

Density Functional Theory Guided Mechanistic Study and Predictive Modeling of Pb(II) Adsorption onto Pretreated Chicken Feather Biomass

Jibunor Udoka Victor¹

jibunorvu@fuotuoike.edu.ng

Federal University Otuoke

Abuchi Elebo²

Federal University of Applied Sciences, Kachia

Anumonye Francis

University of Hull

Ogunyemi Babatunde T.

Federal University Otuoke

Research Article

Keywords: Lead adsorption, pretreated chicken feather biomass, isotherm modeling, kinetic modeling, chemisorption, and physisorption

Posted Date: August 20th, 2026

DOI: <https://doi.org/10.21203/rs.3.rs-10603833/v1>

License:  This work is licensed under a Creative Commons Attribution 4.0 International License.

[Read Full License](#)

Additional Declarations: No competing interests reported.

Density Functional Theory Guided Mechanistic Study and Predictive Modeling of Pb(II) Adsorption onto Pretreated Chicken Feather Biomass

Jibunor Udoka Victor^{1*}, Dr. Abuchi Elebo², Anumonye Francis³ and Dr. Ogunyemi Babatunde T⁴.

¹Department of Chemistry, Faculty of Science, Federal University, Otuoke, Bayelsa State, Nigeria.

²Department of Chemistry, Faculty of Science, Federal University of Applied Sciences, Kachia, Kaduna State, Nigeria.

³Department of Computer Science, Faculty of Science and Engineering, University of Hull, Hull, United Kingdom.

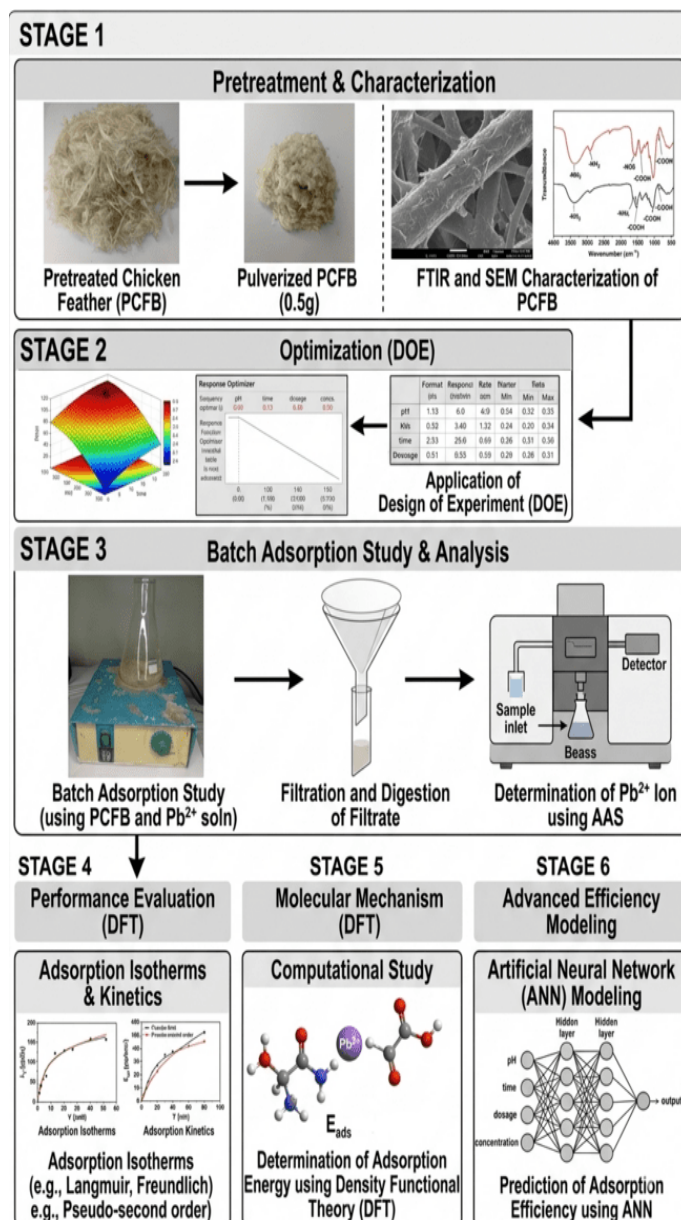
⁴Department of Chemistry, Faculty of Science, Federal University, Otuoke, Bayelsa State, Nigeria.

*Corresponding author's email address: jibunorvu@fuotuke.edu.ng

ABSTRACT

Sustainable valorization of poultry waste offers an attractive strategy for mitigating heavy metal contamination in water. This study integrated experimental, computational, and machine learning investigation of Pb²⁺ adsorption onto ethanol-pretreated chicken feather biomass (PCFB). Batch adsorption was optimized using central composite design, while adsorption mechanisms were elucidated through FTIR, SEM, equilibrium and kinetic modeling, density functional theory, and predictive modeling using response surface methodology (RSM), linear regression (LRM), and artificial neural networks (ANN). FTIR and SEM analyses confirmed the participation of hydroxyl, amino, and sulfur-containing functional groups and pronounced surface morphological changes following Pb²⁺ adsorption. The Freundlich isotherm provided the best description of adsorption equilibrium ($R^2 = 0.9376$), indicating multilayer adsorption on a heterogeneous surface, whereas pseudo second order kinetic ($R^2 = 0.9999$) demonstrated that chemisorption governed the adsorption rate. Regeneration studies showed excellent reusability, with EDTA retaining >77% desorption efficiency after five adsorption-desorption cycles. DFT calculations agree with the experimental observation by exhibiting energetically favorable Pb²⁺ coordination with keratin functional groups through significant charge redistribution and electronic structure modification. Among the predictive models, ANN exhibited superior performance ($R^2 = 0.9473$; RMSE = 0.9641), substantially outperforming RSM and LRM, confirming the highly nonlinear nature of the adsorption system. The combined experimental computational framework establishes PCFB as a regenerable, low cost biosorbent and demonstrates that coupling quantum chemical analysis with machine learning provides a robust strategy for the rational design and optimization of sustainable biosorption systems.

Keywords: Lead adsorption, pretreated chicken feather biomass, isotherm modeling, kinetic modeling, chemisorption, and physisorption.



1.0 Introduction.

The drive for environmental sustainability has emerged as the focal point of global action. Toxic metals (arsenic (As), cadmium (Cd), lead (Pb), mercury (Hg), nickel (Ni), and thallium (Th)) contamination remains one of the most pressing environmental challenges, primarily because they are non-biodegradable, persistent in nature, and ability to aggregate in environmental matrices, causing significant risk to ecosystem integrity and public health. Among these toxic metals, Pb is considered because of its widespread use, non-biodegradability, bioaccumulation, and severe health impacts [1]. Rapid industrialization and anthropogenic activities have predominantly contributed to the increased concentration of lead in the environment. The WHO reported permissible limits (drinking water: 10 ug/L, ambient air: 0.5 ug/m³, and soil: 20 ug/L) of lead metals in the environmental matrix [2]. Exceeding these thresholds poses a direct threat both to human health and ecological stability. Several pieces of literature have reported the health effects of lead exposure; for instance, [3], in their study, reported that lead injection above the permissible limit can cross the placenta and impair the development of the fetus due to its interference with calcium metabolism in pregnant women. Similarly, [4] reported that in 2019, lead exposure accounted for 5.5 million deaths from cardiovascular disease and an annual loss of 765 million IQ points in children globally. [1] reported that lead exposure to children can cause permanent neurodevelopmental consequences in some cases, even at low blood levels. Increased lead concentration in the ecosystem is exacerbated by its mobility and bioaccumulation ability. In response, several techniques (adsorption [5], ion exchange [6], precipitation [7], phytoremediation [8], and reverse osmosis [9]) have been reported for lead recovery from the environment. Among these mentioned techniques, adsorption has been reported to be the most cost-effective and eco-friendly approach.

Adsorption is a surface phenomenon governed by weak van der Waals forces between the adsorbate-adsorbent (physisorption) and/or chemical bond formation between the adsorbate and adsorbent (chemisorption) as they interact [10]. This technique has been employed in various applications wherever surface interactions are used to separate, purify, and protect, such as wastewater treatment [11], air pollution control [12], oil spill remediation

[13], and drug delivery [14]. The effectiveness, fast process, low energy requirement, versatility, eco-friendliness, reversibility, and regeneration make this approach one of the most widely employed separation and purification approaches [15]. Nevertheless, it has its limitations. Conventional adsorbents (e.g., activated carbon, MOFs, and zeolites) often have limitations such as high operational cost, regeneration, and/or secondary pollution risk [16]. These limitations have shifted attention to the development of cheap, sustainable, and environmentally benign adsorbents with high effectiveness. In context, valorization of agricultural and animal derived waste as low-cost adsorbents has gained significant attention.

Poultry waste (e.g., eggshells, feathers, etc.) has been reported to have high adsorption potential. These wastes are often valorized into activated carbon, biochar, fertilizer, animal feed additives, and adsorbents. Chicken feathers, as presented in Fig. 1, offer a sustainable, functional, and efficient adsorbent due to their natural keratin chemistry, modifiable surface properties, and wide applicability. Several agricultural/animal wastes have been reported for adsorption studies. For instance, Sen *et al.* [17], in their study, reviewed the application of agricultural solid wastes for heavy metal ion removal from water and wastewater. The study opined that various solid waste showed great potential to remove metal ions from wastewater under varying conditions. Similarly, Batubara [18], in their study, utilized activated carbon derived from treated sheep remnants and barley husks to remove organic contaminants from aqueous media. The result confirms the merit of using natural waste from plants and animals for water treatment. This current study employed activated carbon derived from chicken feathers for the adsorption of Pb^{2+} ions from aqueous solutions.

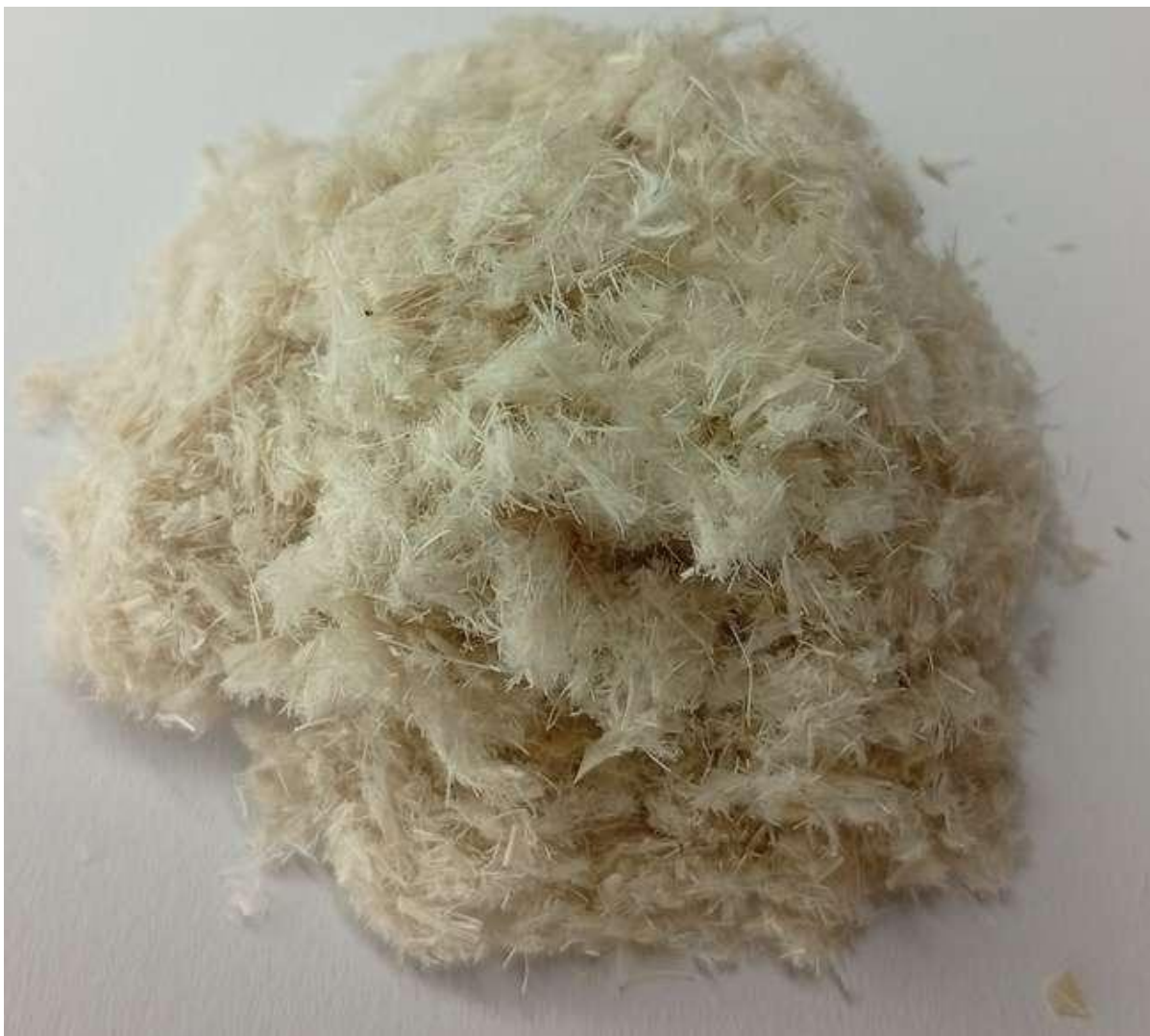


Figure 1: Pretreated Chicken Feather Biomass

The practical application of any adsorbent requires deep insight into the process optimization, which can be achieved through adsorption isotherm and kinetic modeling [19]. An adsorption isotherm provides valuable insight into the mechanism of the adsorption process, investigating whether the adsorption process occurs on a monolayer via chemisorption or multilayer via physisorption or both, revealing the adsorbate-adsorbent affinity. Such equilibrium data are fundamental for understanding the adsorption system/process and identifying the best possible condition to achieve the maximum adsorption performance. Conversely, adsorption kinetics are employed to evaluate the rate of the adsorption process. This data is important as the model directly elucidates the rate-limiting step, which guides the design of adsorbents with improved uptake rates [20]. Ultimately, while isotherm study provides insight into removal efficiency, kinetics provides information on the rate and pathway

by which adsorption occurs. Aggregated adsorption isotherms and kinetics provide complementary information required for the design, optimization, and scaling of adsorption processes. The present study employed Freundlich, Flory-Huggins, Jovanovic, Langmuir, and Temkin isotherms to evaluate the adsorption mechanism, while Elovich, pseudo first order, Pseudo second order, and intraparticle diffusion models were employed to investigate the adsorption kinetics. Thus, the combined application of isotherm and kinetic models is necessary for establishing the best operational strategies for practical environmental application.

2.0 Material and Methods

2.1 Sample collection and preparation.

All chemicals used were of Analar grade. The stock solution of Pb^{2+} ion was prepared in 1 g/L concentration using PbCl_2 and diluted to the required concentration. 0.1M HNO_3 and 0.1M NaOH solutions were used to adjust the pH of the solution mixture. The chicken feather was collected from a local butchery at Swali Market in Bayelsa, Nigeria. The sample was then washed with water and rewashed with deionized water to remove impurities, then oven-dried at 80°C for 72 hrs until constant weight, as described by Heidarinejad *et al.* [21]. The dried sample was pulverized using an agate mortar and soaked in ethanol for 24 hrs, to expose the keratin functional groups and remove lipids, grease, and oily contaminants, then washed with deionized water and oven-dried for 48 hrs to constant weight prior to analysis.

2.2 Characterization

FTIR analysis was carried out using a PerkinElmer Spectrum Two FTIR spectrometer within a wavenumber range of $4000\text{--}400\text{ cm}^{-1}$ to characterize the surface functional group of native and Pb^{2+} ion loaded chicken feather biomass as described by Zubair *et al.* [22]. The surface morphology analysis was investigated using a JEOL JSM-6510LV scanning electron microscope operated under appropriate accelerating voltage at a magnification of x2000 to evaluate surface morphology as described by Alebady *et al.* [23].

2.3 Design of experiment

A central composite design via response surface methodology on Minitab software version 21 was employed to design and optimize the adsorption process by varying the process parameters (dose, concentration, pH, and time) as presented in Table 1 [24]. Experimental runs (30) were generated by the model, which was adopted for the batch adsorption study.

Table 1: Experimental Factor Level Used in Factorial Design

Independent variable	Factor	Coded levels	
		-1	+1
Adsorbent dose (g)	A	0.2	1.0
Concentration (mg/L)	B	20	60
pH	C	2	10
Contact time (min)	D	10	120

2.4 Batch Adsorption Study

In this investigation, 30 batch adsorption experiments were conducted as generated by CCD to study the effect of process parameters on percentage removal of Pb^{2+} ion as described by Spaltonzi *et al.* [25]

The metal uptake capacity (q_e) and adsorption efficiency (A%) were ascertained using equations. 1 and 2, respectively.

$$q_e = \frac{v(C_i - C_f)}{w} \text{----- Eqn. 1}$$

Where;

Q_e = Metal uptake capacity ($mg\ g^{-1}$)

C_i = Initial metal ion concentration (mgL^{-1})

C_f = Final metal ion concentration (mgL^{-1})

w = weight of adsorbent (g)

$$A\% = \frac{C_0 - C_e}{C_0} \times 100 \text{----- Eqn. 2}$$

Where;

%A = Adsorption efficiency

C_0 = Initial metal ion concentration (mgL^{-1})

C_e = equilibrium metal ion concentration (mgL^{-1})

2.5 Desorption and Regeneration Study

The desorption experiment was conducted to evaluate the regeneration potential of Pb^{2+} ion loaded chicken feather biomass [26]. Exactly 2.00 g of the metal-loaded adsorbent was transferred into a conical flask containing 0.1 M of 50 mL H_2SO_4 and EDTA solution, respectively. The reaction mixture was continually stirred at 150 rpm for 1 hr at room temperature using a Corning PC-353 magnetic stirrer. After the stipulated contact time, the biomass was separated via filtration using Whatman filter paper (2.5 μm), and the concentration of desorbed Pb^{2+} ion in the filtrate was quantified using Atomic Adsorption Spectrometry (AAS). The desorption efficiency was calculated after 5 regeneration cycles.

2.6 Adsorption Isotherm

The adsorption capacity of the pretreated chicken feather biomass was elucidated through equilibrium modeling studies. The potential of Flory-Huggins, Freundlich, Langmuir, Jovanovic, and Temkin isotherms was employed to identify which isotherm best describes the interaction between pretreated chicken feather biomass and Pb^{2+} ion. The Freundlich isotherm assumes multilayer adsorption onto a heterogeneous surface [27]. The model is linearly expressed in equation 3;

$$\text{Log } q_e = \text{Log } K_f + \left(\frac{1}{n}\right) \text{Log } C_e \text{----- Eqn. 3}$$

Where K_F represents Freundlich adsorption capacity (L/mg) and n represents adsorption intensity. The plot of $\log q_e$ against $\log C_e$ produces a straight line with slope $1/n$ and intercept K_F .

The Flory-Huggins isotherm assumes a spontaneous process and the possibility of surface coverage by the adsorbate [28]. The model is linearly expressed in equation 4.

$$\text{Log } \frac{\theta}{C_o} = \text{Log } K_{FG} + n \text{Log } (1 - \theta) \text{----- Eqn. 4}$$

Where K_{FG} represents the Flory-Huggins equilibrium constant (L/mg), $\theta = (1 - C_e/C_o)$ represents fractional coverage, and n represents the number of sites occupied by the adsorbed molecules. The plot of $\text{Log } \frac{\theta}{C_o}$ against $\text{Log } (1 - \theta)$ is applied to extrapolate the value for slope n and intercept K_{FG} .

The isotherm was further applied to calculate the Gibbs free energy as expressed in equation 5.

$$\Delta G = -RT \ln K_{FG} \text{----- Eqn. 5}$$

Where ΔG represent the Gibbs free energy of adsorption, T represent the temperature (K), and R represent the universal gas constant.

The Jovanovic isotherm, like the Langmuir isotherm, assumes monolayer adsorption on a limited number of adsorption sites [29]. However, unlike the Langmuir isotherm, Jovanovic introduces an exponential term to account for deviations caused by surface heterogeneity and also assumes that adsorption sites have different binding energies. The linear form of the Jovanovic isotherm is expressed as equation. 6.

$$\ln q_e = \ln q_{max} - K_J C_e \text{----- Eqn. 6}$$

Where, K_J represent the Jovanovic isotherm constant and q_{max} represent the maximum Pb^{2+} ion absorbed. The plot of $\ln q_e$ against C_e , from which slope q_{max} and intercept K_J are extrapolated.

The Langmuir isotherm assumes monolayer adsorption on a uniform surface with no adsorbate-adsorbent interaction [29]. The model is linearly expressed as equation 7.

$$\frac{C_e}{q_e} = \frac{1}{K_L Q^0} + C_e \frac{1}{Q^0} \text{----- Eqn. 7}$$

Where q_e represent the Pb^{2+} ion adsorbed at equilibrium (mg/g), C_e represents the equilibrium concentration of the Pb^{2+} ion (mg/L), K_L represent the Langmuir constant (L/mg), and Q^0 represents the maximum adsorbed Pb^{2+} ion per unit mass of PCFB. The plot of C_e/q_e against C_e produces a straight line from which Q^0 and K_L can be extrapolated from the slope and intercept, respectively. The isotherm further predicts the adsorbate-adsorbent affinity as expressed in the equation. 8.

$$R_L = \frac{1}{1 + K_L C_o} \text{----- Eqn. 8}$$

Where R_L represent the separation factor and C_o represent the initial Pb^{2+} ion concentration. A favourable adsorption is record when the value of R_L is between 0 and 1 i.e $R_L > 1$ represent unfavourable adsorption. However, $R_L = 1$ suggest linear adsorption and $R_L = 0$ suggest irreversible adsorption.

