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# A COMPUTER-BASED METHODOLOGY FOR MODELING THE REMOVAL OF CADMIUM ION FROM INDUSTRIAL WASTEWATER WITH RICE HUSK ASH

**Yasemin ŞİRİN ERYOLDAŞ[1], Faruk Geyik[2], Tuğba TAŞKIN TOK[3]**

[1] Gaziantep University, Faculty of Engineering, Department of Industrial Engineering, Gaziantep, Turkey.
[2] Tarsus University, Faculty of Engineering, Department of Industrial Engineering, Mersin, Turkey.
[3] Gaziantep University, Faculty of Arts and Sciences, Department of Chemistry, Gaziantep, Turkey.
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## ABSTRACT

Rice husk is a significant waste issue due to its high manufacturing rate. The removal of heavy metals from industrial wastewater using the adsorption method is one of the significant usage areas of rice husks. In addition to being more cost-effective than other methods for removing heavy metals from industrial wastewater, using rice husks for this purpose would solve the storage problem of the rice husks. In this study, Gaussian® 0.9 software is utilized to describe and simulate the binding process of the $Cd^{2+}$ ion to the rice husk adsorbent and to perform geometric optimizations to identify the most stable structure. These optimized structures' adsorption energies were computed utilizing the Material Studio® 6.1 software. According to the findings, rice husks can be utilized as an adsorbent in place of more expensive substances. It has been demonstrated that, when compared to experimental procedures, the suggested strategy is both quicker and less expensive.

**Keywords:** rice husk; $Cd^{2+}$ ion; geometry optimization; adsorption simulation.

# PİRİNÇ KABUK KÜLÜ İLE ENDÜSTRİYEL ATIK SUDAN KADMİYUM İYONUNUN GİDERİLMESİNİN MODELLENMESİNE YÖNELİK BİLGİSAYAR TABANLI BİR YÖNTEM

## ÖZET

Pirinç kabuğu, yüksek üretim hızı nedeniyle önemli bir atık sorunudur. Adsorpsiyon yöntemi kullanılarak endüstriyel atık sudan tekstil boyalarının ve ağır metallerin uzaklaştırılması, pirinç kabuğunun önemli bir uygulama alanıdır. Endüstriyel atık sulardan ağır metallerin uzaklaştırılması için diğer yöntemlere göre daha uygun maliyetli olmasının yanı sıra, bu amaçla pirinç kabuğunun kullanılması, pirinç kabuğunun depolanma sorununun çözümü için de etkili bir çözüm yöntemi olmuştur. Bu çalışmada Gaussian ® 0.9 yazılımı $Cd^{2+}$ iyonunun pirinç kabuğundan hazırlanan adsorban yapıya bağlanma süreci belirlemek ve simüle etmek ve en kararlı yapıyı belirlemek üzere geometri optimizasyonu yapmak üzere kullanıldı**.** Bu optimize edilmiş yapıların adsorpsiyon enerjileri, Material Studio® 6.1 yazılımı kullanılarak hesaplanmıştır. Elde edilen bulgulara göre pirinç kabuğu, daha pahalı maddeler yerine adsorban olarak kullanılabilir. Deneysel prosedürlerle karşılaştırıldığında, önerilen metodolojinin hem daha hızlı hem de daha ucuz olduğu kanıtlanmıştır.

**Anahtar Kelimeler:** pirinç kabuğu; $Cd^{2+}$ iyonu; geometri optimizasyonu; adsorpsiyon simulasyonu

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[1] e-posta: yasemineryoldas@gmail.com ORCID ID: 0000-0002-7212-9108 (Sorumlu Yazar)
[2] e-posta: farukgeyik@tarsus.edu.tr. ORCID ID: 0000-0002-2355-0529
[3] e-posta: ttaskin@gantep.edu.tr ORCID ID: 0000-0002-0064-8400

## 1. Introduction

According to the Agricultural Products Markets Reports for 2021 [1], rice production has increased globally overall, with Asian nations dominating the world in rice consumption. Additionally, according to the same report, the world's supply of rice climbed by 2.4% to 735.4 million tons in 2021/22. China produces 212 million tons of paddy and imports 4.5 million tons annually, while India produces 184 million tons. The data on rice exports and imports by countries, as well as data on paddy production, are shown in Figure 1.

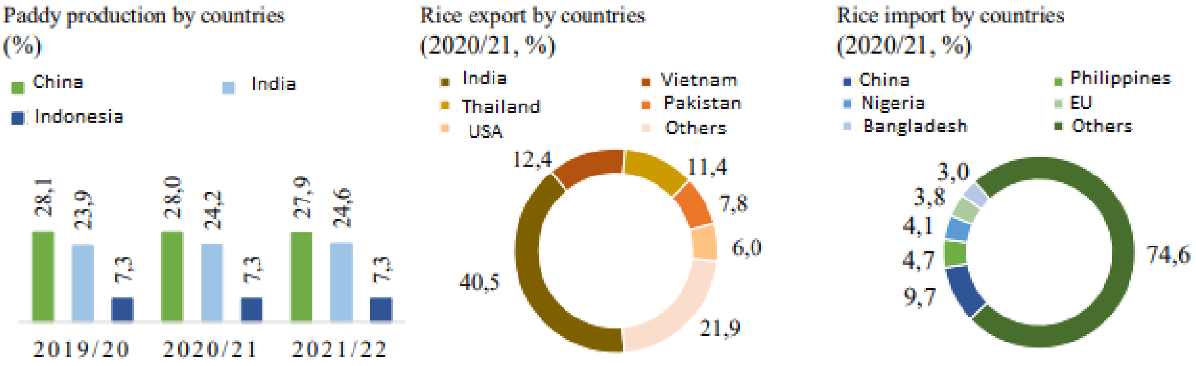

**Figure 1.** Paddy production, rice export, and import data by countries [1].

One of the nations with the highest increases in paddy production during the past ten years is Turkey. The growth in cultivated fields and the improvement in yield per unit area are the causes of this increase. On 125 000 acres of land, 980 000 tons of paddy were produced in 2020–21 [1]. Additionally, 14 158 tons of semi- and fully-milled rice were exported, along with 98 716 tons of paddy, 227 690 tons of semi-milled rice, and 8 000 tons of brown rice [1]. We refer to the 2021 reports of the Agricultural Products Markets [1] for a full report of the data about rice husk (such as consumption, importation, and productivity) in the world and Turkey.

Rice husks ash (RHA) is an agricultural residual or byproduct produced during the milling of rice that is frequently disposed of or underused, having a negative impact on the environment and increasing the cost of producing rice [2]. Due to the increased production of rice for human use, RHA production has also grown [3]. Since its production began, rice husk has mostly been utilized as a fuel in rice mills to create steam for the parboiling process, and around 25% of this rice husk's weight is transformed into RHA [4]. The amount of RHA produced by cogeneration plants is anticipated to rise dramatically due to the world's expanding population and rising demand for rice, a key staple grain. Because there won't be as many landfill places accessible in the future, it will be challenging to dispose of and manage the RHA effectively. Scientists have carried out several studies, and as a consequence of those investigations, it has been discovered that rice husk may be utilized in a variety of industries, from solar panel production to construction. The removal of heavy metal contamination from industrial wastewater using rice husks will be explored in this study.

In this study, the ability of the rice husk to behave as an adsorptive substance was investigated using geometry optimization and absorption simulation approaches. This was accomplished by looking into the mechanism of $Cd^{2+}$ adsorption from industrial wastewater by rice husk. This study's findings supported the idea that using rice husks for adsorption can help with two major issues: first, the large production rates of rice husks, which cause storage problems; and second, it is a less expensive way to remove heavy metals from industrial wastewater. All the studies in the literature focused on experimentally evaluating the adsorption efficiency of the RHA-based absorbents for removal of the heavy metals and the adsorption kinetics of this process experimentally. In terms of the application of geometry optimization and absorption simulation approaches, our study is the first in the literature to offer a computer-based method to identify the binding mechanism of rice husks.

This study is regulated as follows: first, we provided a brief overview of the background of the study and a literature survey about the heavy metal adsorption from industrial wastewater by rice husks. Subsequently, we described the methodology used to handle geometry optimization and adsorption simulation. Then, we demonstrated the results of these simulation processes for removing cadmium ions from industrial wastewater by using an agricultural byproduct. Finally, we summarized the executed study in the conclusion section.