The Temkin isotherm assumes the adsorption heat decreases linearly with coverage as the adsorbate and adsorbent interact (Rajahmundry et al., 2021.). Linearly expressed as equation. 9.

$$q_e = \frac{RT}{b_T} \ln A_T + \frac{RT}{b_T} \ln C_e \text{----- Eqn. 9}$$

Where b_T represents the Temkin constant (J/mol) and A_T represent binding energy (L/g). The plot of q_e against $\ln C_e$ gives a straight line from which slope b_T and intercept A_T are extrapolated.

2.7 Adsorption Kinetic study

The adsorption kinetics describe the rate at which adsorbate molecules are transferred to the surface of the adsorbent from the media. Provides information into how fast equilibrium is attained and the mechanism that controls the adsorption process, i.e., chemical bonding, diffusion, or surface interaction.

The Elovich model assumes no interaction between adsorbed molecules, and they bind on a heterogeneous adsorption surface involving chemical interaction between the adsorbent and adsorbate rather than simple physisorption [31]. The Elovich model is expressed in the equation. 10.

$$q_t = \frac{1}{\beta} \ln(\alpha\beta) + \frac{1}{\beta} \ln(t) \text{----- Eqn. 10}$$

Where q_t is the amount adsorbed at time t (mg/g), α initial adsorption rate (mg/g·min⁻¹), and β desorption/activation constant (g/mg). The plot of q_t against $\ln(t)$ produces slope $\frac{1}{\beta}$ and intercept $\frac{1}{\beta} \ln(\alpha\beta)$.

The intraparticle diffusion model assumes a diffusion-controlled adsorption process. The model implies that if the amount adsorbed q_t is directly proportional to $t^{0.5}$, diffusion is the rate-limiting step [32]. The linear form is expressed in equation. 11.

$$q_t = K_{ID} t^{0.5} + C \text{----- Eqn. 11}$$

Where q_t represents adsorption capacity at time t (mg/g), K_{ID} represents intraparticle diffusion rate constant (mg/g.min^{0.5}) and C represents the intercept related to boundary layer thickness.

The Pseudo First Order (PFO) kinetic model assumes physisorption on a monolayer surface where each adsorbed species acts independently and does not affect adsorption of others [32]. The linear form of PFO is expressed in equation. 12.

$$\log(q_e - q_t) = \log q_e - \frac{k_1}{2.303} t \text{----- Eqn. 12}$$

Where q_e and q_t represent adsorption capacity at equilibrium and time t (mg/g), while K_1 represents pseudo first order rate constant k_1 (min^{-1}). The plot of $\log(q_e - q_t)$ against t produces a straight line with slope k_1 and intercept $\log q_e$.

The Pseudo Second Order (PSO) kinetic model assumes a homogeneous adsorption site governed by surface adsorption via chemisorption [33]. The linear form of the model is presented in equation. 13.

$$\frac{t}{q_t} = \frac{1}{k_2 q_e^2} + \frac{t}{q_e} \text{----- Eqn. 13}$$

Where, K_2 represents the pseudo second order rate constant (g.mg^{-1}). The plot of $\frac{t}{q_t}$ against t produces a straight line with slope $\frac{1}{q_e}$ and intercept $\frac{1}{k_2 q_e^2}$.

2.8 Computational Study

2.8.1 Response Surface Methodology

Response surface methodology (RSM) was employed for statistical valuation of the adsorption experiment data. A design expert on Minitab version 21 software was employed to optimize the process parameter as presented in Table 1 [34]. Regression analysis on Minitab version 21 software was employed to evaluate the interaction between process parameters (A- Dose, B-Conc., C-pH, & D-Time) and response (% removal) using the second-degree polynomial as seen in equation. 14.

$$Y = b_o + \sum_{i=1}^n b_i x_i + (\sum_{i=1}^n b_{ii} x_i)^2 + \sum_{i=1}^{n-1} \sum_{j=i+1}^n b_{ij} x_i x_j + \epsilon \text{----- Eqn. 14}$$

Where Y is the predicted response, x_i and x_j are the input variables, b_o = constant coefficient, b_i = linear coefficient, b_{ij} = interaction coefficient, b_{ii} = quadratic coefficient, and ϵ = random error. The Coefficient of Determination (R^2) was used to evaluate the quality of the model as described by Kothakota *et al.* [35]. The Fisher variation ratio (F-value) was employed to explain the adequacy and significance of the predicted model [36].

2.8.2 Linear Regression (LR) Analysis

Using the MATLAB (R2024b version) Regression Learner App, several linear regression algorithms with various hyperparameter configurations were methodically generated, trained, and assessed in order to determine

which model had the most predictive power [37]. A thorough comparison of linear regression methods under optimal parameter values was made possible by the modeling framework, guaranteeing an impartial evaluation of their predictive efficacy. To increase robustness throughout the validation dataset, reduce prediction errors, and improve model generalization, hyperparameter modification was carried out. The coefficient of determination (R^2), root mean square error (RMSE), mean squared error (MSE), and mean absolute error (MAE) were used to quantitatively evaluate the model's performance. A thorough assessment of the model's predicted accuracy and error characteristics was made possible by these complementary performance indicators. For the adsorption system under study, the best regression model was chosen based on its capacity to maximize the explained variance while concurrently decreasing prediction errors, exhibiting higher predictive reliability and generalization performance.

2.8.3 Artificial Neural Network Analysis

The Artificial Neural Networks (ANNs), a complex mathematical modeling techniques inspired by biological neuron activity, were used to forecast the Pb^{2+} removal efficiency of PCFB. The prediction model employed in this study was developed using MATLAB's Neural Network Toolbox (version R2024b). A feedforward neural network was implemented with a hidden layer and trained using the Levenberg-Marquardt algorithm as described by Elebo [24] with slight modification. The dataset was divided into 70% training, 15% validation, and 15% testing subsets. The network was trained with four experimental input variables: pH, initial Pb^{2+} concentration, adsorbent dosage, and contact time, with the Pb^{2+} adsorption efficiency as the output parameter. A change in the number of hidden layers was seen to influence the ANN model's performance. Too many neurons in the hidden layer could affect the model's ability to learn, consequently resulting in overfitting, while too few neurons may result in poor pattern recognition, consequently producing underfitting. Three statistical performance indicators, coefficient of determination (R^2), root mean square error (RMSE), and mean square error (MSE), were employed to evaluate the predictive performance, accuracy, and reliability of the developed models. Therefore, the model with the high R^2 value closest to unity (1) and lowest MSE and RMSE was selected as the ideal developed model. These ANN parameter validations are presented in Table 2.

2.8.4 Density Functional Theory (DFT)

Density Functional Theory (DFT) calculations using Spartan 14 (version 1.14 software) were employed to elucidate the adsorption mechanism of Pb^{2+} ion onto keratin representative functional groups present in pretreated chicken feather biomass. The computational study was aimed at elucidating the electronic interactions, adsorption behavior, active binding sites, and charge transfer characteristics involved in the biosorption process. The representative keratin structure was modeled using representative amino acid residues and functional groups commonly identified in feather keratin, including amino ($-\text{NH}_2$), carboxyl ($-\text{COOH}$), hydroxyl ($-\text{OH}$), and amide ($-\text{CONH}$) groups. These groups were selected based on experimental characterization obtained from FTIR analysis. The interaction strength between Pb^{2+} ions and the representative keratin functional groups was evaluated using adsorption energy calculation as seen in the equation. 15. [38]

$$E_{\text{ads}} = E_{\text{complex}} - (E_{\text{keratin}} + E_{\text{Pb}^{2+}}) \text{----- Eqn. 15.}$$

Where E_{ads} represents the adsorption energy, E_{complex} is the electronic energy of the keratin- Pb^{2+} complex, E_{keratin} is the electronic energy of the isolated keratin model, and $E_{\text{Pb}^{2+}}$ is the electronic energy of the isolated Pb^{2+} ion. The magnitude suggests the spontaneity and energy favorability of the adsorption process. It also reveals the kind of adsorption involved, either physisorption if the adsorption energies are in the range of -5 and -40 kJ mol^{-1} or chemisorption if the energy is below -40 kJ mol^{-1} .

The Frontier Molecular Orbital analysis was investigated to determine the electronic properties governing adsorption. The HUMO-LUMO energy gap was calculated before and after adsorption, as seen in equation 16.

$$\Delta E = E_{\text{LUMO}} - E_{\text{HOMO}} \text{----- Eqn. 16}$$

The energy gap reveals the electronic stability and reactivity of the molecule. A higher energy gap after adsorption suggests an enhanced electronic stability after adsorption of Pb^{2+} ions by the keratin molecule and vice versa [39]. The charge transfer between keratin active sites and Pb^{2+} ions was evaluated to establish the chemisorption nature of the adsorption process. Adsorption configuration and bond interactions between Pb^{2+} ions and representative keratin functional groups were carefully elucidated and interpreted using Spartan 14V1.14.

Table 2: ANN Model Evaluation Parameters

Performance Parameter	Equation	Equation	Reference
Mean Squared Error (MSE)	$MSE = \frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2$	17	[24]
Root Mean Squared Error (RMSE)	$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2}$	18	[24]
Mean Absolute Error (MAE)	$MAE = \frac{1}{n} \sum_{i=1}^n y_i - \hat{y}_i $	19	[24]
Coefficient of Determination (R^2)	$R^2 = \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{\sum_{i=1}^n (y_i - \bar{y})^2}$	20	[40]
Correlation Coefficient (R)	$R = \frac{\sum_{i=1}^n (y_i - \bar{y})(\hat{y}_i - \bar{\hat{y}})}{\sqrt{\sum_{i=1}^n (y_i - \bar{y})^2 \sum_{i=1}^n (\hat{y}_i - \bar{\hat{y}})^2}}$	21	[40]

Where; y_i is the experimental (actual) value, $\hat{y}_i$ is the ANN predicted value, $\bar{y}$ is the mean of the experimental values, $\bar{\hat{y}}$ is the mean of the predicted value, and n is the number of observations.

3.0 RESULT AND DISCUSSION

3.1 Characterization

3.1.1 SEM Analysis

The surface morphology of the native pretreated chicken feather biomass (PCFB) and the Pb^{2+} loaded chicken feather was investigated using scanning electron microscopy at x2000 magnification. The micrograph revealed distinct morphological modification following Pb^{2+} adsorption, providing direct evidence of the participation of the PCFB surface in the adsorption process. The SEM micrograph of native PCFB (Figure 2a) exhibited a characteristic fibrous keratinous structure with elongated, aligned, and interconnected fibrils, consistent with the morphological characteristics of keratin rich biomaterials [41]. Numerous interfibrillar spaces, microvoids, and surface cavities were observed, indicating a highly heterogeneous surface with abundant accessible adsorption sites. Such structural heterogeneity is advantageous for adsorption because it increases the availability of surface area, enhances intraparticle diffusion, and promotes effective interaction between Pb^{2+} ions and the functional groups embedded within the keratin matrix [39]. The well-defined fibrillar network further demonstrates that

ethanol pretreatment preserved the structural integrity of keratin while exposing additional adsorption sites through partial removal of surface impurities and non-keratinous materials.

Following the adsorption of Pb^{2+} , the SEM micrograph (Figure 2b) showed pronounced morphological alteration. The fibrilla surface became substantially denser and more compact, with numerous granular and cluster deposits distributed along the fiber surface and within the interfibrillar regions. In addition, partial blockage of the pore and the reduction in visible surface roughness were observed after adsorption. The observed morphological transformation is evidence of Pb^{2+} adsorption on the keratin surface; however, the immobilization of the Pb^{2+} was not merely electrostatic interaction but also occurred through surface complexation between the Pb^{2+} ion and functional groups present in the keratin matrix, such as amino (-NH), carboxyl (-COOH), hydroxyl (-OH), and sulfur containing groups. The increase in surface compactness may be attributed to the formation of metal-keratin complexes, which altered the original morphology of the feather fibers.

The present findings are consistent with previous studies on keratin rich biomass. For instance, Zhang *et al.* [42] reported that feather derived keratin exhibited a rough and porous fibrillar structure before adsorption, which became smoother and densely occupied with particle deposits after Cd^{2+} uptake, confirming successful surface complexation. Similarly, Zhu *et al.* [43] demonstrated that protein-based biomass developed a compact surface with reduced pore visibility after adsorption of trace metals, indicating extensive occupation of active binding sites and strong chemisorptive interactions. Comparable morphological transformation has also been reported by Khan *et al.* [44] for chemically modified feather keratin, where the disappearance of open fibrillar channels and the appearance of granular deposits were associated with efficient Pb^{2+} adsorption through amino, carboxyl, and sulfur containing functional groups.

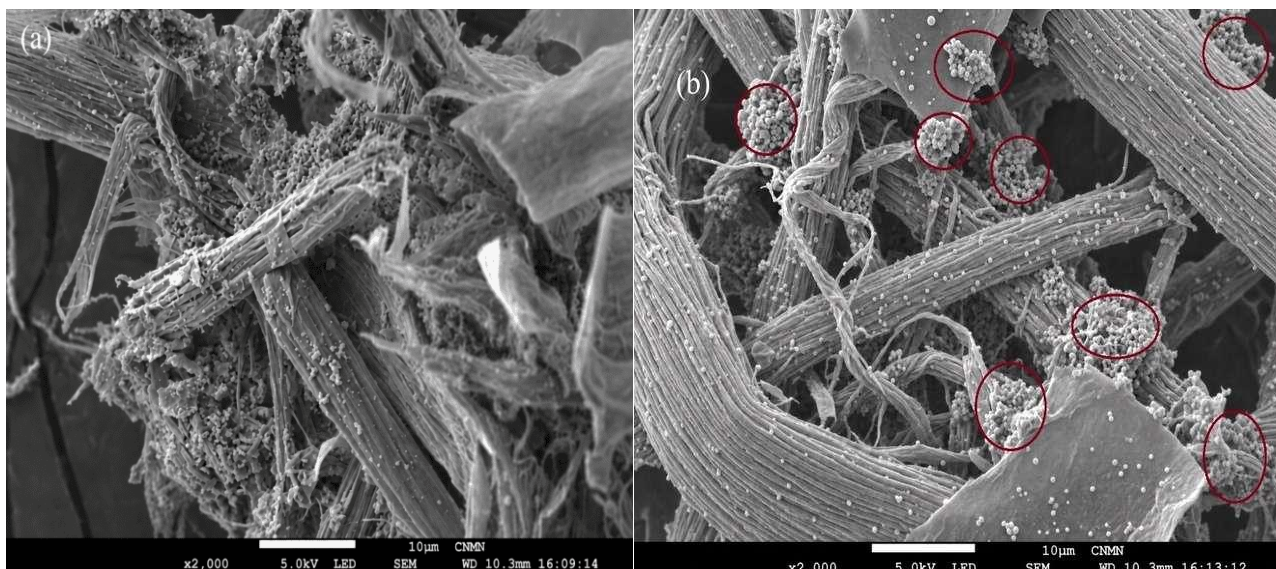


Figure 2: SEM Micrograph of Native (a) and Heavy Metal Loaded (b) chicken feather

3.1.2 Fourier Transformed Infrared (FTIR) Spectroscopy analysis

FTIR was employed to investigate the changes in functional groups of chicken feathers following heavy Pb^{2+} ion adsorption. The spectra of PCFB and Pb^{2+} ion loaded chicken feather are presented in Figure 3a and 3b, respectively. The FTIR spectrum of PCFB exhibited characteristic absorption bands of keratin, a fibrous structure protein abundant in feathers. A broad band at 3388 cm^{-1} was assigned to the O-H stretching vibration of hydroxyl. The weak band at 2925 cm^{-1} correspond to the O-H stretching vibration of alcohol groups. The appearance of a peak at 2176 cm^{-1} corresponding to S-C=N stretching of the thiocyanate group. The sharp peaks at 1640 cm^{-1} corresponding to N-H bending suggest the amine group. The weak peak at 1393 cm^{-1} corresponds to O-H bending of the alcohol group. The peak at 1104 cm^{-1} correspond to C-N stretching of the amine group. The peaks at 866 and 744 cm^{-1} correspond to C-Cl stretching of alkyl halides.

Upon adsorption of Pb^{2+} ions (Figure 2b), O-H stretching exhibits a significant shift from 3388 cm^{-1} to 3275 cm^{-1} after Pb^{2+} adsorption as seen in Table 3, which suggests a formation of surface complexation between Pb^{2+} ions and hydroxyl/carboxylic functionalities. The shift towards a higher wavenumber suggests changes in the hydrogen bonding environment during adsorption. The shift of a medium peak from 2925 to 2928 cm^{-1} corresponding to O-H stretching further strengthens the participation of the hydroxyl group in immobilization of the Pb^{2+} ion on the keratin surface. The appearance of a medium peak at 2928 cm^{-1} corresponding to S-C=N of

the thiocyanate group suggests the contribution of the thiocyanate group in Pb^{2+} ion immobilization. In addition, a shift in N-H bending from 1640 cm^{-1} to 1634 cm^{-1} after Pb^{2+} ion adsorption suggests coordination interaction between Pb^{2+} ions and the nitrogen atom of the amine group, resulting in weakening of the bond environment. The appearance of a peak at 1512 cm^{-1} , corresponding to NO_2 stretching after Pb^{2+} ion adsorption, suggests coordination interaction between Pb^{2+} ions and oxygen atoms of the nitro group, resulting in weakening of the bond environment and possible formation of Pb-O complexes. The appearance of weak peaks at 1242 cm^{-1} and a shift from 1104 to 1071 cm^{-1} suggest C-N related vibration modes and possibly amide III associated functional groups within the keratin matrix, suggesting the participation of nitrogen- and oxygen-containing functional groups in the adsorption process through coordination interaction with Pb^{2+} ions. The appearance of a medium peak at 530 cm^{-1} corresponding to the metal-oxygen group indicates the formation of metal oxide after Pb^{2+} ion adsorption.

The present study is consistent with previous studies on proteins and keratin based biosorbents. For instance, Zahara *et al.* [45] reported that the main active sites that allow feather keratin to immobilize heavy metals through complexation, electrostatic attraction, and ion exchange include thiol (-SH), disulfide (-S-S-), amino (- NH_2), amide, and carboxyl (-COOH) groups. Similarly, Akhtar *et al.* [46] observed notable changes in the O-H, N-H, and amide bands following Pb^{2+} adsorption onto keratin-derived biochar and opined that Pb^{2+} complexation is governed by functional groups comprising oxygen and nitrogen.

The more observed spectral shifts in the current work, especially in the hydroxyl and amide regions as seen in Table 3, along with the emergence of the Pb-O vibration, indicate stronger surface complexation and more efficient use of keratin functional groups after ethanol pretreatment, which explains the remarkably high Pb^{2+} removal efficiencies attained during the batch adsorption experiments.

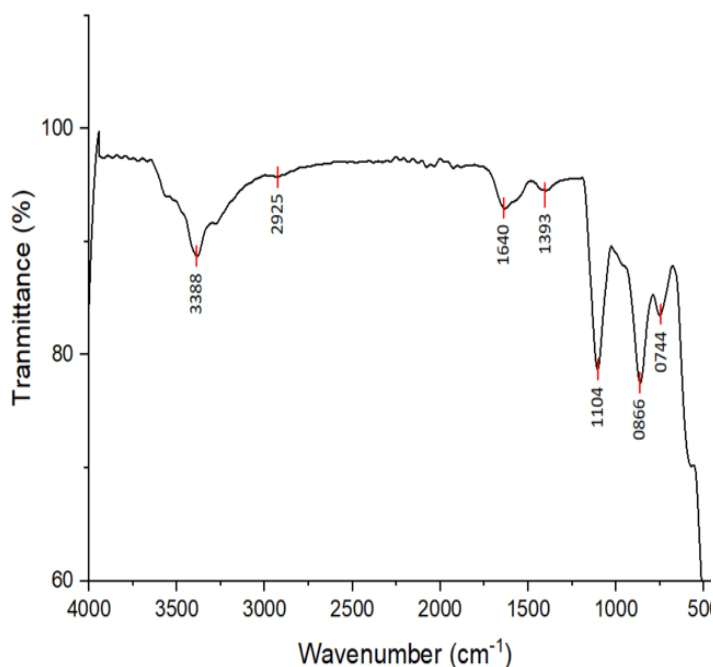


Figure 3a: FTIR of Ethanol Pretreat Chicken Feather Biomass

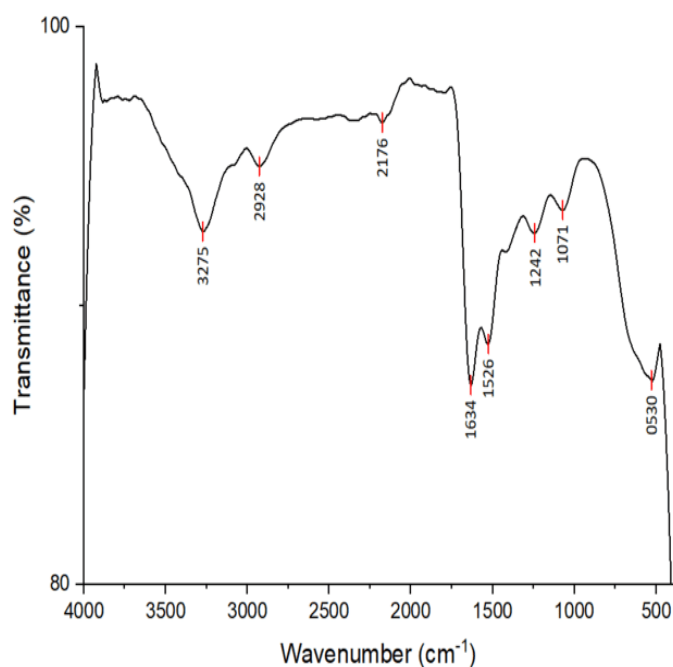


Figure 3b: FTIR of Pb²⁺ loaded Chicken Feather Biomass

Table 3: Assignment of IR bands of Functional Groups in Pretreated and Pb²⁺ Loaded Chicken Feather Biomass respectively.