## 2. Background of the Study

The oldest known toxins are metals, which, depending on their concentration, can be detrimental to living things. Mining operations, the use of fossil fuels, the increasing rate of industrialization, etc. are all contributing factors to today's rise in heavy metal pollution [7]. The different kinds of metals emitted to the environment by the fundamental industries are listed in Table 1.

**Table 1.** Heavy metal distribution in industrial wastewater [8].

| **INDUSTRY** | Fe | Zn | Cu | Ni | Pb | Sn | Hg | Cr | Mn | Cd |
|---|---|---|---|---|---|---|---|---|---|---|
| Coating Industry | - | - | + | + | - | - | + | + | - | + |
| Leather Industry | - | - | - | - | - | - | - | + | - | - |
| Metal Industry | - | + | + | - | + | + | + | + | - | + |
| Fertilizer Industry | + | + | + | + | + | + | + | + | + | + |
| Iron-Steel Industry | + | + | + | + | + | + | + | + | - | + |
| Energy Production | - | + | + | + | + | + | + | + | - | + |
| Chlor-Alkali Production | + | + | - | - | + | + | + | + | - | + |
| Petrochemistry | + | + | - | - | + | + | + | + | - | + |
| Glass, Cement Industry | - | - | - | - | - | - | - | + | - | - |
| Textile Industry | - | - | - | - | - | - | - | + | - | - |
| Paper Industry | - | + | + | + | + | + | + | + | - | - |

Laws to protect the environment are now necessary around the world, including in Turkey, due to the rise in demands for scarce water resources and their exploitation. Today, less than 3% of water is suitable for consumption. As a result, safety measures must be implemented before the contaminated water is discharged into the surrounding environment. Given that industrial wastewater may include significant levels of hazardous contaminants, the WHO and legislation have set lower limits for the concentrations of heavy metals in the wastewater. For the list of the maximum values for heavy metals in marine ecosystems, industrial wastewater, and drinking water that the TSE-226, EU, WHO, and other organizations have permitted, we refer to [9] and [10].

Due to these adverse consequences, wastewater containing heavy metals must be filtered. Some techniques used for filtration include adsorption, chemical sedimentation, ion exchange, and reverse osmosis. These methods, however, fall well short of being affordable and useful in terms of facilities, technology, and other criteria. Because of this, attention was given to employing biowastes as adsorbents to remove heavy metals from wastewater, such as rice husks [11].

## 3. Literature Review

A byproduct of agriculture, rice husk is a plentiful natural resource. Due to its heat insulation characteristics and the high silica ratio of its structure, it finds use in a variety of industries, from the energy sector to the construction industry. For a detailed analysis of the application of rice husk ash in different areas, we refer to [12]. There is a large literature on the usage of rice husk ash for the adsorption of heavy metals from an aqueous medium that must be analyzed in depth, and we think it should be the focus of a different study. However, we will summarize the most important and the most recent studies in this section.

The potential use of rice husk as a biosorbent for the removal of heavy metal ions (Cr, Pb, Zn) present in aqueous solutions was investigated by Priya et al. [13]. And according to the findings of their experiments, rice husk powder can be used as a cheap adsorbent to remove heavy metal ions from industrial wastewater. Moreover, their experimental findings indicated that the amount of metal ion adsorption increases in direct proportion to the pH of the solution, the amount of rice husk powder used, and the duration of contact. In contrast, the adsorption effectiveness decreases when the temperature and the concentration of heavy metal ions rise.

Javed et al. [14] used RHA and iron-oxide-modified RHA adsorbents to extract arsenic from drinking water. In the study of Chanda et al. [15], silica is extracted from RHA and used to synthesize the zeolite Faujasite (FAU). This adsorbent is then used for batch-wise adsorptive removal of Cr(VI) and Pb(II) ions from an aqueous medium. Bahrami et al. [16] synthesized a biosorbent using RHA modified by hexadecyltrimethylammonium bromide surfactant (HDTMAB-RHA) to remove nitrate ions from the aqueous medium.