Frequency	PCFB (cm ⁻¹)	Pb ²⁺ Load PCFB (cm ⁻¹)	Assignment	Class of compounds
3200 – 3550	3388	3275	O-H stretching	Alcohol
2700 – 3200	2925	2928	O-H stretching	Alcohol
2190 - 2260	-	2176	S-C≡N stretching	Thiocyanate
1580 – 1650	1640	1634	N-H bending	Amine
1626 - 1662			C=C Stretching	Alkene
	-	1526	N-O stretching	Nitro compound
1380 - 1410	1393		O-H bending	Alcohol
1200 - 1275	-	1242	C-N Stretching	Amine
1020 - 1250	1104	1071	C-N stretching	Amine
885 - 895	866	-	C-Cl stretching	Alkyl halide
665 - 730	744	-	C-Cl stretching	Alkyl halide
400 - 600	-	530	Metal oxygen (inorganic)	

3.2 Batch Adsorption Study

The batch adsorption trials showed that ethanol-pretreated chicken feather biomass had a remarkable Pb²⁺ removal efficiency, as the adsorption efficiencies range from 81.54 to 99.46% throughout the experimental region as seen in Table 4. Adsorbent dosage had a major impact on adsorption efficiency; removal increased

from 95.21% at 0.2 g to a high of 99.46% at 0.8 g before falling to 97.57% at 1.0 g. This suggests that too much biomass loading promotes particle aggregation and decreases the efficient use of active sites. The removal efficiency decreased from 98.86 to 92.22% when the initial Pb^{2+} concentration was increased from 20 to 100 mg L^{-1} . This was due to the gradual saturation of the available adsorption sites at higher metal loadings. The pH of the solution had a significant impact on adsorption; the maximum removal (96.85%) was recorded at pH 9, while adsorption efficiency decreased significantly to 81.54% at pH 11, most likely as a result of Pb^{2+} hydrolysis and the creation of hydroxyl complexes that hinder adsorption. Rapid Pb^{2+} absorption occurred within the first 45 minutes (98.53%), after which adsorption approached equilibrium and remained nearly constant up to 120 minutes (98.35%), showing quick adsorption kinetics. Contact time had a relatively smaller impact. The combination of high Pb^{2+} concentration (100 mg L^{-1}), acidic pH (2), adsorbent dosage (0.6 g), and short contact time (10 min) resulted in the lowest removal efficiency (82.50%), indicating the synergistic influence of the process variables. The consistently high removal efficiencies (>90% in the majority of experimental runs) show that keratin functional groups have a strong affinity for Pb^{2+} and reveal a nonlinear interaction among adsorption variables. These findings support the use of sophisticated predictive models, such as response surface methodology and artificial neural networks, to accurately describe the adsorption process.

3.3 Desorption and Regeneration Study

The desorption and regeneration performance of Pb^{2+} loaded pretreated chicken feather biomass was evaluated over five consecutive adsorption-desorption cycles using 0.5 M HCl and 0.5 M EDTA as eluents [47]. As presented in Table 5, the biosorbent exhibited excellent reusability, maintaining consistently high Pb^{2+} ion removal efficiency throughout regeneration cycles. EDTA superior desorption efficiencies ranging from 77.80 - 81.23 %, whereas HCl yielded comparatively lower values between 64.38 – 64.62 %. The highest desorption efficiency for EDTA was recorded in the first cycle (80.17%), while the lowest value (78.70%) occurred in the third cycle exhibiting only a marginal decline in regeneration performance after repeated use. In contrast, HCl exhibited relatively stable but consistently lower desorption efficiency, suggesting that its regeneration capacity was limited by the strength of the Pb^{2+} biosorbent interactions.

The superior regeneration performance of EDTA can be attributed to its strong chelating affinity towards Pb^{2+} ions. EDTA forms highly stable and soluble Pb-EDTA complexes, thereby effectively disrupting the coordination bond between Pb^{2+} ions and the active sites of the keratin surface. This observation suggests that a substantial portion of Pb^{2+} ion adsorption on PCFB predominantly occurred through reversible surface complexation and coordination interaction rather than irreversible chemisorption alone. In contrast, HCl regenerated the biosorbent predominantly through proton exchange mechanism, where excess H^+ ions displaced the adsorbed Pb^{2+} ions from the active binding sites. Although effective, however, protonation may not completely disrupt stronger metal-ligand coordination interactions, explaining the comparatively lower desorption efficiency obtained with HCl. Similar regeneration behavior has been reported in previous studies for keratin and lignocellulosic based biosorbent, where EDTA consistently outperformed mineral acids because of its greater ability to complex and mobilize strongly adsorbed heavy metals ions [44]; [48].

The slight reduction in desorption efficiency observed after repeated regeneration cycles, particularly with HCl, may be attributed to incomplete desorption of Pb^{2+} ions, gradual blockage of adsorption sites, minor structural alterations of the keratin matrix, or leaching of surface active functional groups during repeated acidic treatment. Nevertheless, the relatively small decrease in regeneration efficiency demonstrates that the structural integrity and adsorption functionality of PCFB were largely preserved throughout the regeneration process. The ability to retain more than 77% desorption efficiency with EDTA after five consecutive cycles confirms the chemical stability of the biosorbent and highlights its potential for repeated application in wastewater treatment. The effectiveness of EDTA in removing adsorbed Pb^{2+} indicates that metal uptake was primarily governed by surface complexation involving carboxyl, amino, hydroxyl, and sulfur containing functional groups within the keratin moieties.

Comparable observation was reported by Saini *et al.* [49], who opined that EDTA regenerated keratin-based biosorbent more effectively than HNO_3 due to formation of stable metal-chelate complexes. Similarly, Chen *et al.* [50] opined that agricultural waste derived biosorbent retained over 75% of their initial adsorption capacity after multiple EDTA regeneration cycles, confirming that reversible coordination interaction dominates

Pb^{2+} adsorption and facilitate efficient desorption. The regeneration efficiency obtained in the present study are consistent with these reports and further demonstrate that PCFB possesses excellent operational stability, high reusability, and considerable economic potential for sustainable Pb^{2+} remediation from contaminated systems.

Table 4: CCD Matrix Experimental Design for Pb (II) Removal using PCFB

Runs	Dose	Conc.	pH	Time	Adsorption Efficiency (%)	RSM (%)	LRM (%)	ANN (%)
1	0.2	60	7	60	95.212	92.963	93.81	94.79
2	0.4	60	7	60	95.525	93.337	94.07	94.96
3	0.6	60	7	60	96.217	93.711	94.33	95.78
4	0.8	60	7	60	99.458	94.085	94.59	98.96
5	1	60	7	60	97.565	94.459	94.85	97.42
6	0.8	20	7	60	98.860	95.137	96.27	98.71
7	0.8	40	7	60	96.475	94.611	95.43	95.79
8	0.8	60	7	60	92.382	94.085	94.59	91.69
9	0.8	80	7	60	95.315	93.559	93.75	94.49
10	0.8	100	7	60	92.221	93.033	92.90	92.13
11	0.8	20	2	60	96.150	93.692	93.44	96.21
12	0.8	20	3	60	92.790	93.981	94.01	90.23
13	0.8	20	5	60	88.630	94.559	95.14	87.16
14	0.8	20	7	60	93.990	95.137	96.27	93.78
15	0.8	20	9	60	96.850	95.715	97.40	94.78
16	0.8	20	11	60	81.540	96.293	98.54	80.98
17	0.8	20	9	10	95.745	93.420	95.05	95.71
18	0.8	20	9	20	93.810	93.879	95.52	91.97
19	0.8	20	9	30	96.320	94.338	95.99	95.79
20	0.8	20	9	45	98.525	95.027	96.70	97.79
21	0.8	20	9	60	96.580	95.715	97.40	94.91
22	0.8	20	9	120	98.345	98.469	98.23	97.93
23	0.6	100	2	10	82.500	88.919	87.46	82.41
24	0.2	40	2	120	93.750	94.798	94.64	91.98
25	1	80	5	120	95.246	96.109	95.71	95.14
26	0.4	100	5	10	90.331	89.412	88.90	90.19
27	0.6	80	3	30	90.455	90.652	89.81	89.79
28	0.2	40	3	20	89.882	90.497	90.50	89.25
29	0.4	100	11	20	90.620	91.605	92.76	89.78
30	1	80	11	45	94.122	94.401	95.56	93.98

Table 5: Pb²⁺ Desorption by PCFB

Cycles	Amount before biosorption (mgL ⁻¹)	Amount after biosorption (mgL ⁻¹)	Biosorption (%)	Amount Desorbed by 0.5 M HCl	Amount Desorbed by 0.5 M EDTA	% Desorbed by 0.5 M HCl	% Desorbed by 0.5 M EDTA
1	60	1.11	98.15	37.98	47.21	64.49	80.17
2	60	1.09	98.18	38.02	47.85	64.54	79.82
3	60	1.12	98.13	38.05	46.34	64.62	78.70
4	60	1.08	98.20	37.93	45.84	64.38	79.49
5	60	1.16	98.07	38.03	46.43	64.63	78.91

3.4 Computational Analysis

3.4.1 Response Surface Methodology Analysis

Central composite design (CCD) via response surface methodology was employed to evaluate the effect of process initial Pb²⁺ concentration (A), solution pH (B), adsorbent dosage (C), and contact time (D) on Pb²⁺ removal by PCFB as presented in Table 4. The relationship between operational variables and Pb²⁺ ion adsorption efficiency by PCFB was examined using multiple linear regression model's (LRM) equation as seen in equation 22. The regression coefficients as seen table 6, revealed that dosage, pH, and contact time positively influenced Pb²⁺ removal with coefficient values of 1.87, 0.289, and 0.049 respectively, while initial Pb²⁺ concentration exerted a slight negative influence (-0.0263). This trend is consistent with the establish adsorption behavior of biosorbent, where increasing adsorbent dosage provides additional active binding sites, higher pH enhances metal ion complexation through deprotonation of functional groups, and longer contact time facilitates equilibrium attainment, while elevated initial metal concentration promotes competition for the finite number of adsorption sites [51].

Despite the expected coefficient trends, none of the predictor variables were statistically significant ($P > 0.05$) as seen in their p-values of 0.613, 0.350, 0.102, and 0.324 for dose, pH, contact time, and concentration respectively. This indicates that within the examined experimental domain, these variables' individual linear contributions were insufficient to explain Pb^{2+} removal. The absence of correlation between independent variable was corroborated by the low variance inflation factor ($VIF = 1.08 - 1.22$), indicating that the estimated regression coefficients were stable and unbiased. A VIF of 1 indicates no correlation between independent variables, while a VIF above 5 to 10 indicates multicollinearity the compromise model reliability [52].

The overall predictive performance of the linear model was poor, with a coefficient of determination (R^2) of 22.62% and an adjusted R^2 of 10.24% as seen in Table 7, demonstrating that the fitted linear equation only partially explained the variation in Pb^{2+} removal efficiency. More significantly, the 10-fold cross-validation R^2 and predicted R^2 were both 0.00%, indicating weak predictive power and low generalization to unseen experimental data. Although contact time exhibited the largest regression coefficient among the investigated variables, the overall regression model was statistically insignificant ($F = 1.83$, $P = 0.155$) as seen in table 8, indicating that the linear relationship between the selected process variables and adsorption efficiency was inadequate.

Similar observation has been reported by Bayou *et al.* (2022), who opined that conceptional linear regression explained less than 30% of the variability in heavy metal adsorption by agricultural biosorbent because adsorption was governed by nonlinear interactions between physiochemical variables. Similarly, Mondal, [53], demonstrated that linear statistical models poorly describe Cd^{2+} adsorption onto keratin-rich biosorbents, whereas nonlinear machine learning algorithm substantially improved prediction accuracy.

The Durbin-Watson statistic of 1.86 together with the non-significant lack-of-fit test ($P = 0.454$) demonstrated that the regression residuals were randomly distributed and that the principal assumptions of linear regression satisfied. However, the existence of one significant observation with a high standardized residual (-3.93) (Table 9) suggest that the dataset contains localized nonlinear behavior which could not be adequately represented by

the first order regression equation. Since the regression assumption remains valid, the poor predictive performance of the model cannot be attributed to statistical violations but rather the inability of a linear model to capture the complex adsorption mechanism governing Pb^{2+} uptake.

Holistically, these results show that a straightforward linear connection is insufficient to explain Pb^{2+} adsorption onto prepared chicken feathers. Instead, the adsorption process may be controlled by intricate nonlinear interactions including surface heterogeneity, diffusion, and metal-binding mechanisms typical of keratin-based biosorbents, according to the LRM model's poor explanatory and predictive ability. Similar findings have been reported by Elamraoui, [54], who observed that adsorption by keratinous and lignocellulosic biosorbents is inherently nonlinear because multiple adsorption mechanisms occur simultaneously. Therefore, it is anticipated that sophisticated nonlinear techniques such artificial neural networks (ANN) or adaptive neuro-fuzzy inference systems (ANFIS) may offer better predictive performance and a more accurate description of the adsorption process.

The pareto analysis (Figure 4), identified contact time as the most influential process variable affecting Pb^{2+} adsorption onto PCFB, followed by Pb^{2+} concentration, solution pH, and adsorbent dosage. However, no single process variable had a statistically significant linear effect on adsorption efficiency ($P > 0.05$), as none of the standardized effects surpassed the significance threshold (2.060). The predominance of contact time emphasizes the significance of adsorption kinetics and mass transfer in facilitating Pb^{2+} diffusion and interaction with the keratin functional groups before attainment of equilibrium. These findings are consistent with report by Zhang *et al.* [42] who identified contact time as the dominant factor controlling heavy metals adsorption by protein based biosorbent despite the absence of statistically significant first order effects. The inability of the pareto analysis to identify dominant linear effects further support the conclusion that Pb^{2+} uptake results from the combination of several interacting physiochemical mechanism rather than a single controlling variable.

Residual diagnostics (Figure 5), demonstrated that the assumptions of multiple linear regression were generally satisfied. The residuals exhibited approximate normality, randomly dispersion around zero, and exhibited constant variance with no evidence of autocorrelation, as confirmed by the Durbin-Watson statistic of 1.86. Although one statistically significant outlier was identified, the isolated occurrence is more likely attributed to experimental variability or localized nonlinear adsorption behavior, than a systematic model inadequacy. A comparative residual patterns have been reported in recent adsorption modelling studies where regression assumptions were satisfied despite poor predictive accuracy, emphasizing that statistical validity alone does not guarantee model suitability for highly nonlinear adsorption system [36]. Collectively, the Pareto and residual analyses shows that the regression model's poor predictive performance results from its inability to fully capture the intricate and nonlinear adsorption mechanisms controlling Pb^{2+} sequestration by the keratin-based biosorbent rather than from statistical assumptions being broken. These findings provide strong justification to employ a more sophisticated nonlinear modeling techniques, such as artificial neural networks (ANN) and adaptive neuro-fuzzy inference systems (ANFIS) which are better suited for describing complex adsorption systems characterized by strong variable interactions and nonlinear response surfaces.

Table 6: Regression Coefficients

Term	Coef	SE Coef	T-Value	P-Value	VIF
Constant	89.39	3.65	24.47	0.000	
Dose	1.87	3.64	0.51	0.613	1.22
Conc.	-0.0263	0.0262	-1.01	0.324	1.09
pH	0.289	0.303	0.95	0.350	1.17
Time	0.0459	0.0270	1.70	0.102	1.08

Regression Equation (%): $89.39 + 1.87 \text{ Dose} - 0.0263 \text{ Conc.} + 0.289 \text{ pH} + 0.0459 \text{ Time}$ ----- Eqn 22

Table 7: Model Summary

S	R-sq	R-sq(adj)	R-sq(pred)	10-fold S	10-fold R-sq
4.04567	22.62%	10.24%	0.00%	4.35560	0.00%

Table 8: Analysis of Variance

Source	DF	Adj SS	Adj MS	F-Value	P-Value
Regression	4	119.64	29.91	1.83	0.155
Dose	1	4.30	4.30	0.26	0.613
Conc.	1	16.57	16.57	1.01	0.324
pH	1	14.85	14.85	0.91	0.350
Time	1	47.17	47.17	2.88	0.102
Error	25	409.19	16.37		
Lack-of-Fit	22	372.25	16.92	1.37	0.454
Pure Error	3	36.93	12.31		
Total	29	528.83			
Durbin-Watson Statistic		1.86			

Table 9: Fits and Diagnostics for Unusual Observations

Obs	Response (%)	Fit	Resid	Std Resid	
16	81.54	96.29	-14.75	-3.93	R

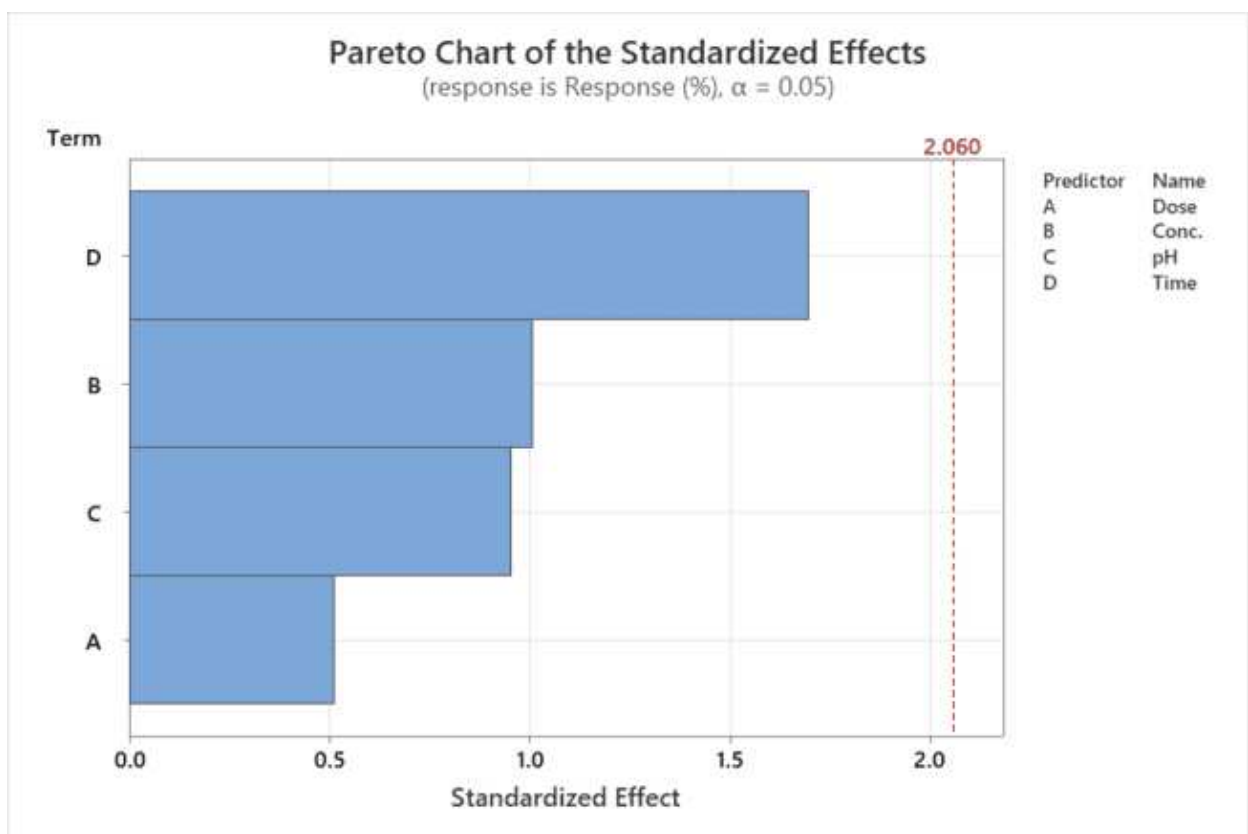


Figure 4: Parato Chart Analysis of the Mean effect

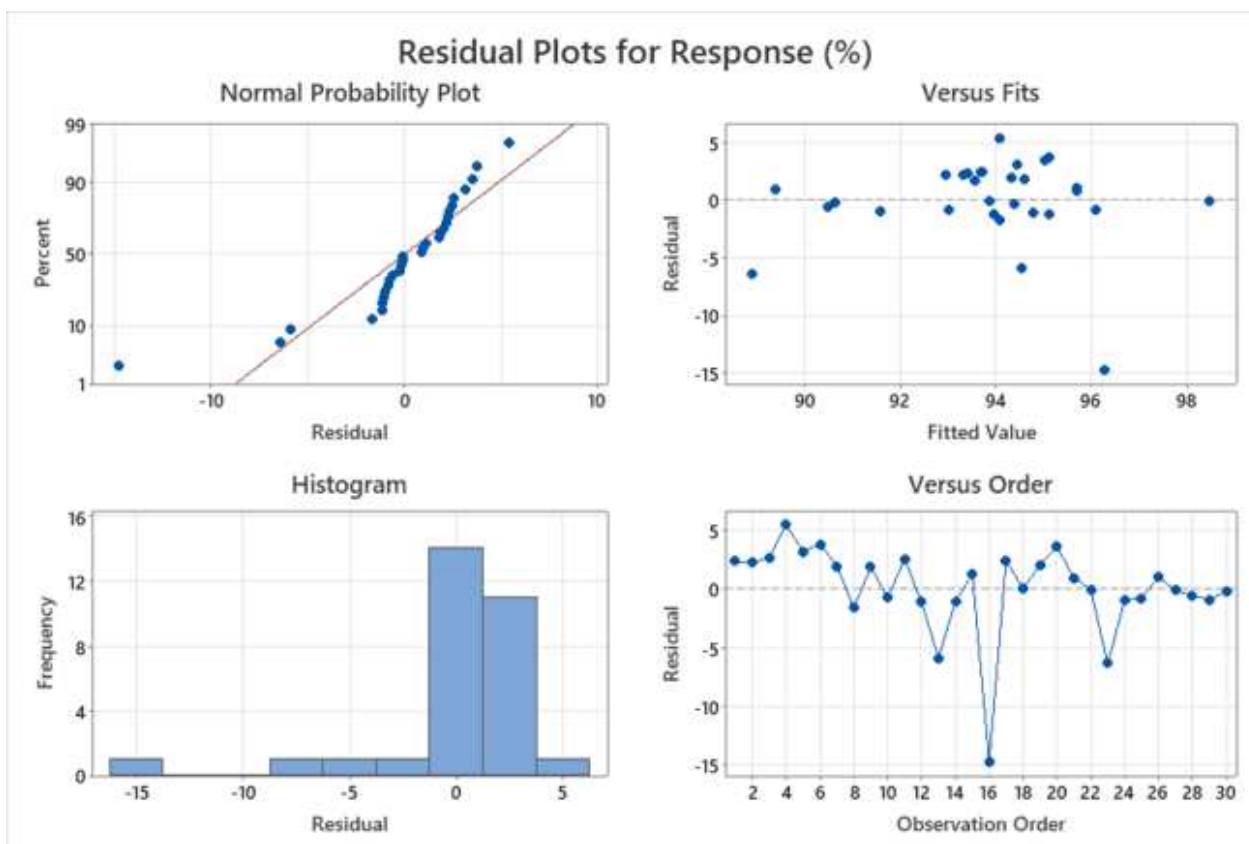


Figure 5: Residual Analysis and Model Adequacy Diagnostics

3.4.2 Linear Regression Analysis

The candidate linear regression models (LRM) exhibited substantial variation in predictive performance, with Model 16.3 identified as the optimal model used base on external validation as seen in Table 10. This model produced the lowest RMSE of 4.26, MSE of 18.11, and MAE of 2.85, together with the highest validation R^2 value of 0.05 among the evaluated models as seen in Figure 6. Despite outperforming the remaining linear models, the coefficient of determination indicates that only 5% of the variability in Pb^{2+} adsorption efficiency was explained by the predictor variables, demonstrating weak explanatory and predictive capability. In contrast, the remaining models yielded negative validation R^2 values (-24.98 to -0.17), indicating prediction errors greater than those obtained using the mean response as a predictor, which is a recognized indicator of poor model generalization and inadequate predictive performance.