Montalvo-Andía et al. [17] investigated the absorption process of Cadmium (Cd) ions by utilizing untreated and chemically modified rice husk, and their results proved that the rice husk is an easily managed, low-cost, and efficient biosorbent. RHA and parboiled-RHA that have undergone chemical treatment are used by Gamboa et al. [18] as adsorbents to remove Cr(VI) from wastewater. Their experimental results confirmed that the RHA is an economical and environmentally friendly bio-material that effectively eliminates Cr (VI) from diluted aqueous solutions.

Hossain et al. [19] synthesized potassium hydroxide (KOH)-activated novel rice husk (RH)-based adsorbents and used them on synthetic wastewater to remove hazardous heavy metal ions (such as $Pb^{2+}$, $Fe^{3+}$, $Cu^{2+}$, $Zn^{2+}$, $Mn^{2+}$) using fixed-bed flow column adsorption. It can be said that the considerable capacity of these novel absorbents to adsorb heavy metals and dyes will lead to a new understanding of adsorption mechanisms and the creation of next-generation commercial adsorbents for the treatment of industrial wastewater.

Because rice husk ash is a porous substance with a high silica content, Nurandini [20] further demonstrated that it has a significant ability to absorb heavy metals in water. The goal of this study was to determine the optimum amount of rice husk ash that could be used as an adsorbent and the maximum amount of $Hg^{2+}$ ions that could be absorbed from the column adsorption process utilizing RHA.

For further information on the adsorption properties of rice husk and studies on this subject, we refer to [8] and the latest review study [13], and we refer to [21] and [22] for rice husk usage for the removal of textile dyes from industrial wastewater. We can infer from the literature that chemical adjustments have a favorable impact on the adsorption capacity of these agricultural sorbents.

All the studies mentioned above focused on experimentally evaluating the adsorption efficiency of the RHA-based absorbents for removal of the heavy metals based on some criteria such as adsorbent dosage, pH, pollutant concentration, and interaction time. Additionally, they studied the adsorption kinetics of this process experimentally. In our study, we used computer programming to show the adsorptive feature of rice husks. This is the first study in the literature to provide a computer-based strategy for optimizing the binding mechanism of rice husk through the use of geometry optimization and using absorption simulation techniques for modeling $Cd^{2+}$ adsorption from industrial effluent by rice husk.

## 4. Materials and Methods

The proposed methodology starts with creating the molecular projections of the polyacrylamide, combination structure, and rice husk on the computer-generated media. The expected 36 structures that will arise when Cd has been adsorbed are then shown and optimized.

A two-step process can be used to summarize the optimization of a structure [9]. The first one is called an energy assessment (for a given conformation, an energy statement must be described and analyzed), and the second one is called a conformation adjustment (the conformation is modified to find the minimum energy value; this value could be discovered after a single adjustment or after thousands of iterations). The size of the structure and the complexity of the algorithm influence the number of iterations.

Comparing the structures with various optimization energies, the most stable structure is found to have the lowest energy. Additionally, it was discovered that Cd binds to the adsorbent at that location. The geometry optimization process will be explained in Section 4.1 in detail. All of this research was completed using the Gaussian 0.9 software package, Semi-Empirical/PM3MM module.

As a next step, the adsorption capability of rice husk covered with polymers is examined using the Material Studio 6.1 software. Using the Adsorption Locator module of this application, we computed the adsorption energies of 36 hypothetical structures on an unmodified rice husk. After that, the structures with the highest adsorption energies were identified, along with the adsorption energies at which the Cd ion binds in single, double, quadruple, and sextant bonds.

Adsorption Locator modules, which we utilized to simulate the adsorption of Cd ions to rice husk adsorbent, are based on three hypotheses. These ideas include the Metropolis Monte Carlo method [23, 24], the generation of substrate-adsorbate configurations [25], and the Simulated Annealing Algorithm [26]. We selected the Simulated Annealing Algorithm for the adsorption energy calculations.

The primary principle of the Simulated Annealing algorithm was influenced by the annealing theory. This algorithm simulates the cooling process that occurs in molten materials. First, the algorithm begins with an initial solution (Q) and a temperature value (T). Then, based on the employed neighbor structure, it identifies the neighbor of the current solution and determines the objective function value of the neighbor solution at each iteration.

The Boltzmann-type exponential probability distribution, which is controlled by a temperature parameter T, determines whether these new neighbor solutions are accepted. The acceptance likelihood (p) of a given solution is:

$$p = 1, \qquad \text{if } Q_{new} < Q_{current} \qquad \text{or}$$

$$p = e^{-(Qnew\ -\ Qcurrent)\ /\ T}, \qquad \text{in another case}$$

The best solution is then left unchanged if none of the conditions are met, and the temperature value is updated at the end of each iteration. For a detailed explanation of the Simulated Annealing algorithm, we refer [9] and [26].

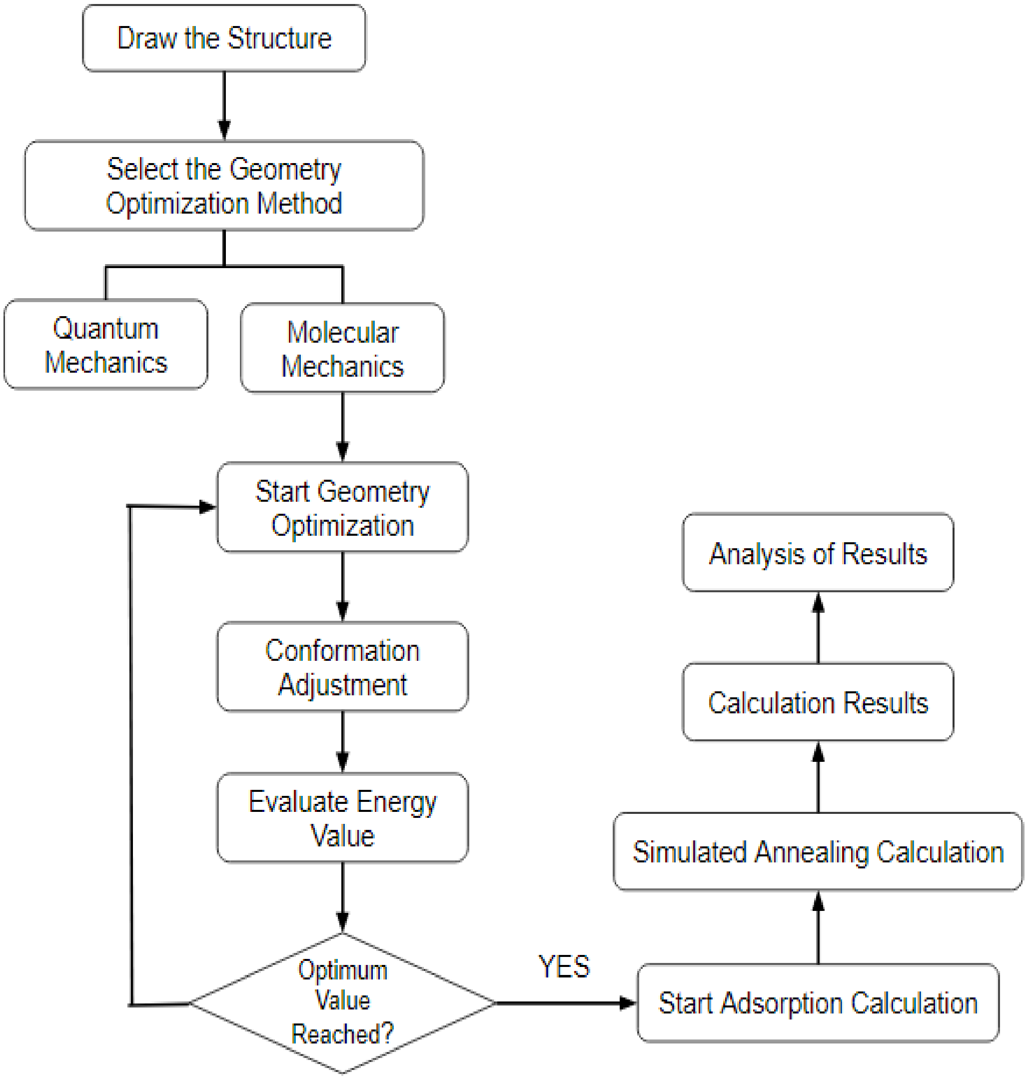

**Figure 2.** Flowchart of the proposed methodology.

After adsorption energies are calculated via the Adsorption Locator tool, these results are analyzed, and the structure with the highest energy value is chosen. The adsorption simulation process will be explained in Section 4.2 in detail.