The validation predicted versus actual response plot as seen in Figure 7, corroborates these statistical findings. Although several observations are distributed close to the line of perfect prediction, the noticeable dispersion

around the 1:1 reference line indicates considerable discrepancies between predicted and experimental Pb^{2+} adsorption efficiencies. The presence of both overestimation and underestimation without an obvious directional trend suggest that the residuals are randomly distributed, implying the absence of systematic prediction bias. However, the magnitude of the deviation confirms that the model captures only the overall trend of the adsorption process while failing to explain a substantial proportion of the experimental variability.

Similarly, the response plot (Figure 8) shows that the predicted response generally follows the experimental trend, with relatively small residuals for most validation samples. Nevertheless, several observations exhibit comparatively large residuals, particularly at lower adsorption efficiencies, underscoring localized prediction errors and reduced model reliability under specific operating conditions. These observations are consistent with the low validation R^2 of 0.05, confirming that the linear regression model is unable to adequately describe the complex response surface governing Pb^{2+} adsorption.

The limited performance of the linear regression model is consistent with previous adsorption studies, which demonstrated that adsorption systems are inherently nonlinear because of simultaneous interactions among process variables and the heterogeneous nature of adsorption sites. Consequently, nonlinear modelling approaches generally provide more accurate predictions than conventional linear regression. For instance, Vitek and Mancini. [55] reported nonlinear regression produced more reliable adsorption parameter estimation than linearized models by avoiding the distortions introduced during linear transformation of adsorption data. Similarly, comparative investigation of metal ion biosorption onto calcium alginate and dye adsorption onto rice husk concluded that nonlinear regression consistently outperformed linear methods in describing adsorption behavior and estimating model parameters with greater accuracy [56].

The Model 16.3 represent the best performing linear regression under the studied conditions and it provides an appropriate linear baseline for comparison. However, its low explanatory power and persistent prediction errors demonstrate that first order linear regression is inadequate for modelling Pb^{2+} adsorption onto ethanol pretreated chicken feather biomass. These findings indicate that the adsorption process is governed by nonlinear

interactions among adsorbent dosage, solution pH, initial metal concentration, and contact time, thereby providing strong justification for the application of nonlinear machine learning models, to achieve more accurate and robust prediction of biosorption performance.

Table 10: Performance Evaluation of Linear Regression Models

Model Number	Model Type	Status	RMSE (Validation)	MSE (Validation)	R-Squared (Validation)	MAE (Validation)
7	Linear Regression	Trained	22.31	497.52	-24.98	12.00
16.1	Linear Regression	Trained	4.74	22.48	-0.17	3.28
16.2	Linear Regression	Trained	10.73	115.19	-5.02	6.38
16.3	Linear Regression	Trained	4.26	18.11	0.05	2.85
16.4	Stepwise Linear Regression	Trained	5.26	27.66	-0.44	3.93

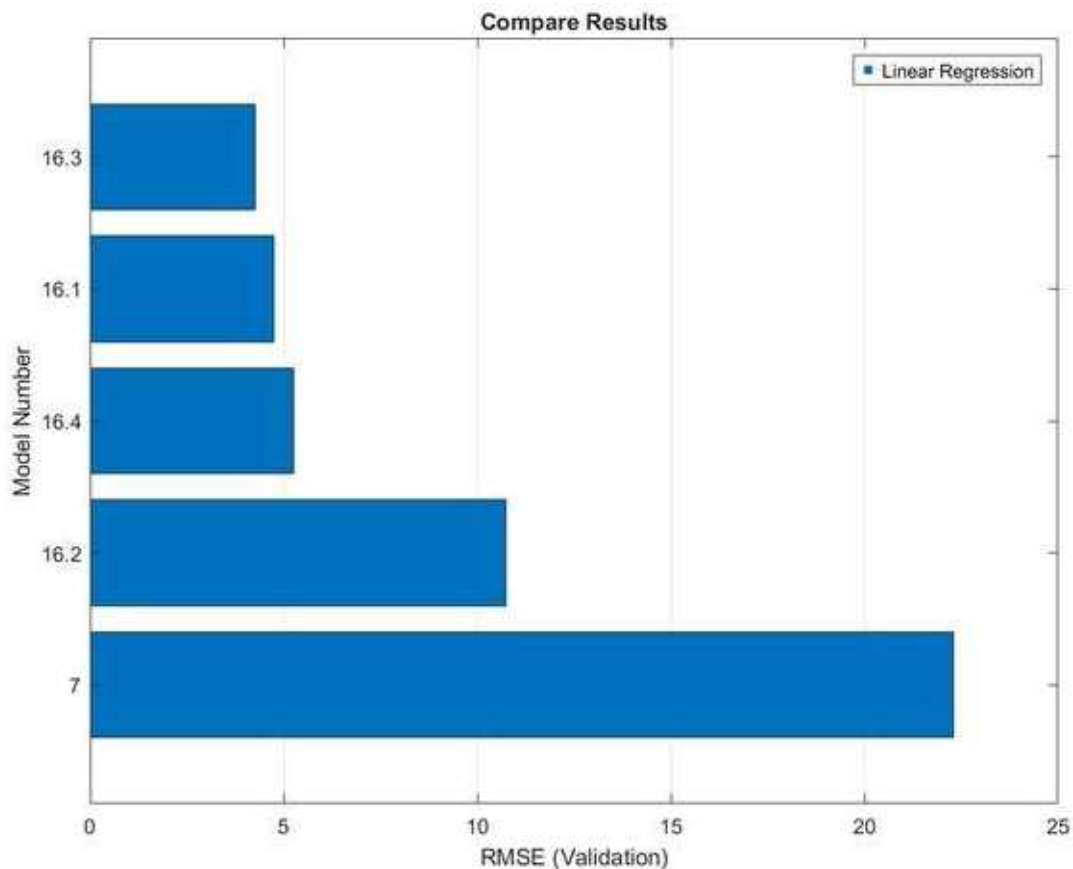


Figure 6: Comparison Validation of RMSE for Potential Linear Regression Models

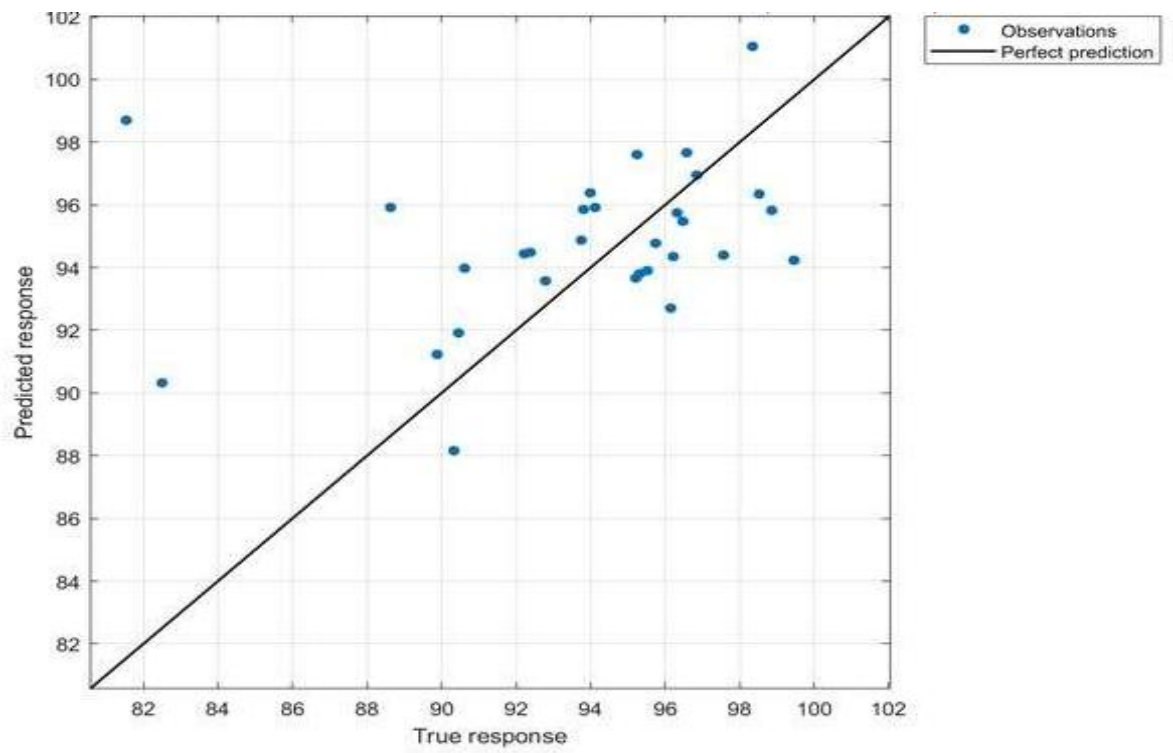


Figure 7: Validation plot of Develop LRM

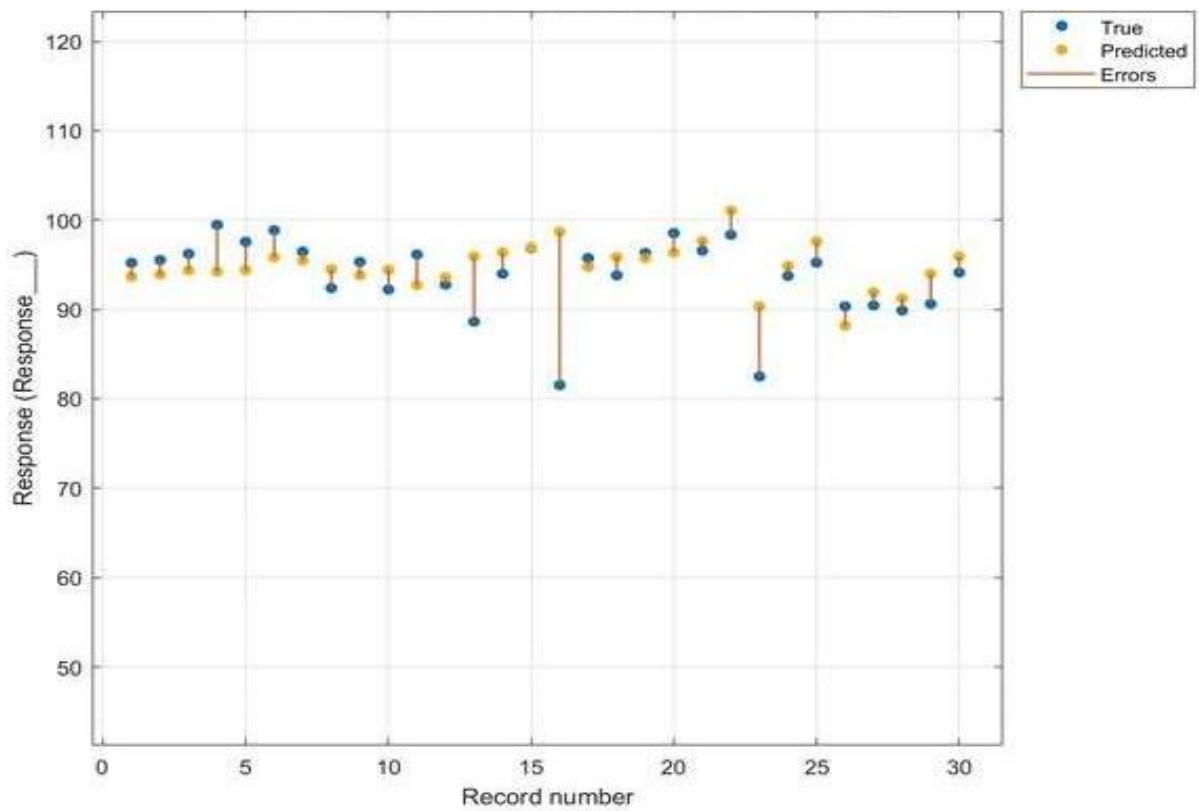


Figure 8: Model Prediction Accuracy Assessment

3.4.3 Artificial Neural Network (ANN) Analysis

An artificial neural network (ANN) with a 4:8:1 architecture was constructed to predict the adsorption of Pb^{2+} ions onto PCFB as seen in figure 9. A satisfactory prediction with little error was indicated by the RMSE value of 1.27 and the R^2 value of 0.94. However, investigations of neural networks with hidden layers ranging from 1 to 25 neurons have been reported in the literature [57]. As a result, the number of hidden neurons has a substantial impact on the neural network's performance, as shown in table 11. While fewer neurons overwhelm the network's capacity for learning and prediction, a model with many hidden neurons is very flexible and may lead to overfitting of the dataset. The number of optimal neurons was thus determined by model optimization, which involved evaluating the trained network's performance against different hidden layer neurons.

The table 12 displays the developed ANN model's training procedure. The network completed 14 training epochs in about 3 seconds, and during which the performance mean squared error decreased from 136 to 0.761, demonstrating the model converged rapidly and with high predicted accuracy. Additionally, the gradient decreased from 369 to 1.09×10^{-5} , indicating that the optimization algorithm approached a stable minimum. During training, the Lavenberg Marquardt damping parameter (u) dropped from 1.0×10^{-3} to 1.0×10^{-5} , indicating effective optimization. In order to avoid overfitting and improve the model's generalization performance, the early stopping criterion was satisfied when the training terminated after six (6) consecutive validation checks without improvement.

The ANN validation performance and adaptability are presented in Figure 10. The dotted lines represent the line of best fit, while the colors blue, green, and red, respectively, represent the different RMSE values related to the ANN training, validation, and test. The RMSE measures the average difference between the experimental values and the ANN predicted value in relation to the regression line. Stronger agreement between the ANN predictions and the experimental observations is indicated by a smaller RMSE, which indicates that the predicted data lie closer to the line of best fit [58].

Figure 11 shows the developed ANN model used to predict Pb^{2+} ions adsorption onto PCFB. The satisfactory model adopted for this study was the model whose uniformity between the experimental data and predicted

values had close agreement, which yielded the highest R^2 value closest to unity. The Pb^{2+} adsorption experimental R^2 values in the current study showed that the output layer was closely predicted by the model, since the model produced the highest R^2 value (0.94) that was nearest to unity and its uniformity between the experimental data and predicted values showed close agreement, therefore leading to a better and more significant model as shown in Table 4.

Consistent with the current study, ANN as a powerful prediction tool has been reported in previous study. For instance, Mansouri *et al.* [59] opined that an ANN model with a mean squared error (MSE) of 0.0015 and an R^2 of 0.9951 satisfactorily predicted adsorptive desulfurization using zeolites. Similarly, Tariq *et al.* [60], opined that ANN modeling with iterative optimization produced extremely accurate predictions that closely matched experimental findings when forecasting the adsorption capacity of 3-nitrophenol utilizing carbonaceous material derived from biomass waste. The work highlights the significance of various correlation methods for thorough insights into competitive adsorption dynamics while demonstrating the effectiveness of deep learning in optimizing adsorption operations. After being refined across 228 epochs, the 5-14-1 learning architecture showed excellent performance with high R^2 values and mean squared error (MSE) values of 4.07, 18.406, and 6.2122 for training, testing, and total datasets, respectively.

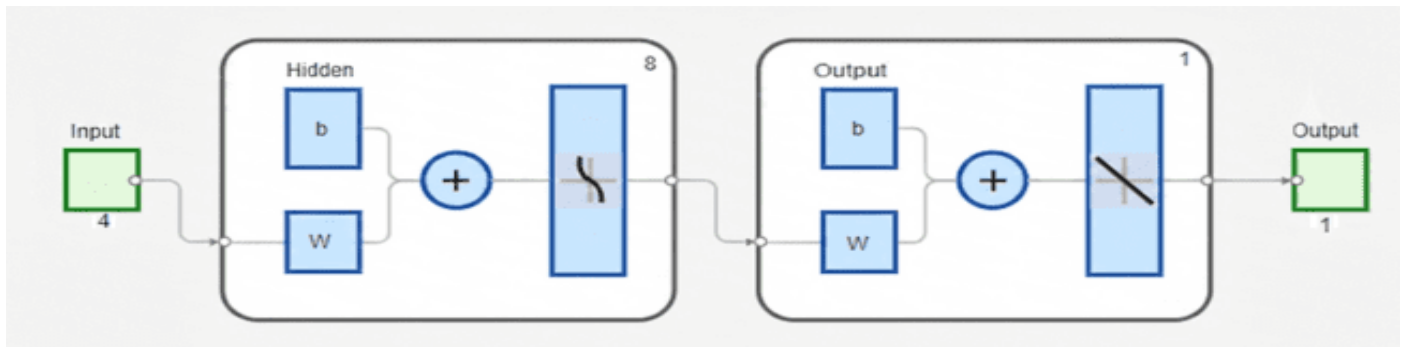


Figure 9: Proposed Architecture for predicting Pb^{+2} Adsorption onto PCFB

Table 11: Comparative Evaluation of Different ANN Network Architecture's Performance

Topology	MSE	RSME	R ²
4:8:1	1.618	1.27	0.94
4:10:1	1.669	1.29	0.91
4:12:1	2.060	1.43	0.92
4:16:1	2.094	1.45	0.92
4:20:1	2.273	1.51	0.90

Table 12: ANN Training Process

Unit	Initial Value	Stopped Value	Target Value
Epoch	0	14	1000
Elapsed	-	00:00:03	-
Performance	136	0.761	0
Gradient	369	1.09×10^{-5}	1×10^{-7}
Mu	0.001	1×10^{-5}	1×10^{10}
Validation Checks	0	6	6