We summarized the overall methodology that we utilized in our investigation in Figure 2. All experiments were run on an Intel® Core TM i5-3317U CPU @ 1.7 GHz with 8GB RAM computer.

### *4.1. Geometry Optimization*

The technique of iterating on a molecule to determine the lowest energy state where it is stable or to define the reaction's intermediate products is known as geometry optimization [27]. In order to do geometry optimization, the method starts with a set of cartesian coordinates for a chemical and looks for a new set of coordinates with the least amount of potential energy. If the energy has decreased to its lowest level or the target structure has taken on a particular shape, the program converges and presents the results of the computations. The given error is checked, the geometry data is managed, and an appropriate value must be input for the following run if the program does not converge.

There are two markers for the effectiveness of the optimization: the number of iterations required to converge to the minimum and the time it takes to assess the energy expression. Additionally, there are various standard algorithms for a structure's geometry optimization. These algorithms are [28]:

- Steepest Descents [29]
- Conjugate Gradient [30]
- Newton- Raphson methods [31]

The number of optimization cycles and the root-mean-square gradient are two convergence criteria that can be utilized in optimization calculations. Since it might be challenging to predict the precise number of cycles required for good geometry optimization, the root-mean-square gradient can be utilized to end the optimization process. When mixing optimization techniques are used, the cycle number can be utilized as a termination. The default number of cycles is determined by the Gaussian 0.9 software to be 15 times the number of atoms.

The molecular structures of polyacrylamide and rice husk were simulated in this section. Subsequently, the Gaussian 0.9 package program was used to model the start-up geometries of the prepared adsorbent from polyacrylamide and rice husks and the probable structures that would occur when Cd was adsorbed.

### *4.2. Adsorption Simulation*

As we have already stated, it is crucial to effectively and safely purify industrial wastewater. As a substitute, it has been extensively researched to use agricultural and inexpensive products as sorbents. Recent research has focused primarily on agricultural materials and their byproducts, such as rice husk, sawdust, treated orange trash, etc. [32-34].

Subsequently, we examined the adsorption property of polymer-coated rice husks using the Material Studio 6.1 software. Using the Adsorption Locator function, we computed the adsorption energies of our 36 potential structures. After that, the structures with the highest adsorption energies were identified, along with the adsorption energies at which the Cd ion binds in single, double, quadruple, and sextant bonds.

The Adsorption Locator is used to discover low-energy adsorption locations on the adsorbent and simulate the adsorption of pure adsorbates or adsorbate combinations. In adsorption calculation studies, there are some advantages to using a computer program as opposed to an experimental study, such as cost and time savings, the ability to develop new materials faster than through experimentation, a reduction in researcher workload, an increase in productivity, etc.

## 5. Results

### *5.1. Results of the Geometry Optimization*

In this part of the study, we attempted to explain the binding mechanism of $Cd^{2+}$ to the adsorbent, prepared by combining polyacrylamide and rice husks. Figure 3 demonstrates the reaction mechanism of the prepared adsorbent. adsorbent that will be employed in the Cd adsorption process. The rice husk is designated by the R in the adsorbent.