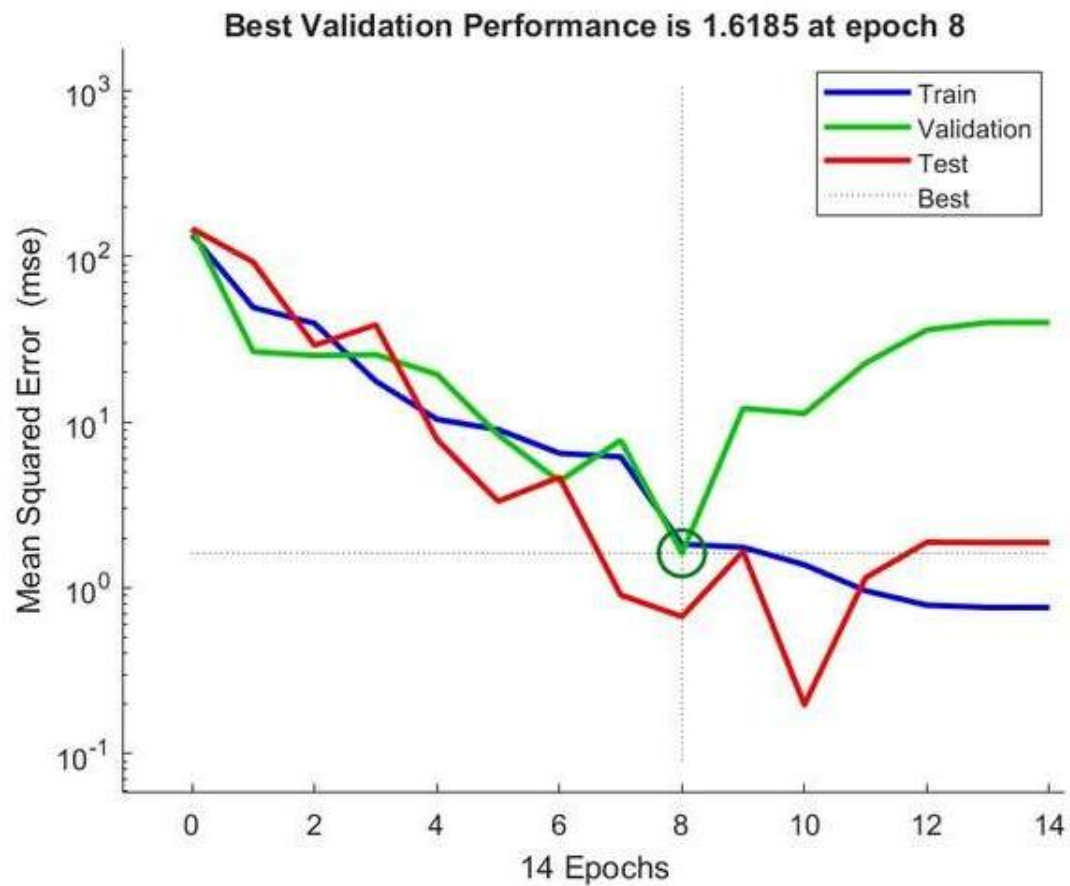


Figure 10: ANN Training and Validation Performance

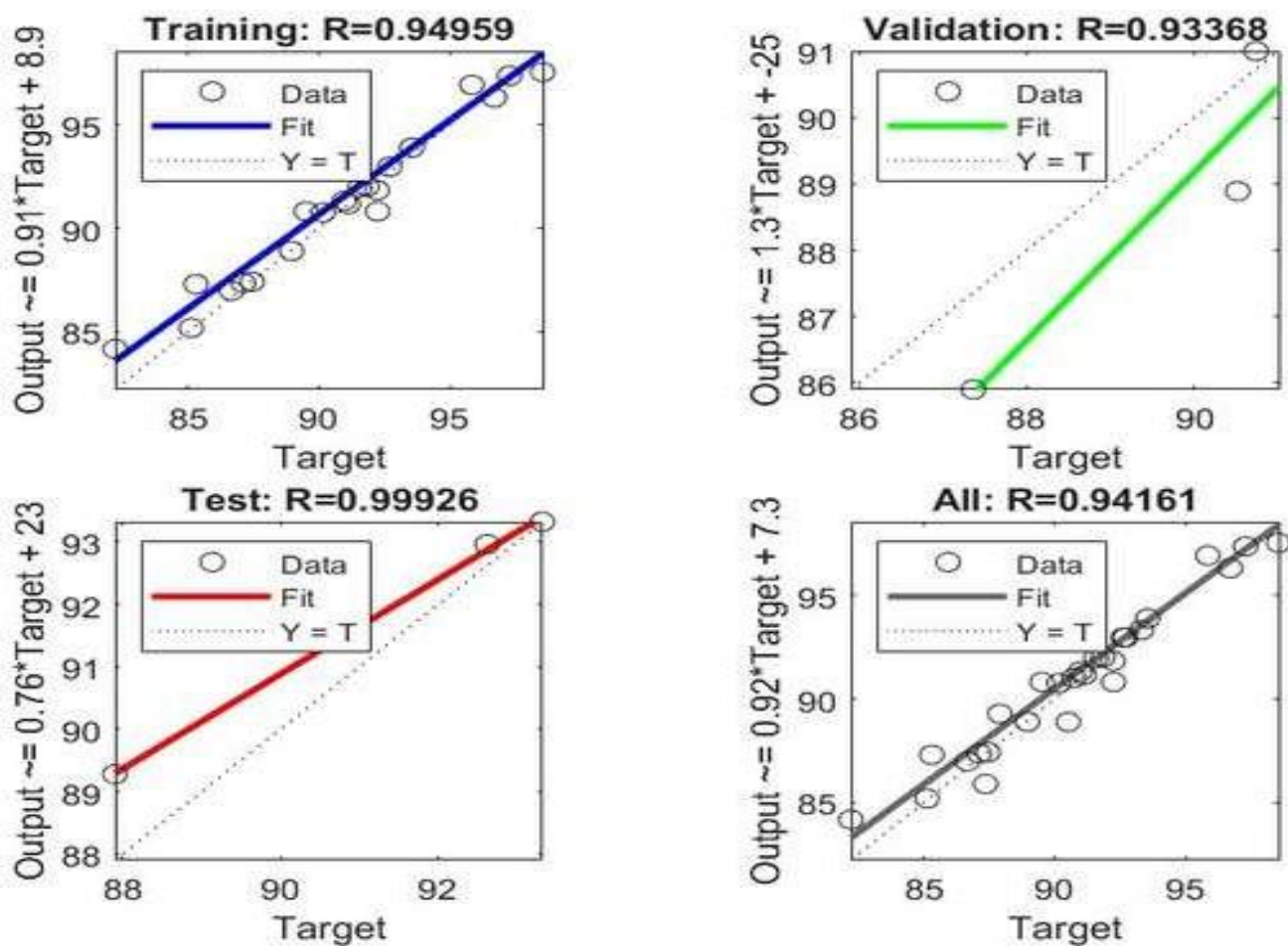


Figure 11: Developed ANN Model

3.4.4 Comparative Evaluation of ANN, LRM and RSM Developed models

The predictive performance of the developed artificial neural network (ANN), linear regression model (LRM), and response surface methodology (RSM) models was evaluated using the coefficient of determination (R^2), mean squared error (MSE), and root mean squared error (RMSE) derived from the experimental and predicted Pb^{2+} removal efficiencies as presented in Table 13. Among the three models, the ANN exhibited the highest predictive accuracy, achieving an R^2 of 0.9473, with the lowest prediction errors MSE of 0.9295, and an RMSE of 0.9641. The high R^2 coupled with the minimal prediction errors demonstrates the excellent capability of the ANN to capture the complex nonlinear interactions between the process factors governing Pb^{2+} adsorption process. This superior performance reflects the adaptive learning ability of ANN, which are capable of modeling

intricate input-output relationship without assuming a predefined mathematical form. Conversely, RSM model showed considerably poorer predictive performance with R^2 value of 0.2262, MSE of 13.64 and, RMSE of 3.69, indicating that the second-order polynomial equation generated from the central composite design was unable to sufficiently describe the experimental response over the examined experimental conditions. Similarly, the linear regression model (LRM) yielded the poorest predictive performance, with the lowest R^2 (0.1630) and the highest prediction errors (MSE = 14.7549 and RMSE = 3.8412), demonstrating that the simple linear relationship cannot adequately describe the complexity of the adsorption mechanism.

Pb^{2+} adsorption onto ethanol-pretreated chicken feather biomass is driven by complex nonlinear connections that are better represented using machine learning approaches than traditional statistical regression techniques, as demonstrated by the ANN's notable advantage over both RSM and LRM. Although the ANN offered excellent predictive capability, the comparatively low R^2 values for the RSM and LRM indicate that complex nonlinear interactions among the operating variables dominate the adsorption process, making traditional regression-based models less appropriate for accurate prediction

These findings are consistent with previous study by Hafeez *et al.* [61] who reported superior predictive capabilities of ANN over conventional regression models for adsorption systems. They opined that ANN predicted Pb^{2+} adsorption onto magnetic montmorillonite/CoFe₂O₄ composite more accurately than RSM, achieving an R^2 of 0.998 with lower RMSE values, and concluded that ANN was a more reliable optimization tool for complex adsorption processes. Similarly, Igberase [62], demonstrated that ANN consistently outperformed RSM in modelling the simultaneous adsorption of Pb^{2+} and Ni^{2+} onto modified chitosan beads, reporting excellent prediction accuracies with R^2 values up to 1.00 during training, and significant lower prediction errors, which they attributed to the ability of ANN to effectively learn nonlinear adsorption behavior.

These recent findings reinforce the growing consensus that machine learning models, particularly ANN, provide more accurate, reliable, and generalizable prediction of adsorption performance than conventional RSM and

LRM, making them highly suitable for the design, optimization, and scale-up of biosorption processes involving heterogeneous biomaterials such as ethanol pretreated chicken feather biomass.

Table 13: Comparative Performance Evaluation of the Developed Predictive Models

Model	R ²	MSE	RMSE
RSM	0.22	13.63	3.69
LRM	0.16	14.75	3.84
ANN	0.94	0.93	0.96

3.4.5 Density Function Theory (DFT) Analysis

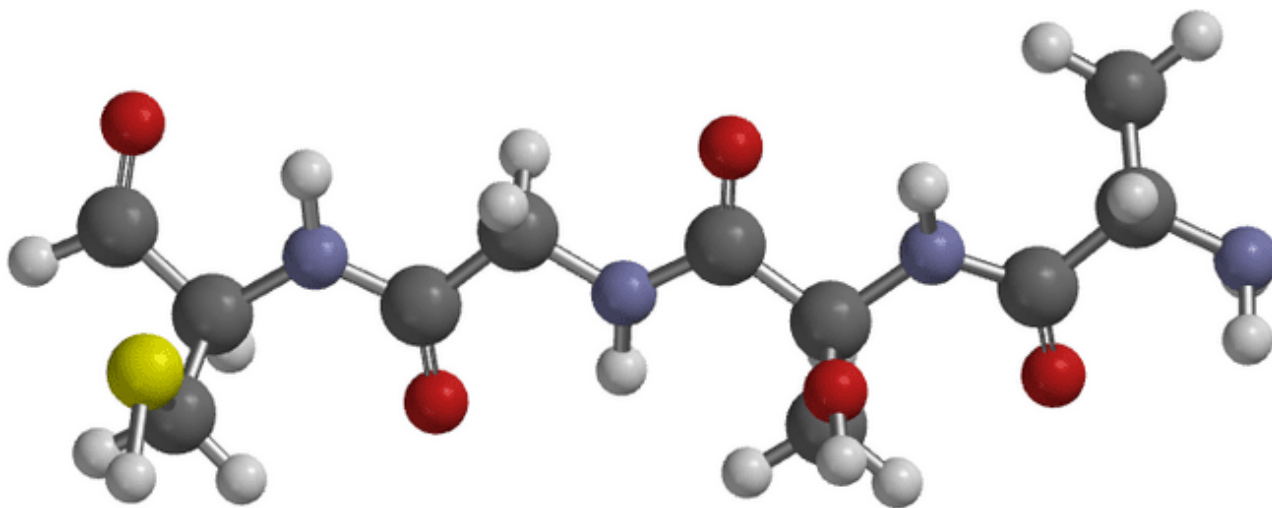


Figure 12: Optimized Keratin Representative Structure

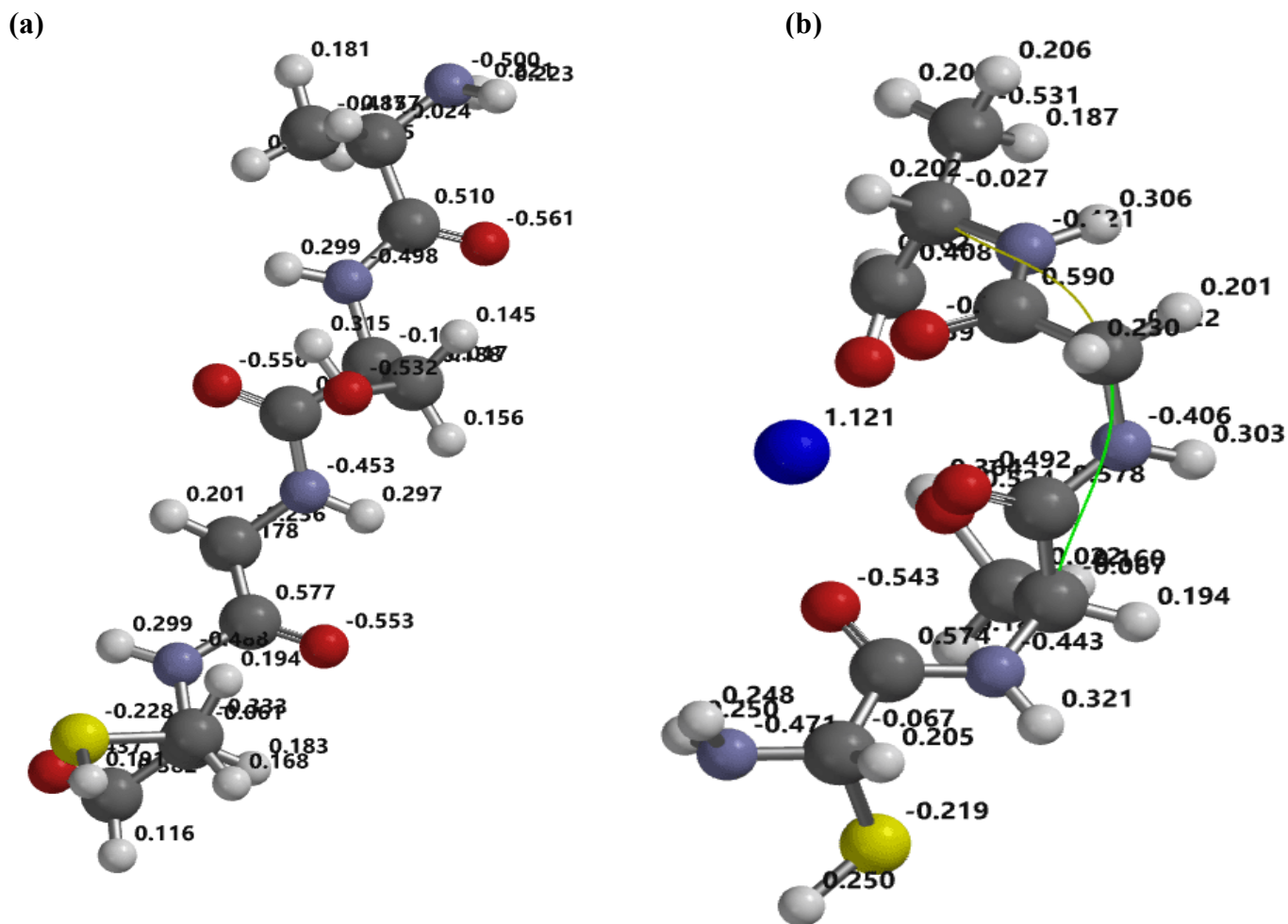


Figure 13: Millikan charge of Keratin (a) and Mulliken Charge of Pb^{2+} -Keratin complex (b)

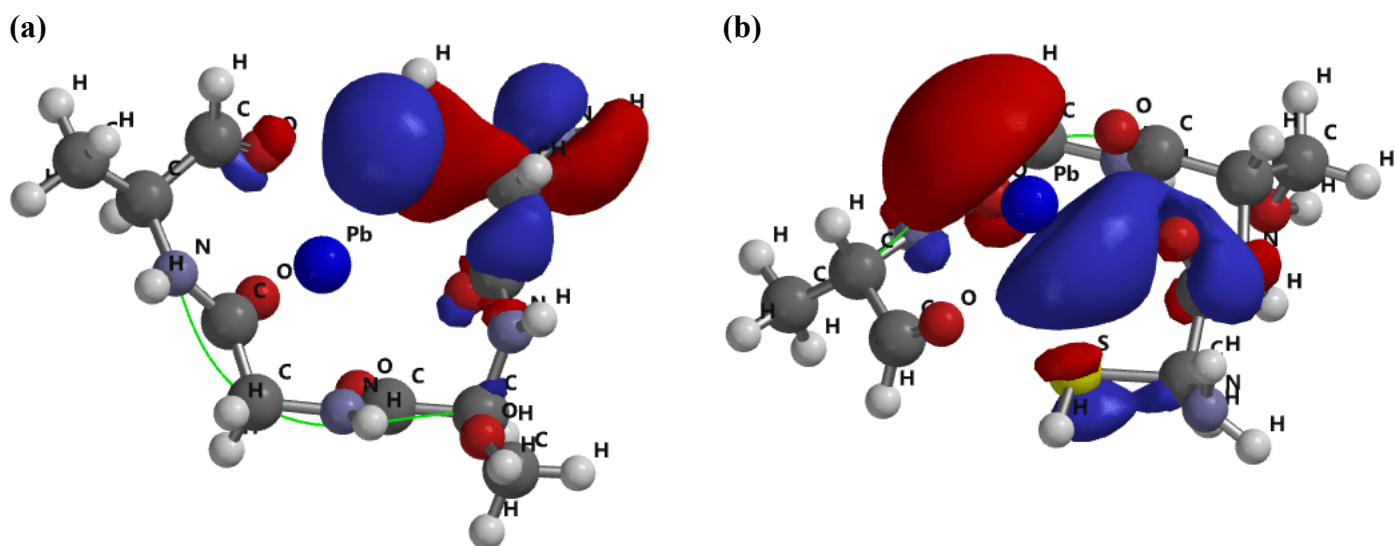


Figure 14: The Frontier Molecular Orbital for HOMO (a) and LUMO (b)

The representative keratin model used in this study was constructed using Spartan 14 V1.14 software (Figure 12), from four amino acid residue namely cysteine, glycine, alanine, and serine because they constitute the major components of feather β -keratin and collectively replicate its essential structural and electronic characteristics [3]. Cysteine contributes thiol (-SH) functional groups that serve as precursors to the disulfide cross-links that give keratin its mechanical stability and structural integrity, as well as sulfur donor sites with a great affinity for heavy metal ions. Glycine and alanine preserve the characteristic β sheet framework of feather keratin owing to their high abundance within the protein structure, whereas serine introduces polar hydroxyl (-OH) groups that participate in hydrogen bonding and influence the electron density around potential adsorption sites. Collectively, these amino acid residues provide the main sulfur-, oxygen-, and nitrogen-containing functional groups that dominate metal ion coordination, thereby offering a chemically representative and computationally efficient molecular model for elucidating the adsorption mechanism of Pb^{2+} at the molecular level.

Prior to chemical quantum calculations, the keratin model was initially subjected to geometry optimization and molecular mechanics energy minimization in order to obtain eliminate steric strain and obtain the ground state structure corresponding to the lowest energy molecular configuration. A conformational search was then used to identify the global minimum energy conformer, which serve as the input structure for quantum chemical calculations. Density functional theory (DFT) geometry optimization at the B3LYP/6-31G* level was then used to precisely identify the electronic structure and energy profile of the optimized keratin model. The Pb^{2+} -keratin complex was treated to the same computational methods in order to preserve methodological consistency and enable a direct comparison of the energetic properties before and after metal coordination.

The calculated DFT descriptors (Table 14) demonstrate that Pb^{2+} adsorption significantly alters the electronic structure and stability of the keratin model. The calculated adsorption energy of $-470.65 \text{ kJ mol}^{-1}$, indicates that complex formation is highly thermodynamically favorable and reflect strong chemical interactions between Pb^{2+} and the active adsorption sites of keratin. Such a large negative adsorption energy is consistent with chemisorption involving coordinate bond formation rather than weak physisorption. The LUMO – HOMO energy gap decreased from 9.36 eV for pure keratin to 7.70 eV after adsorption corresponding to 17.7%

reduction. A narrower energy gap generally signifies increase molecular reactivity and enhanced charge transfer between the adsorbent and adsorbate, indicating that coordination of Pb^{2+} facilitates electron delocalization within the keratin framework [38].

Similarly, both the HOMO (Figure 14a) and LUMO (Figure 14b) energies shifted to lower levels after Pb^{2+} adsorption, suggesting stabilization of the electronic structure after complex formation. The reduction in HOMO's energy indicates that, the occupied orbitals became more stable, following electron density redistribution, thereby reducing the electron donating tendency of the isolated keratin molecule. When a complex is formed, the electronic structure is reorganized, as indicated by the stabilization of the LUMO. These electronic changes, together with the highly negative adsorption energy and formation of Pb-donor atom bonds, provides strong evidence for stable coordination between Pb^{2+} and the functional groups present in PCFB.

The dipole moment increased from 3.32 Debye to 4.06 Debye after Pb^{2+} adsorption, indicating a significant redistribution of electron density upon complex formation. The increased molecular polarity indicates strong electrostatic interactions between Pb^{2+} and the donor atoms of keratin, particularly sulfur, nitrogen and oxygen atoms. An increase in dipole moment after adsorption is usually associated with enhanced charge separation and stronger metal-ligand interactions, supporting the occurrence of a chemisorption mechanism dominated by electron sharing between the adsorbent and the metal ion [63].

Collectively, the DFT descriptors consistently demonstrate that Pb^{2+} adsorption induces significant electronic rearrangement within the keratin framework. The highly favorable adsorption energy, reduction in the HOMO-LUMO energy gap, stabilization of frontier molecular orbitals, and increased dipole indicates that adsorption proceeds predominantly through charge transfer interaction involving sulfur, nitrogen and oxygen containing functional moieties. These findings further reaffirm the formation of a stable Pb^{2+} -keratin coordination complex and the chemisorption mechanism inferred from the experimental adsorption and kinetic studies.

The present findings are consistent with recent computational investigation of heavy metal adsorption on keratinous and protein based biomaterials. For instance, Fernandez *et al.* [64], reported that DFT calculations for

Pb²⁺ adsorption on amino acid rich biopolymeric adsorbent exhibited highly negative adsorption energies accompanied by reduced HOMO-LUMO energy gaps, indicating enhanced electronic interaction and spontaneous chemisorption through oxygen and nitrogen containing functional groups. Similarly, Costa *et al.* [65], opined that coordination of Pb²⁺ with sulfur and oxygen rich biomolecular ligands resulted in stabilization of frontier molecular orbitals, increased dipole moments, and significant charge redistribution, confirming that electron transfer is the principal driving force for stable Pb²⁺ complex formation. El Messaoudi *et al.* [66] also reported similar observation, he observed that DFT descriptors, including negative adsorption energies, reduced energy gaps, and increased molecular polarity, provided convincing evidence of strong chemisorption interactions between heavy metal ions and protein derived biosorbents. Collectively, these studies support the present results and reinforce the suitability of DFT as a reliable tool for elucidating the molecular mechanism governing Pb²⁺ adsorption on keratin based biosorbents

Table 14: DFT computation Descriptors of Keratin and Pb²⁺-Keratin complex

Descriptors	Keratin	Pb	Pb ²⁺ -Keratin complex
Electronic Energy	-880.38 kJ/mol	2108.65 kJ/mol	772.92 kJ/mol
E-HUMO	-9.63 ev	-23.31 ev	-15.66 ev
E-LUMO	-0.27 ev	-12.40 ev	-7.96 ev
Dipole moment	3.32 debye	0.00	4.06 debye
Energy of Adsorption (E _{ads})	-470.65 kJ mol ⁻¹		
Energy Gap (ΔE)	9.36 ev	10.91 ev	7.7 ev

The Mulliken charge analysis showed that Pb²⁺ adsorption induced significant electron density redistribution within the representative keratin model (Figure 13a and 13b), demonstrating charge transfer between the metal ion and the adsorbent (Table 15). The largest reduction in negative charge occurred at O₅ (Δ = +0.102 e), N₃ (Δ = +0.092 e), N₄ (Δ = +0.079 e), and O₃ (Δ = +0.064 e) identifying these heteroatoms as the principal electron-donating centers involved in Pb²⁺ coordination. Conversely, sulfur (Δ = +0.009 e) and the remaining nitrogen

atoms exhibited only minor charge redistribution, suggesting secondary contributions to the adsorption process. Interestingly, O₁ became more negatively charged ($\Delta = -0.106$ e), indicating that this atom participated primarily in intramolecular electronic polarization rather than direct Pb²⁺ coordination. Such redistribution of electron density is consistent with adsorption induced orbital interaction and confirms that complex formation is accompanied by extensive electronic rearrangement within the keratin framework [50].

These findings suggest that Pb²⁺ adsorption is controlled by multidentate coordination involving several oxygen and nitrogen donor sites, thereby stabilizing the adsorbed complex through the observed electronic redistribution. This observation is consistent with the Hard and Soft Acids and Bases (HSAB) theory, which predict that Pb²⁺, a borderline-soft Lewis acid, preferentially interact with electron rich oxygen and nitrogen donor site present in protein based adsorbents. The Mulliken charge analysis supports the suggested adsorption mechanism by offering quantum chemical evidence that Pb²⁺ adsorption happens through multidentate coordination accompanied by significant electronic restructuring of the keratin framework. Consistent with the present study Ayad *et al.* [67], reported DFT investigation where Mulliken charge redistribution was identified as direct evidence of electron transfer during adsorption, oxygen containing functional groups were identified to serve as the predominant active sites because of their high electron density and strong coordination ability. Similarly, Qi and Guan [68], demonstrated that adsorption induced charge redistribution significantly modifies the electron environment surrounding adsorption centers, thereby enhancing complex stability and adsorption strength.

Furthermore, the optimized bond distance (Table 16) provides additional structural evidence supporting the proposed adsorption mechanism. The calculated Pb–O bond lengths range (2.407 to 2.732 Å), is consistent with stable Pb–O coordination reported for lead-organic complexes. Furthermore, the relatively short Pb–N bond distances of N₄ (2.405 Å) and N₂ (2.571 Å), confirms that these amide nitrogen atoms form a direct coordination with Pb²⁺. Conversely, the longer Pb–S distance of 5.907 Å and the Pb–N₁/Pb–N₃ distances of approximately 4.19 Å significantly exceeded the lengths of coordination bonds, demonstrating that these atoms contributed minimally, if at all to direct Pb²⁺ coordination. Collectively, these findings support the Mulliken population

analysis, confirming that oxygen atoms are the primary coordination centers while nitrogen atoms provide additional stabilization through auxiliary coordination. The agreement between the electronic and geometric descriptors demonstrates that adsorption is predominantly governed by simultaneous charge transfer and structural rearrangement, resulting in the formation of a thermodynamically stable adsorption complex.

This present study is consistent with previous report by Ganguly *et al.* [69] who reported DFT studies where variation in Mulliken atomic charges together with optimized metal ligand bond length were used to identify adsorption active sites and explain the enhanced stability of metal complexes following adsorption. These consistencies further validate the proposed adsorption mechanism and reinforce the reliability of the present DFT calculations.

Table 15: Milliken Charge before and After adsorption of Pb²⁺

Element	Before Adsorption	After Adsorption	Difference
S	-0.228	-0.219	+0.009
N ₁	-0.488	-0.471	+0.017
N ₂	-0.453	-0.443	+0.01
N ₃	-0.498	-0.406	+0.092
N ₄	-0.500	-0.421	+0.079
O ₁	-0.437	-0.543	-0.106
O ₂	-0.553	-0.524	+0.029
O ₃	-0.556	-0.492	+0.064
O ₄	-0.532	-0.533	-0.001
O ₅	-0.561	-0.459	+0.102

Table 16: Bond Distance

Element	Bond Distance (Å)
Pb-S	5.907
Pb-N ₁	4.189
Pb-N ₂	2.571
Pb-N ₃	4.189
Pb-N ₄	2.405
Pb-O ₁	2.407
Pb-O ₂	2.732
Pb-O ₃	2.507
Pb-O ₄	2.407
Pb-O ₅	2.694

3.5 Adsorption Isotherm

The image in Fig. 15 represents the Freundlich isotherm for Pb^{2+} ion sorption. The correlation parameters are presented in Table 17. The correlation coefficient (R^2) = 0.9376 shows the Freundlich isotherm explains the experimental data. This suggests the adsorption of Pb^{2+} ion ions by PCFB occurred on a multilayer heterogeneous surface. Which strongly suggest PCFB possess a non-uniform active site. The heterogeneity factor (n) = 2.353495 suggest a favorable adsorption process since $1 < n < 10$ [49]; [16]. This result implies that the surface binding sites have moderate heterogeneity and increasing Pb^{2+} ion concentration leads to saturation effect and energy distribution across site since $1/n < 1$. The Freundlich isotherm constant (K_F) = $0.8993 (mg/g)(L/mg)^{0.5}$ suggest a relatively moderate adsorbate-adsorbent affinity [27].

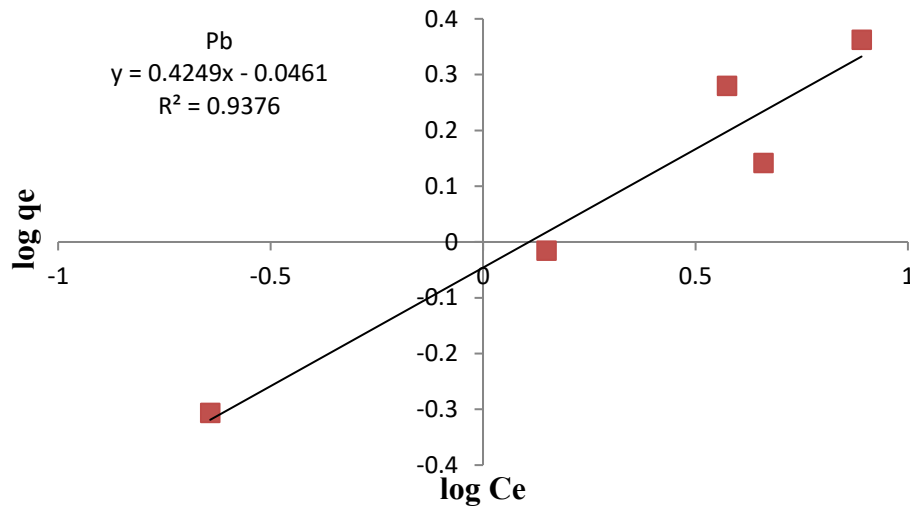


Figure 15: Freundlich Isotherm of Pb^{2+} ion Sorption onto pretreated Chicken Feather biomass

The Flory-Huggins isotherm for Pb^{2+} ion sorption is illustrated in Fig. 16 while the isotherm parameters are presented in Table 17. The data revealed $R^2 = 0.8505$, $K_{FH} = 656.15 (Lmg^{-1})$ $n = 0.7752$ and $G = -16kJmol^{-1}$ as presented. This result suggests that 85% of the variation in the experimental data can be explained by this model. The values of the equilibrium parameter (K_{FG}) and degree of surface coverage (n), indicates high adsorbate-adsorbent affinity while the adsorption process followed a heterogeneous multilayer mechanism with an adsorbate molecule occupying less than one site [33]. This implies favorable adsorption with high surface

coverage. The Gibbs free energy value confirms the process was spontaneous which also falls within the range typical (-20 – 0 kJ/mol) for physisorption process [70].

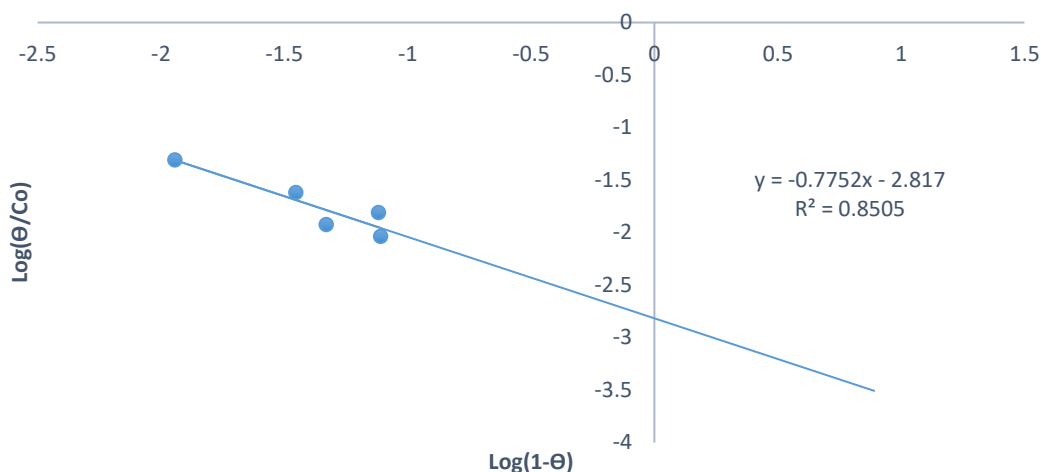


Figure 16: Flory-Huggins Isotherm of Pb (II) ions Sorption onto pretreated Chicken Feather biomass

The Jovanovic isotherm for Pb^{2+} ion sorption is illustrated in Figure 17, while the isotherm parameters are presented in Table 17. The result revealed that the $R^2 = 0.7979$, $K_J = 0.1855$ and $Q_{\text{max}} = 1.5600 \text{ mgg}^{-1}$. This suggest that statistically 79.79% variation in the experimental data can be explained by this isotherm i.e the data showed a good fit. The value for K_J suggests a positive correlation between adsorbate concentration and amount adsorbed at equilibrium, which implies the adsorption is favourable what a maximum adsorption capacity of 1.56 mg/g (reflecting saturation capacity of the adsorbent at equilibrium) [29].

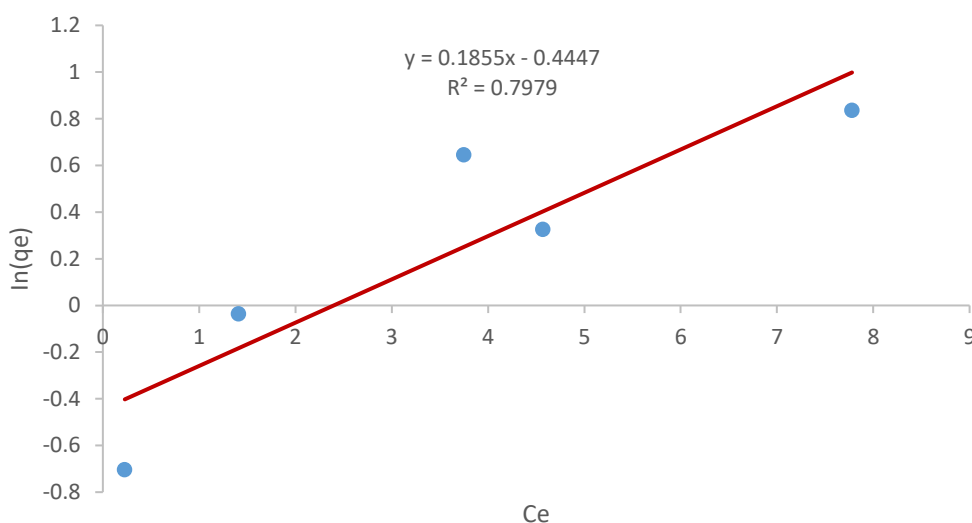


Figure 17: Jovanovic Isotherm for Pb^{2+} ion sorption onto Pretreated Chicken Feather Biomass

The image in Figure 18, illustrates the Langmuir isotherm for Pb^{2+} ion sorption onto PCFB, while the isotherm parameters are presented in Table 17. The result revealed that $R^2 = 0.841$, $K_L = 0.5248 \text{ mg/L}$, $Q_0 = 0.087 \text{ mg/g}$ and $R_L = 2.58131$. This result suggests that Langmuir isotherm can account for 84.1% variation in the experimental data [71]; [72]. Nonetheless, the value of the Langmuir constant (K_L) suggests a moderate adsorbate-adsorbent affinity as seen in the relatively low maximum monolayer adsorption capacity (Q_0) (0.087 mg/g) and unfavorable adsorption process as seen in the separation factor $R_L > 1$.

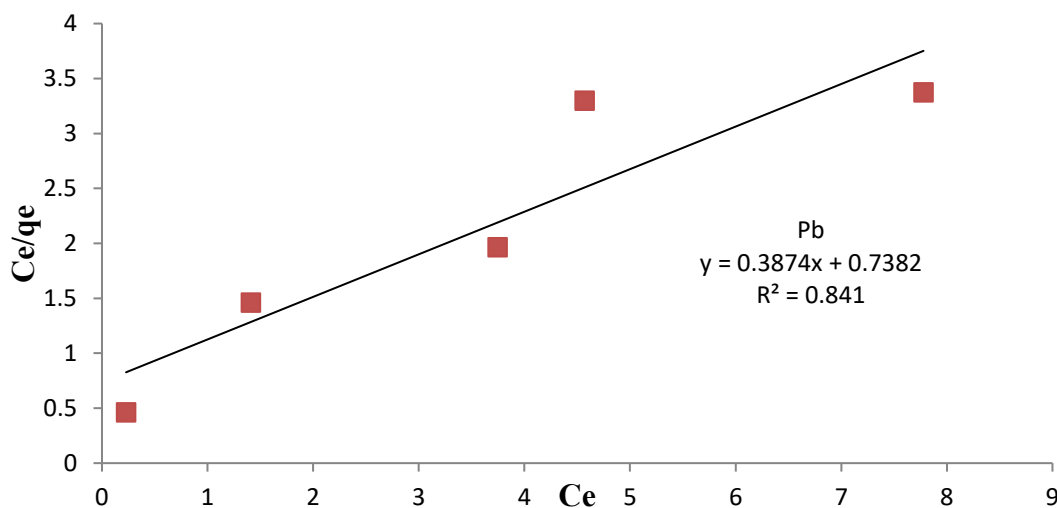


Figure 18: Langmuir Isotherm of Pb (II) ions Sorption onto Pretreated Chicken Feather Biomass

The image in Figure 19 illustrates the Temkin isotherm for Pb^{2+} ion sorption, with the isotherm parameters presented in Table 17. The result revealed $R^2 = 0.8257$, $A_T = 9.40367 \text{ L/g}$ and $b_T = 48.812 \text{ J/mol}$. This result suggests that Temkin model account for 82.57% variation in the experimental data. The values for Temkin binding constant (A_T) and heat of adsorption (b_T) suggest a favorable adsorption process with strong adsorbate-adsorbent affinity and repulsive interaction between the adsorbed molecules [72]. The heat of adsorption decreases with increasing surface coverage.

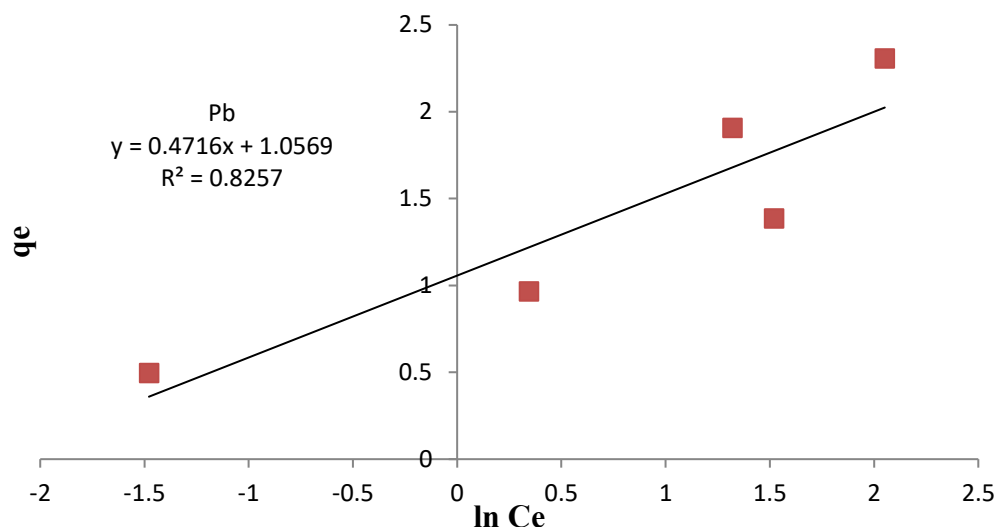


Figure 19: Temkin Isotherm of Pb ²⁺ ions Sorption onto Pretreated Chicken Feather Biomass

Table 17: Correlation parameters of Langmuir, Freundlich, Temkins, Flory-Huggins and Jovanovic Isotherms for selected Heavy Metal ions adsorption onto Pretreated Chicken Feather Biomass

Models	Descriptors	Values
Freundlich Isotherm	R ²	0.9376
	n ₁	2.353495
	K _F	0.8993 (mg/g)(L/mg) ^{0.5}
Flory-Huggins Isotherm	R ²	0.8505
	K _{FH}	656.15 L/mg ⁻¹
	n ₂	0.7752
	ΔG	-16 kJ/mol
Jovanovic Isotherm	R ²	0.7979
	K _J	0.1855 L/mg
	Q _{max}	1.5600 mg/g
Langmuir Isotherm	R ²	0.841
	K _L	0.5248 L/mg
	Q _o	0.087 mg/g
	R _L	2.58131
Temkin Isotherm	R ²	0.8257
	A _T	9.40367 L/g
	b _T	4812.812 J/mol

In this present study, Freundlich isotherm ($R^2 = 0.9376$) best describe the adsorption of Pb²⁺ ion onto PCFB, indicating that the adsorption occurred predominantly on a heterogeneous surface through multilayer adsorption with non-uniform distribution of active sites. The Freundlich constant ($n = 2.35$, $K_F = 0.8993$) further demonstrate favourable adsorption, moderate surface heterogeneity, and appreciable adsorbate-adsorbent affinity. The value

of $n > 1$ suggests that the adsorption process was energetically favourable over the concentration range investigated. These observations are consistent with heterogeneous chemical composition of keratin, which possess amino, carboxyl, hydroxyl and sulfur moieties capable of providing adsorption sites with different binding energies [73].

The Flory-Huggins isotherm ($R^2 = 0.8505$) further supports heterogeneous multilayer adsorption with high surface coverage, favourable adsorbate-adsorbent affinity. The negative Gibbs free energy ($\Delta G = -16 \text{ kJ/mol}$) confirms that Pb^{2+} adsorption is thermodynamically spontaneous. The magnitude of ΔG also suggest that physisorption also contributed substantially to the overall Pb^{2+} coordination process. However, when considered alongside DFT results, which exhibited direct Pb-O and Pb-N coordination, the adsorption mechanism is more appropriately described as mixed physisorption-chemisorption, whereby electrostatic attraction and van der Waals forces facilitates the initial uptake of Pb^{2+} , followed by localized coordination with oxygen and nitrogen containing functional groups [22]. The Jovanovic isotherm ($R^2 = 0.7979$) predicted a maximum adsorption capacity of 1.56 mg/g, indicating that though adsorption was favourable, the equilibrium adsorption capacity remained relatively low under the investigated conditions. This comparatively lower fit suggests that assumptions of an ideal homogeneous surface with negligible lateral interactions are less suitable for describing Pb^{2+} adsorption onto PCFB.

Similarly, the Langmuir isotherm ($R^2 = 0.841$) explained only 84.1% of the experimental variation, while the low monolayer adsorption capacity ($Q_0 = 0.087 \text{ mg/g}$) and $R_L > 1$ suggested monolayer adsorption was unfavourable within the studied experimented conditions. This deviation from Langmuir assumption further confirms the heterogeneous nature of the keratin surface [74].

Although the Temkin isotherm ($R^2 = 0.8257$) exhibited a poorer fit than the Freundlich isotherm model, it nevertheless indicated favourable Pb^{2+} adsorption with relatively strong affinity between Pb^{2+} ion and PCFB. The Temkin parameters further suggest that the heat of adsorption decreases progressively with increasing surface coverage due to interactions between the adsorbed species, indicating that the adsorption energies

declines as the adsorption site becomes occupied [75]. This observation complements the Freundlich isotherm, which provides the best fit to the experimental data, further confirming that adsorption occurred on a heterogenous biosorbent with active sites of varying adsorption energies.

Consistent with the present study, Zahara *et al.* [45] reported Freundlich dominated adsorption mechanism of keratin based biosorbent and other proteinaceous adsorbents, where surface heterogeneity arising from diverse functional groups facilitated multilayer adsorption of heavy metals rather than ideal monolayer adsorption.

The isotherm evaluation of the present study demonstrates that Pb^{2+} adsorption onto PCFB is predominantly heterogenous and multilayer in nature, with the Freundlich model proving the most satisfactory description of the equilibrium data. The combined evidence from the Freundlich, Flory-Huggins, Temkin, and DFT analysis indicates that adsorption proceeds through a mixed mechanism involving both physisorption and chemisorption.

3.3 Kinetic study

The graphical illustration in Figure 20, depicts the Pseudo first order (PFO) kinetic for Pb^{2+} ion sorption onto PCFB, while the kinetic parameters are presented in Table 18. The result revealed $R^2 = 0.8929$, $Q_e = 0.028893$ mg/g and $K_1 = 0.026945 \text{ min}^{-1}$. The result from the R^2 value showed that the experimental data moderately fitted PFO kinetic i.e PFO partially describe the adsorption kinetics. The values for Q_e and K_1 shows a low adsorption capacity (0.028893mg/g) at a very slow rate ($0.026945 \text{ min}^{-1}$), which suggest limited surface area or porosity on the PCFB and/or competition with other ions or insufficient active site for Pb^{2+} ion sorption (Nasser Mohamed *et al.*, 2024).

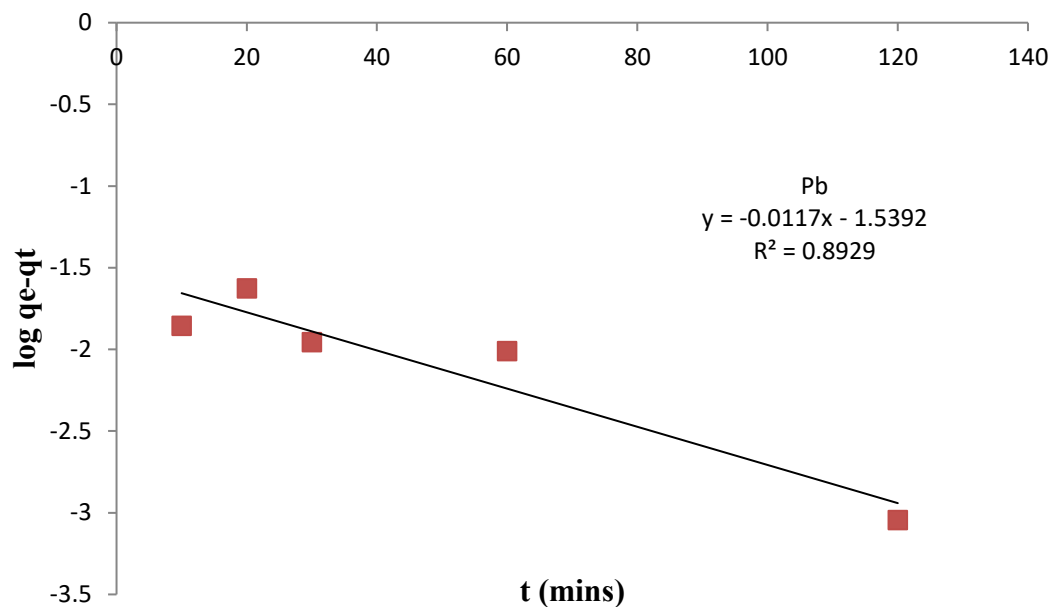


Figure 20: Pseudo First Order of Pb²⁺ ion Sorption onto Pretreated Chicken Feather Biomass

The Graphical illustration in Figure 21, represents the Pseudo second order (PSO) kinetics for Pb²⁺ ion sorption onto PCFB while the kinetic parameters are presented in Table 18. The result showed the $R^2 = 0.9999$, $Q_e = 0.493852$ mg/g and $K_2 = 2.944714$ g/mg.min. The R^2 value indicates an excellent correlation with the PSO kinetics model. The Q_e and K_2 values indicates a maximum adsorption capacity (0.493852 mg/g) at a rate constant (2.944714 min⁻¹). This implies the adsorption of Pb²⁺ ion by PCFB is fast efficient and chemisorption driven [76].

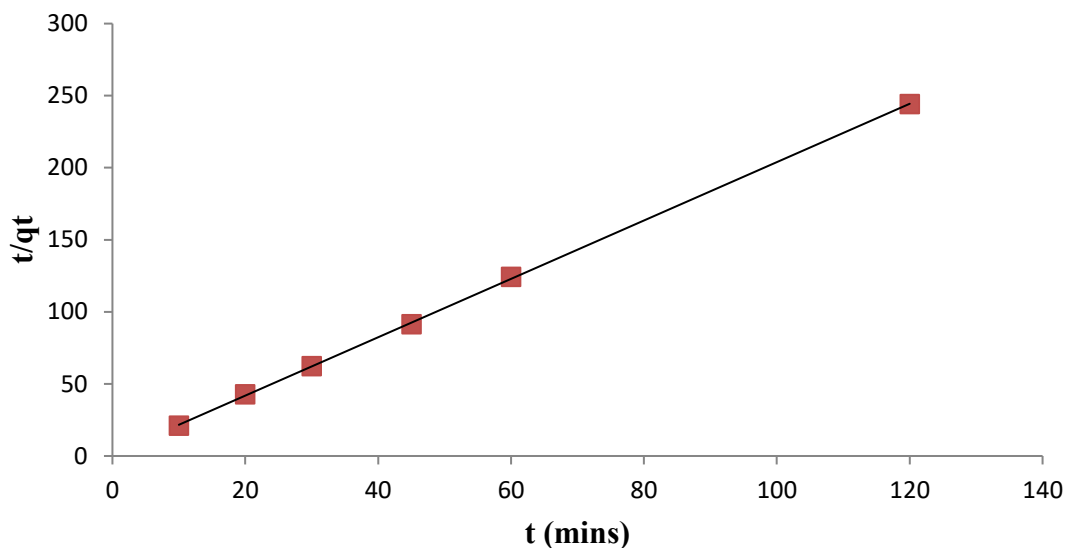


Figure 21: Pseudo Second Order of Pb^{2+} ion ions Sorption onto Pretreated Chicken Feather Biomass

The graphical illustration in Figure 22, illustrates the Elovich model for Pb^{2+} ion sorption onto PCFB while the kinetic parameters are presented in Table 18. The result showed $R^2 = 0.4852$, Elovich adsorption rate (α)= 4.93 $mg.g^{-1}.min^{-1}$ and desorption constant (β)= 0.014461 $g.mg^{-1}$. The R^2 value indicate a poor correlation with Elovich model. The result also shows a moderately high initial adsorption rate and very low desorption constant which suggest stronger Pb^{2+} ion binding to PCFB surface (Benjelloun *et al.*, 2021). Nevertheless, this descriptor may not be reliable because of the very poor data correlation ($R^2 = 0.4852$) with the Temkin model [19].

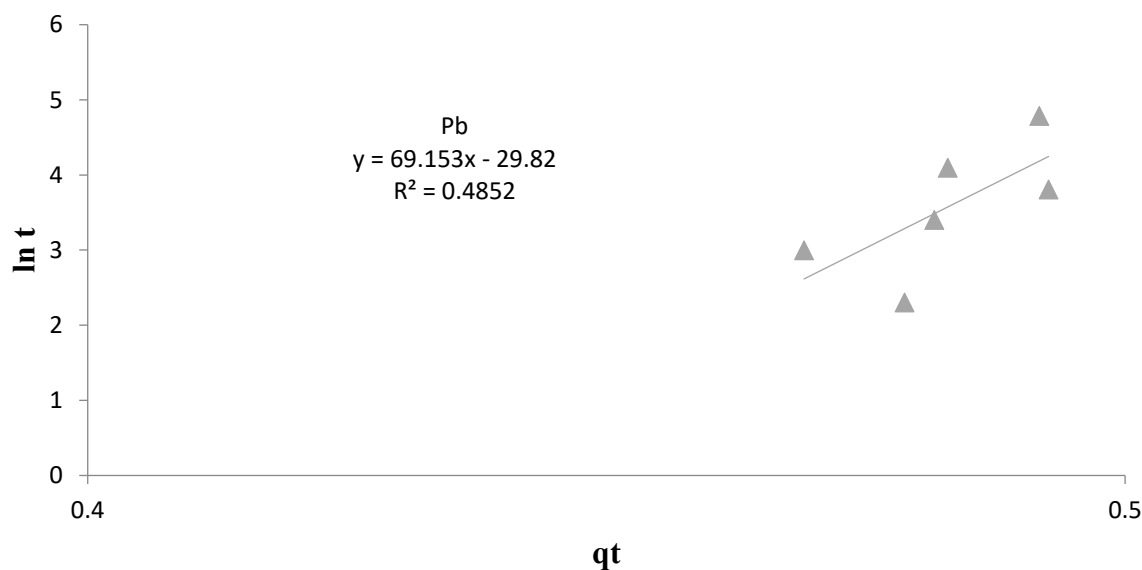


Figure 22: Elovich Model for Pb^{2+} ions Sorption onto PCFB

The graphical illustration in Figure 23, represents the Weber-Morris intraparticle diffusion model, the kinetic descriptors are presented in Table 18. The result showed that a correlation coefficient (R^2) = 0.4956, Intraparticle diffusion constant $K_{ID} = 0.0017 \text{ mg/g.min}^{0.5}$ and Intercept $C = 0.4684$. The R^2 value data shows a very poor correlation with intraparticle diffusion model. The Intraparticle diffusion constant and intercept suggest a very slow diffusion rate and a minor boundary layer effect i.e intraparticle diffusion is a predominant mechanism controlling the adsorption process [77]. Nonetheless, the poor data correlation of this model suggests the descriptor generated may not be reliable for mechanistic interpretation.

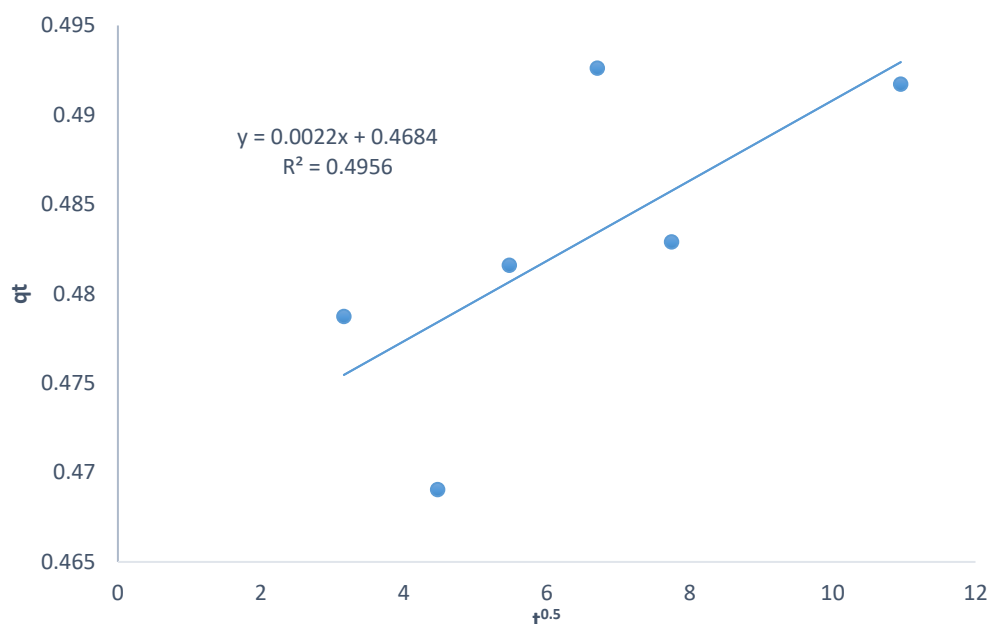


Figure 23: Intraparticle diffusion model for Pb^{2+} ion sorption onto Pretreated Chicken Feather biomass

Table 18: Rate Constants and Correlation Coefficient Values of Pseudo First Order, Pseudo Second Order, Elovich and Intraparticle diffusion Model for Pb ions Adsorption onto Pretreated Chicken Feather Biomass

Kinetic Model	Descriptors	Value
Pseudo First Order	R^2	0.8929
	Q_e	0.028893 mg/g
	K_1	0.026945 min^{-1}
Pseudo Second Order	R^2	0.9999
	Q_e	0.493852 mg/g
	K_2	2.944714 g/mg.min
Elovich Model	R^2	0.4852
	α	4.93 mg/g.min
	β	0.014461 mg/g

Intraparticle diffusion Model	R^2	0.4956
	K_{ID}	0.0017 mg/g.min ^{0.5}
	C	0.4684

The kinetic evaluation of the present study demonstrated that Pb^{2+} adsorption on PCFB was best described by the pseudo second order (PSO) model ($R^2 = 0.9999$), with a high rate constant ($k_2 = 2.94$ g/mg/min) and an equilibrium adsorption capacity (0.494 mg/g), indicating rapid adsorption governed predominantly by chemisorption through interaction between Pb^{2+} ions and the active functional groups of the keratin matrix. Conversely, the pseudo first order model exhibited a lower correlation ($R^2 = 0.893$) and substantially underestimated the adsorption capacity ($q_e = 0.029$ mg/g), demonstrating that physisorption was not the dominant mechanism. The poor fit obtained for Elovich ($R^2 = 0.485$) and Weber-Morris intraparticle diffusion ($R^2 = 0.496$) models further demonstrated that neither heterogeneous surface chemisorption nor intraparticle diffusion alone controlled the adsorption rate, suggesting that surface chemical interactions constituted the primary rate limiting step. These findings are consistent with previous studies on keratin rich and other bio derived adsorbent, which similarly identified PSO kinetics as the most appropriate model for describing the adsorption of metal ion, reflecting the dominant role of chemisorption mediated by amino, carboxyl, hydroxyl, and sulfur containing functional groups, while intraparticle diffusion contributed only as a secondary transport process ([20]; [78]. Similarly, Shubha *et al.* [79], reported that Pb^{2+} adsorption onto functionalized bio-based adsorbent followed PSO kinetics, indicating that chemical interaction dominated the adsorption process. Likewise, Banasaz and Ferraro [80] observed that keratin derived biosorbent exhibited excellent conformity with the PSO model owing to the strong affinity of sulfur and nitrogen containing functional groups for Pb^{2+} ions. In the same vein, demonstrated that poultry feather based biosorbent removed Pb^{2+} predominantly through chemisorption, with PSO providing the highest predictive accuracy, while intraparticle diffusion acted only as a secondary transport mechanism.

The kinetic findings demonstrated that chemisorption was the dominant rate limiting mechanism governing Pb^{2+} adsorption onto PCFB.

4.0 Conclusion

This study demonstrated that ethanol pretreated chicken feather biomass is an efficient sustainable and regenerable biosorbent for Pb^{2+} removal from aqueous media. Experimental characterization confirmed that ethanol pretreatment enhanced the accessibility of keratin derived hydroxyl, amino, and sulfur containing functional groups, which served as the principal binding sites for Pb^{2+} ions. Equilibrium studies established that adsorption occurred predominantly on a heterogenous surface following the Freundlich isotherm, whereas pseudo second order kinetic identified chemisorption as the dominant rate controlling mechanism. The satisfactory regeneration performance obtained with EDTA further demonstrates that operational stability and reusability of the biosorbent, supporting its practical applicability.

Beyond conventional adsorption studies, the integration of DFT calculations with machine learning provided molecular and process level insight into the adsorption mechanism. Quantum chemical analysis validated the experimentally proposed coordination interactions through favourable electronic stabilization and charge transfer between Pb^{2+} ions and keratin functional groups. Simultaneously, comparative modelling demonstrated that ANN substantially outperformed RSM and linear regression, confirming that Pb^{2+} adsorption is governed by complex nonlinear interactions that cannot be adequately represented by conventional statistical models.

Holistically, the findings establish an integrated experimental computational workflow for understanding and predicting heavy metal biosorption. This approach not only advances the mechanistic understanding of keratin based biosorbent but also provides a rational framework for the design, optimization and scale up of sustainable adsorption technologies for wastewater remediation.

References

- [1]. Abdelhaffez, G., Eltaher, M., Ibrahim, A., Environments, A. E.-, 2026. Sustainable Heavy Metal Removal from Model Aqueous Solutions and Industrial Wastewater Using Softwood Sawdust as Eco-Friendly and Cost-Effective. *Environments*, 2026• *mdpi.Com*. Retrieved August 3, 2026, from <https://www.mdpi.com/2076-3298/13/7/385>
- [2]. Abdulwasiiu Olawale, S., Bonilla-Petriciolet, A., Ileana Mendoza-Castillo, D., Charles Okafor, C., Sellaoui, L., & Badawi, M. (2022). Thermodynamics and mechanism of the adsorption of heavy metal ions on keratin biomasses for wastewater detoxification. *Journals.Sagepub.Com* <https://doi.org/10.1155/2022/7384924>
- [3]. Abookleesh, F. (2025). Approaches to the Development and Utilization of Rapeseed Protein-Based Bioplastics for Sustainable Food Packaging Applications. <https://ualberta.scholaris.ca/items/199dd1fe-a4ec-456b-9a28-d299cb4010f2>
- [4]. Adedipe, D., Bayode, A., Ore, O. (2025). Progress in the application of graphene-based nanomaterials for gas adsorption and mitigation of air pollution. *Advances*, 2025• *Pubs.Rsc.Org*. Retrieved August 3, 2026, from <https://pubs.rsc.org/ra/article-abstract/15/38/31032/907655>
- [5]. Akhtar, M., Ali, S., Zaman, W. (2024). Innovative adsorbents for pollutant removal: exploring the latest research and applications. *Molecules*, 2024• *Mdpi.Com*. Retrieved August 3, 2026, from <https://www.mdpi.com/1420-3049/29/18/4317>
- [6]. Akhtar, M., Anum, J., Rehman, A. (2026). Green-Synthesized Carbon Quantum Dots for Environmental Monitoring of Heavy Metals: A Critical Review of Mechanisms and Performance. *Journal of Engineering, Science and Technological Trends*, 2026• *Journals.Scopua.Com*. Retrieved August 3, 2026, from <https://journals.scopua.com/index.php/JESTT/article/view/111>
- [7]. Alafnan, S., Awotunde, A., Glatz, G., Adjei, S., Alrumaih, I., & Gowida, A. (2021). Langmuir adsorption isotherm in unconventional resources: Applicability and limitations. *Journal of Petroleum Science and Engineering*, 207. <https://doi.org/10.1016/J.PETROL.2021.109172>
- [8]. Alebady, M., Hamama, H., Mahmoud, S. (2024). Effect of various surface coating methods on surface roughness, micromorphological analysis and fluoride release from contemporary glass ionomer restorations. *BMC Oral Health*, 2024• *Springer*, 24(1). <https://doi.org/10.1186/s12903-024-04234-5>
- [9]. Aouaini, F., Dhaouadi, F., Sellaoui, L., Badawi, M., Piscitelli, A., Erto, A., & Lamine, A. Ben. (2022). Adaptation of advanced physical models to interpret the adsorption isotherms of lead and cadmium ions onto activated carbon in single-compound and binary systems. *Environmental Science and Pollution Research*, 29(41), 62507–62513. <https://doi.org/10.1007/S11356-022-20173-6>
- [10]. Ayad, A., Harrou, A., Himri, A. El, Benali, M., Dira, S Aparicio, Gutiérrez, A., Soldera, A., Gharibi, E. (2026). Polarity-Driven Selective Adsorption of Quercetin on Kaolinite: An Integrated DFT and Monte Carlo Study. *Materials*, 2026• *Mdpi.Com*. Retrieved August 3, 2026, from <https://www.mdpi.com/1996-1944/19/2/368>
- [11]. Banasaz, S., Ferraro, V. (2024). Keratin from animal by-products: structure, characterization, extraction and application—a review. *Polymers*, 2024• *Mdpi.Com*. Retrieved August 3, 2026, from <https://www.mdpi.com/2073-4360/16/14/1999>
- [12]. Batubara, A., Hasan, H., Moniem, M. A., Masoud, M. S., Mostafa, A., & Gamal, M. (2023). Usage of natural wastes from animal and plant origins as adsorbents for the removal of some toxic industrial dyes and heavy metals in aqueous media. *Journal of Water Process Engineering*, 2023• *Elsevier*. Retrieved August 3, 2026, from <https://www.sciencedirect.com/science/article/pii/S2214714423007249>

- [13]. Cao, H., Ma, X., Wei, Z., Tan, Y., Chen, S., Ye, T., Yuan, M., Xu, F. (2022). Behavior and mechanism of the adsorption of lead by an eco-friendly porous double-network hydrogel derived from keratin. *Chemosphere*, 2022• Elsevier. Retrieved August 3, 2026, from <https://www.sciencedirect.com/science/article/pii/S004565352103558X>
- [14]. Chakraborty, R., Asthana, A., Singh, A. K., Verma, R., Sankarasubramanian, S., Yadav, S., Carabineiro, S. A. C., & Susan, M. A. B. H. (2022). Chicken feathers derived materials for the removal of chromium from aqueous solutions: kinetics, isotherms, thermodynamics and regeneration studies. *Journal of Dispersion Science and Technology*, 43(3), 446–460. <https://doi.org/10.1080/01932691.2020.1842760>
- [15]. Chandra Mandal, G., Mandal, A., & Chakraborty, A. (2022). The toxic effect of lead on human health: A review. *Human Biology and Public Health*, 2022• Human-Biology-and-Public-Health ..., 3, 1–11. <https://doi.org/10.52905/hbph2022.3.45>
- [16]. Chauhan, M., Saini, V. K., & Suthar, S. (2020). Enhancement in selective adsorption and removal efficiency of natural clay by intercalation of Zr-pillars into its layered nanostructure. *Journal of Cleaner Production*, 258. <https://doi.org/10.1016/J.JCLEPRO.2020.120686>
- [17]. Chen, Z., Yang, H., Su, Z., Wang, X., Chen, X., & Pang, N. (2026). Ferric pyrophosphate-activated N and S self-doped keratin biochar derived from rabbit hair enables efficient Cr (VI) removal: synergistic effect of Fe (II) with N and S. *Biochemical Engineering Journal*, 2026• Elsevier. Retrieved August 3, 2026, from <https://www.sciencedirect.com/science/article/pii/S1369703X26000902>
- [18]. Chu, K. H., Hashim, M. A., Bashiri, H., Debord, J., Harel, M., & Bollinger, J. C. (2023). The Flory-Huggins Isotherm and Water Contaminant Adsorption: Debunking Some Modeling Fallacies. *Industrial and Engineering Chemistry Research*, 62(2), 1121–1131. <https://doi.org/10.1021/ACS.IECR.2C03799>
- [19]. Costa, A., Filho, S., de Aguiar Filho, S., Santos, T. J., & Pereira, D. H. (2021). Theoretical insights about the possibility of removing Pb²⁺ and Hg²⁺ metal ions using adsorptive processes and matrices of carboxymethyl diethylaminoethyl. *Journal of Molecular Liquids*, 2021• Elsevier. Retrieved August 3, 2026, from <https://www.sciencedirect.com/science/article/pii/S0167732221004554>
- [20]. Debord, J., Harel, M., Bollinger, J. C., & Chu, K. H. (2022). The Elovich isotherm equation: Back to the roots and new developments. *Chemical Engineering Science*, 262. <https://doi.org/10.1016/J.CES.2022.118012>
- [21]. Debord, J., Harel, M., Bollinger, J. C., Debord, J., & Chu, K., H. (2022). The Elovich isotherm equation: Back to the roots and new developments. *Chemical Engineering Science*, 2022• Elsevier. Retrieved August 3, 2026, from <https://www.sciencedirect.com/science/article/pii/S0009250922005966>
- [22]. Dharmarathna, S., & Priyantha N. (2024). Investigation of boundary layer effect of intra-particle diffusion on methylene blue adsorption on activated carbon. *Energy Nexus*, 2024• Elsevier. Retrieved August 3, 2026, from <https://www.sciencedirect.com/science/article/pii/S2772427124000251>
- [23]. Elamraoui, S., Asdiou, N., Achaby, E. I., Kounbach, S., Benhida, R., Achak M., & Kaim B. R. (2025). Unveiling the adsorptive potential of natural biopolymers for olive mill wastewater treatment: a synergistic approach using RSM-BBD, mixture design, kinetics. *International Journal of Molecular Sciences*, 2025• Mdpi.Com. Retrieved August 3, 2026, from <https://www.mdpi.com/1422-0067/26/16/7738>
- [24]. Elbager, M. A., Asmaly, H. A., Al-Suwaiyan, M., Ibrahim, A. I., & Dafallah, H. (2025). High Performance Batch Adsorption of Methylene Blue Using Desert Date Seed Shell Activated Carbon:

- Characterization and Response Surface Methodology Optimization. *Water, Air, and Soil Pollution*, 236(4). <https://doi.org/10.1007/S11270-025-07880-9>
- [25]. Elebo, A. (2025a). Machine learning and experimental design interrogation for modelling corrosion inhibition of mild steel (ASISI 1018) by expired clindamycin: weight loss, artificial neural network, electrochemical, computational and surface topology investigations. *Results in Chemistry*, 17. <https://doi.org/10.1016/j.rechem.2025.102571>
- [26]. Elebo, A. (2025b). Machine learning and experimental design interrogation for modelling corrosion inhibition of mild steel (ASISI 1018) by expired clindamycin: weight loss, artificial neural network, electrochemical, computational and surface topology investigations. *Results in Chemistry*, 17. <https://doi.org/10.1016/J.RECHEM.2025.102571>
- [27]. Fernández, J., Fernández, J. A. H., Prieto Palomo J. A., Toloza, T. (2025). Theoretical/experimental study of the heavy metals in poly (vinylalcohol)/carboxymethyl starch-g-poly (vinyl imidazole)-based magnetic hydrogel. *Journal of Composites Science*, 2025• *Mdpi.Com*. Retrieved August 3, 2026, from <https://www.mdpi.com/2504-477X/9/4/193>
- [28]. Ganguly, P., Manoj, A., Dhanushkodi, S., Ganguly, P., Manoj, A., Dhanushkodi, S. R., Gurusamy, G., & Kundu S. (2025). Electrode selection framework for oxygen evolution reaction catalysts involving density functional theory and finite element method. *RSC Advances*, 2025• *Pubs.Rsc.Org*. Retrieved August 3, 2026, from <https://pubs.rsc.org/ra/article-abstract/15/36/29389/907599>
- [29]. Hafeez, S., Ishaq, A., Intisar, A., Mahmood, T., Din M. I., Ahmed, E., Tariq, M. R., & Abid M. A. (2024). Predictive modeling for the adsorptive and photocatalytic removal of phenolic contaminants from water using artificial neural networks. *Heliyon*, 2024• *Cell.Com*. Retrieved August 3, 2026, from [https://www.cell.com/heliyon/fulltext/S2405-8440\(24\)13982-5](https://www.cell.com/heliyon/fulltext/S2405-8440(24)13982-5)
- [30]. Halli, P., Agarwal, V., Partinen, J., & Lundström, M. (2020). Recovery of Pb and Zn from a citrate leach liquor of a roasted EAF dust using precipitation and solvent extraction. *Separation and Purification Technology*, 236. <https://doi.org/10.1016/J.SEPUR.2019.116264>
- [31]. Haridharan, N., Sundar, D., Kurrupasamy, L., Anandan, S., Liu, C. H., & Wu, J. J. (2022). Oil spills adsorption and cleanup by polymeric materials: A review. *Polymers for Advanced Technologies*, 33(5), 1353–1384. <https://doi.org/10.1002/PAT.5636>
- [32]. Heidarinejad, Z., Dehghani, M. H., Heidari, M., Javedan, G., Ali, I., & Sillanpää, M. (2020). Methods for preparation and activation of activated carbon: a review. *Environmental Chemistry Letters*, 18(2), 393–415. <https://doi.org/10.1007/S10311-019-00955-0>
- [33]. Hennequin, L. M., Tan, S. yin, Jensen, E., Fennell, P., & Hallett, J. P. (2022). Combining phytoremediation and biorefinery: Metal extraction from lead contaminated Miscanthus during pretreatment using the ionoSolv process. *Industrial Crops and Products*, 176. <https://doi.org/10.1016/J.INDCROP.2021.114259>
- [34]. Huber, F., Berwanger, J., Polesya, S., Mankovsky, S., Ebert, H., & Giessibl, F. J. (2019). Chemical bond formation showing a transition from physisorption to chemisorption. *Science*, 366(6462), 235–238. <https://doi.org/10.1126/SCIENCE.AAY3444>
- [35]. Illés, I., & Kékesi, T. (2022). Efficient deposition of indium by cementation from chloride solutions. *Hydrometallurgy*, 2022• *Elsevier*. Retrieved August 3, 2026, from <https://www.sciencedirect.com/science/article/pii/S0304386X21002553>
- [36]. Isgoren, M., Fersiz, S., & Gengec, E. (2025). A novel, simply prepared biosorbent for the removal of cationic dye: characterization, isotherm, kinetic and thermodynamic study. *Journal of Dispersion Science and Technology*, 2025• *Taylor & Francis*. Retrieved August 3, 2026, from <https://www.tandfonline.com/doi/abs/10.1080/01932691.2025.2558143>

- [37]. Kavand, M., Eslami, P., & Razeh, L. (2020). The adsorption of cadmium and lead ions from the synthesis wastewater with the activated carbon: Optimization of the single and binary systems. *Journal of Water Process Engineering*, 2020• Elsevier. Retrieved August 3, 2026, from <https://www.sciencedirect.com/science/article/pii/S2214714420300301>
- [38]. Kothakota, A., Pandiselvam, R., Siliveru, K., Pandey J. P., Sagarika N., Srinivas C. H. S., & Kumar A. (2021). Modeling and optimization of process parameters for nutritional enhancement in enzymatic milled rice by multiple linear regression (MLR) and artificial neural. *Foods*, 2021• Mdpi.Com. Retrieved August 3, 2026, from <https://www.mdpi.com/2304-8158/10/12/2975>
- [39]. Kyriazos, T., Poga, M., Kyriazos, T., & Poga, M. (2023). Dealing with multicollinearity in factor analysis: the problem, detections, and solutions. *Open Journal of Statistics*, 2023• Scirp.Net, 13, 404–424. <https://doi.org/10.4236/ojs.2023.133020>
- [40]. Lanphear, B., Navas-Acien, A., & Bellinger, D. C. (2024). Lead Poisoning. *New England Journal of Medicine*, 391(17), 1621–1631. <https://doi.org/10.1056/NEJMRA2402527>
- [41]. Lazarus, B., Chadha, C., Velasco-Hogan, A., Barbosa J. D. V., Jasiuk I., & Meyers M., A. (2021). Engineering with keratin: A functional material and a source of bioinspiration. *Iscience*, 2021• Cell.Com. Retrieved August 3, 2026, from [https://www.cell.com/iscience/fulltext/S2589-0042\(21\)00766-5](https://www.cell.com/iscience/fulltext/S2589-0042(21)00766-5)
- [42]. Longo, E. (2021). Heterostructures Based on the Large-Area Sb₂te₃ Topological Insulator For Spin-Charge Conversion. <https://boa.unimib.it/handle/10281/311358>
- [43]. Mabuza, M., Premllall, K., & Daramola M. O. (2022). Modelling and thermodynamic properties of pure CO₂ and flue gas sorption data on South African coals using Langmuir, Freundlich, Temkin, and extended Langmuir. *International Journal of Coal Science & Technology*, 2022• Springer, 9(3), 45. <https://doi.org/10.1007/s40789-022-00515-y>
- [44]. Mahmoud, M. E., El-Said, F., Ibrahim, A. A., & Elnashar, A. S. (2024). Effective removal of hexavalent chromium from water by sustainable nano-scaled waste avocado seeds: adsorption isotherm, thermodynamics, kinetics, and error. *Biomass Conversion and Biorefinery*, 2024• Springer, 14(13), 14725–14743. <https://doi.org/10.1007/s13399-022-03619-2>
- [45]. Mansouri, M., Shayanmehr, M., & Ghaemi, A. (2025). Exploring the adsorption desulfurization efficiency using RSM and ANN methodologies. *Scientific Reports*, 2025• Nature.Com. <https://doi.org/10.1038/s41598-025-05688-5>
- [46]. Maung, S., Ayub, A., Xu, W., Wang, J., Li, & Yue, Z. (2026). A green and scalable strategy for heavy metal remediation in acid mine drainage: Experimental and quantum chemical insights into NTA-modified biochar. *Separation and Purification Technology*, 2026• Elsevier. Retrieved August 3, 2026, from <https://www.sciencedirect.com/science/article/pii/S1383586626013365>
- [47]. Messaoudi, N. El, Miyah, Y., Georgin, J., Franco, DSP., Yilmazoğlu, M., Kouka, T., & Messali M (2025). Sustainable casein-derived materials for water purification: opportunities, challenges, progress, and perspectives. *Reactive and Functional Polymers*, 2025• Elsevier. Retrieved August 3, 2026, from <https://www.sciencedirect.com/science/article/pii/S138151482500464X>
- [48]. Berggren, M. (2024). Coefficients of determination measured on the same scale as the outcome: Alternatives to R² that use standard deviations instead of explained variance. *Psychological Methods*, 2024• Psycnet.Apa.Org. Retrieved August 3, 2026, from <https://psycnet.apa.org/record/2025-03746-001>
- [49]. Sen T. K. (2023). Agricultural solid wastes based adsorbent materials in the remediation of heavy metal ions from water and wastewater by adsorption: a review. *Molecules*, 2023• Mdpi.Com. Retrieved August 3, 2026, from <https://www.mdpi.com/1420-3049/28/14/5575>

- [50]. Mondal, N. K., Palui, S., Sen, K., Debnath, P., & Mondal, A. (2026). Sustainable Cr(VI) Aqueous Detoxification using Keratin-Based Adsorbents: Integration of Taguchi Design and Computational Modelling. *Water, Air, and Soil Pollution*, 237(4). <https://doi.org/10.1007/S11270-025-08920-0>
- [51]. Motaleb, K. Z. M. A., Islam, S., Faheem, M. S., Khan, A., Hasan, M. B., Jamshaid, H., Janutėnienė, J., & Tadžijevs, A. (2025). Valorisation of bio-waste for the development of sustainable technical textiles. *Textile Progress*, 57(3), 117–217. <https://doi.org/10.1080/00405167.2025.2569218>
- [52]. Murty, V. R., Nayak, M., & Mulky, L. (2026). Heavy metal remediation using biomass derived adsorbents: Pre-treatment strategies for enhanced performance. *Separation Science and Technology (Philadelphia)*, 61(8), 1214–1237. <https://doi.org/10.1080/01496395.2025.2607092>
- [53]. Musa Abubakar, A., Arowo, M. N., Selele, M. I., Houndedjihou, D., & Nayem, Z. (2024). Jovanovic and Sips Isotherm Parameters of Mango Seed Shell Cadmium Ion Sorption from Aqueous Solution. *Ojs.Wiserpub.Com* AM Abubakar, MNT Arowo, MI Selele, D Houndedjihou, Z Nayem Sustainable Chemical Engineering, 2025•ojs.Wiserpub.Com, 35–55. <https://doi.org/10.37256/sce.6120255830>
- [54]. Naranjo, V., Hendricks, M., & Jones, K. S. (2020). Lead toxicity in children: an unremitting public health problem. *Pediatric Neurology*, 2020• Elsevier, 113, 51–55. <https://doi.org/10.1016/j.pediatrneurol.2020.08.005>
- [55]. Nasser, S. M., Abbas, M., & Trari, M. (2024). Understanding the rate-limiting step adsorption kinetics onto biomaterials for mechanism adsorption control. *Progress in Reaction Kinetics and Mechanism*, 2024• Journals.Sagepub.Com, 49, 1–26. <https://doi.org/10.1177/14686783241226858>
- [56]. Nighojkar, A., Zimmermann, K., Ateia, M., Barbeau, B., Mohseni, M., Krishnamurthy, S., & Dixit S. (2023). Application of neural network in metal adsorption using biomaterials (BMs): a review. *Environmental Science: Advances*, 2023• Pubs.Rsc.Org. Retrieved August 3, 2026, from <https://pubs.rsc.org/va/article-abstract/2/1/11/794429>
- [57]. Qi, L., & Guan J (2026). Charge redistribution of atomic catalysts in Electrocatalysis., *Advanced Functional Materials*, 2026• Wiley Online Library. Retrieved August 3, 2026, from <https://advanced.onlinelibrary.wiley.com/doi/abs/10.1002/adfm.202527230>
- [58]. Rajahmundry, G., Garlapati, C., Kumar, P., Alwi, R. S., & Vo D. N. (2021). Statistical analysis of adsorption isotherm models and its appropriate selection. *Chemosphere*, 2021• Elsevier. Retrieved August 3, 2026, from <https://www.sciencedirect.com/science/article/pii/S0045653521006457>
- [59]. Raji, Z., Karim, A., Karam, A., & Khalloufi S. (2023). Adsorption of heavy metals: mechanisms, kinetics, and applications of various adsorbents in wastewater remediation—a review. *Waste*, 2023•mdpi.Com. Retrieved August 3, 2026, from <https://www.mdpi.com/2813-0391/1/3/46>
- [60]. Saha, S., Zubair, M., Khosa, M. A., Song, S., & Ullah, A. (2019). Keratin and Chitosan Biosorbents for Wastewater Treatment: A Review. *Journal of Polymers and the Environment*, 27(7), 1389–1403. <https://doi.org/10.1007/S10924-019-01439-6>
- [61]. Sekeroglu, B., & Dimililer, K. (2020). Review and analysis of hidden neuron number effect of shallow backpropagation neural networks. *Neural Network World*, 2020• Academia.Edu. Retrieved August 3, 2026, from <https://www.academia.edu/download/68435469/NNW.2020.30.008.pdf>
- [62]. Shams, S., Jahani, A., Kalantary, S., Moeinaddini, M., & Khorasani, N. (2021). The evaluation on artificial neural networks (ANN) and multiple linear regressions (MLR) models for predicting SO₂ concentration. *Urban Climate*, 2021• Elsevier. Retrieved August 3, 2026, from <https://www.sciencedirect.com/science/article/pii/S2212095521000675>

- [63]. Shanmugasundar, G., Vanitha, M., Čep, R., Kumar, V., Kalita, K., & Ramachandran M. (2021). A comparative study of linear, random forest and adaboost regressions for modeling non-traditional machining. *Processes*, 2021• *Mdpi.Com*. Retrieved August 3, 2026, from <https://www.mdpi.com/2227-9717/9/11/2015>
- [64]. Shubha, A., Sharmita, G., Sustainable, R., & Manaswi R. (2024). Recent advances in preparation and biomedical applications of keratin-based biomaterials. *Biotechnology for Sustainable Materials*, 2024• *Springer*, 1(1). <https://doi.org/10.1186/s44316-024-00016-9>
- [65]. Siadati, S. A., Ebrahimzadeh, M. A., Yazdian-Robati, R., & Babanezhad, E. (2024). A theoretical approach on the possibility of using α -phagraphene, g- X_3N_4 nanosheets, and C19X fullerenes for adsorption and drug delivery of a proteasome inhibitor drug. *Diamond and Related Materials*, 147. <https://doi.org/10.1016/J.DIAMOND.2024.111344>
- [66]. Singh, M., Rayaz, M., & Rao, A. (2024). Application of novel phytosorbent to sequester chromium(VI) and lead(II) from aqueous phase: Optimization, equilibrium and kinetics. *Environmental Progress and Sustainable Energy*, 43(1). <https://doi.org/10.1002/EP.14266>
- [67]. Spaolonzi, M. P., de Farias, M. B., da Silva, M. G. C., & Vieira, M. G. A. (2022). Adsorption of cefazolin on organoclay: experimental design, characterization, and a complete batch study. *Environmental Science and Pollution Research*, 29(46), 70209–70227. <https://doi.org/10.1007/S11356-022-20830-W>
- [68]. Tariq, R., Abatal, M., Vargas, J., & Vázquez-Sánchez A. Y. (2024). Deep learning artificial neural network framework to optimize the adsorption capacity of 3-nitrophenol using carbonaceous material obtained from biomass waste. *Scientific Reports*, 2024• *Nature.Com*, 14, 20250. <https://doi.org/10.1038/s41598-024-70989-0>
- [69]. Igberase, E. (2024). The adsorption of Pb^{2+} and Ni^{2+} ions utilizing modified chitosan beads: A response surface methodology and neural network modelling study. *Desalination and Water Treatment*, 2024• *Elsevier*. Retrieved August 3, 2026, from <https://www.sciencedirect.com/science/article/pii/S1944398624003266>
- [70]. Upadhyay, K., Viramgami, A., Balachandar, R., Pagdhune, A., Sen, S., & Sarkar, K. (2022). A comparative health assessment of occupationally lead exposed individuals with blood lead levels range across upper acceptable limit. *Indian Journal of Community Medicine*, 47(3), 343–346. https://doi.org/10.4103/IJCM.IJCM_756_21
- [71]. Vashista, S., Arora, A., & Sah, M. K. (2024). Catalysing Sustainability with Keratin-Derived Adsorbent Materials for Enhanced Heavy Metal Remediation. *Korean Journal of Chemical Engineering*, 41(7), 1901–1921. <https://doi.org/10.1007/S11814-024-00168-4>
- [72]. Vellingiri, S., Kumar Tata, R., Manne, S., Natarajan, A., Ismail, S. O., Murugan, A., Paulraj, P., & Kumar Jeyaramalingam, S. (2026). Predicting wire electrical discharge machined surface roughness of C355/silicon nitride/graphene hybrid nanocomposites using simulation, statistical and machine. *Scientific Reports*, 2026• *Nature.Com*. <https://doi.org/10.1038/s41598-026-41376-8>
- [73]. Villena-Martínez, E., Alvizuri-Tintaya, P., Lora-García, J., & Torregrosa-López, J. I. (2022). Reverse osmosis modeling study of lead and arsenic removal from drinking water in tarija and La paz, Bolivia. *Processes*, 2022•*mdpi.Com*. Retrieved August 3, 2026, from <https://www.mdpi.com/2227-9717/10/9/1889>
- [74]. Vitek, R., & Masini, J. C. (2023). Nonlinear regression for treating adsorption isotherm data to characterize new sorbents: Advantages over linearization demonstrated with simulated and experimental. *Heliyon*, 2023• *Cell.Com*. Retrieved August 3, 2026, from [https://www.cell.com/heliyon/fulltext/S2405-8440\(23\)02335-6](https://www.cell.com/heliyon/fulltext/S2405-8440(23)02335-6)

- [75]. Younas, F., Mustafa, A., Farooqi, Z. U. R., Wang, X., Younas, S., Mohy-Ud-din, W., Hameed, M. A., Abrar, M. M., Maitlo, A. A., Noreen, S., & Hussain, M. M. (2021). Current and emerging adsorbent technologies for wastewater treatment: Trends, limitations, and environmental implications. *Water (Switzerland)*, 13(2). <https://doi.org/10.3390/W13020215>
- [76]. Zahara, I., Irfan, M., Zubair, M., Siddique, T., & Ullah, A. (2023). Removal of divalent cations and oxyanions by keratin-derived sorbents: Influence of process parameters and mechanistic studies. *Science of the Total Environment*, 2023• Elsevier. Retrieved August 3, 2026, from <https://www.sciencedirect.com/science/article/pii/S0048969723029091>
- [77]. Zhang, J., Noor, Z. Z., Baharuddin, N. H., Setu, S. A., Mohd Hamzah, M. A. A., & Zakaria, Z. A. (2024). Removal of Heavy Metals by Pseudomonas sp. – Model Fitting and Interpretation. *Current Microbiology*, 81(10). <https://doi.org/10.1007/S00284-024-03832-4>
- [78]. Zhu, P., Chu, Y., Li, F., & Chen, L. (2025). Biodegradable and Reusable Sponge Material Prepared from Pea Protein for the Effective Removal of Heavy Metals. *ACS Applied Materials and Interfaces*, 17(18), 26534–26550. <https://doi.org/10.1021/ACSAMI.4C22940>
- [79]. Zubair, M., Roopesh, M., & Ullah, A. (2025). Green Nanoengineered Keratin Derived Bio-Adsorbent for Heavy Metals Removal from Aqueous Media. *Advanced Sustainable Systems*, 2025• Wiley Online Library. Retrieved August 3, 2026, from <https://advanced.onlinelibrary.wiley.com/doi/abs/10.1002/adsu.202400491>

STATEMENT AND DECLARATIONS

Funding: The author declare that no funding, grants or other support was received during the preparation of this manuscript

Author's Contribution

All the authors contributed to the study. Material preparation, data collection and analysis were performed by Jibunor Udoka Victor and Anumonye Francis. The first draft of the manuscript was written by Jibunor Udoka Victor and proofread by Dr. Abuchi Elebo, and Dr. Ogunyemi Babatunde T., all authors commented on previous versions of the manuscript. All authors read and approved the final manuscript.

Ethical Approval: Since the chicken feather biomass was collected as waste from a commercial chicken butchery in Swali Market, Yenagoa, Bayelsa State, Nigeria, ethical approval was not necessary for this work.

Consent to Participate: Since the chicken feather biomass was gathered as poultry waste from a local chicken butchery at Swali Market in Yenagoa, Bayelsa State, Nigeria, ethical approval was not necessary for this work. For this study, no live animals were utilized, handled, or sacrificed. As a result, no human subjects nor animal experimentation were used in the study, and informed consent was not relevant.

Consent to Publish: This is not applicable for this specific section

Competing Interest: The authors declare that they have no financial or non-financial competing interests that could have influenced the work reported in this manuscript

Data Availability Statement: All data generated or analysed during this study are included in this published article.

Clinical Trial Number: Not applicable.

Permissions or Credit: All images and figures are either original work or reproduced/adapted with appropriate permission and credit to the original source.