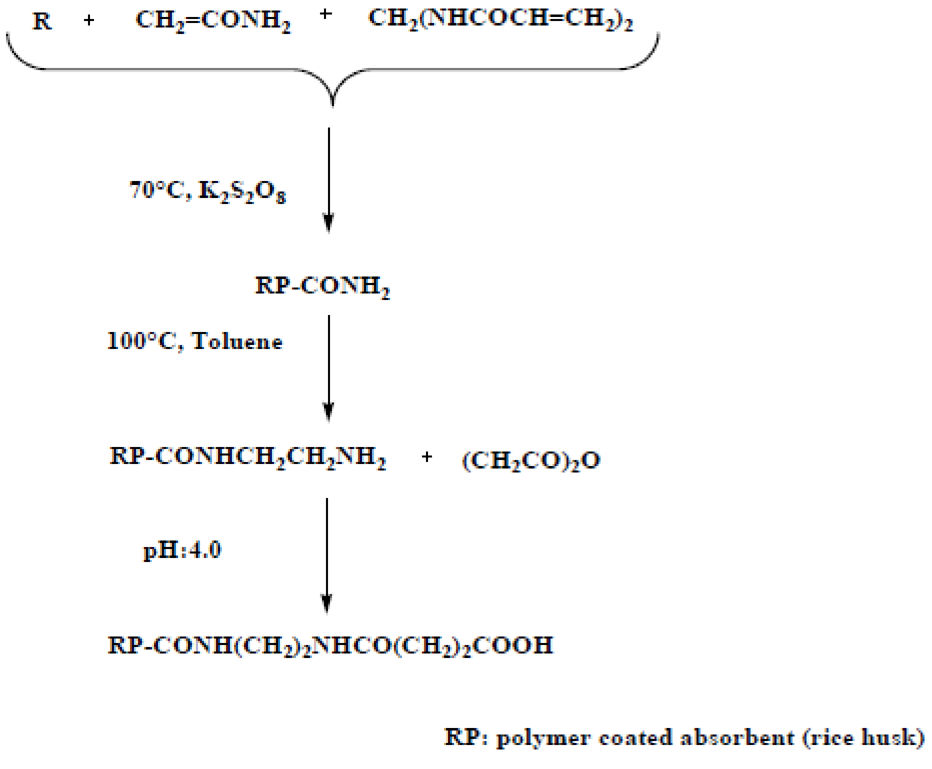

**Figure 3.** Prepared adsorbent [35].

The next step was to determine the likely areas where the Cd atom would bind to the adsorbent once the structure of the rice husk and the generated adsorbent had been established. We then presented potential molecular structures using the package program, followed by geometry optimizations to find the most stable structure.

The structure that requires the least amount of optimization energy would be the most stable. These steps enable the identification of the region where Cd binds to the structure. As these probable structures were being determined, the functional groups (typically phosphate (PO4), amide (NH2), thiols (SH), carboxylate (COO), and hydroxide (OH)) that connect the metal ion to the biomaterial surface were taken into consideration [36].

A geometry's potential energy for a molecule is described by Rappié et al. [37] as "a sum of bonded ($E_R$, $E_\theta$, $E_\Phi$ , $E_w$ ) interactions and nonbonded $E_{vdw}$ + $E_e$ ) interactions [37]:

$E = E_R + E_\theta + E_\Phi + E_w + E_{vdw} + E_e$ Equation 1.

$E_R$ = The valence interactions consist of bond stretching

$E_\theta$ = Angle bend term

$E_\Phi$= Torsional term

$E_w$=Inversion parameter

$E_{vdw}$ = Van der waals energy

$E_e$ = Electrostatic energy"

The software was utilized to determine the energy value because it is impossible to calculate it manually. The calculated optimization energies as an outcome of the geometry optimization are shown in Table 2. If we had to describe the representations in the table, we would say that "rice husk ash- polyacrylamide-Cd-O1 (1)" represents the primary condition where the Cd ion has a single bond with an O ion, and "rice husk ash- polyacrylamide-Cd-O1 (2), (3), and (4)" represent the Cd ion having four single bonds with different O ions. One of the four instances of the Cd ion having a double bond with an O ion is shown as "rice husk ash- polyacrylamide-Cd-O2 (3)". So, while the numbers around the atom indicate whether the bonding is single, double, quadruple, or sextet, the numbers in parenthesis reveal how many various ways of bonding are in these numbers.

**Table 2**. Optimization energies of prepared adsorbent, polyacrylamide, rice husk ash, and all potential Cd-bound molecules.

| **Structures** | **Optimization Energies(kcal/mol)** | **Structures** | **Optimization Energies (kcal/mol)** |
|---|---|---|---|
| Rice husk ash | 2,5 | Rice husk ash-polyacrylamide-Cd-N2(1) | 83 |
| RHA- polyacrylamide | 68 | Rice husk ash-polyacrylamide-Cd-N2(2) | 82 |
| polyacrylamide -cis | 11 | Rice husk ash-polyacrylamide-Cd-N2(3) | 88 |
| polyacrylamide -trans | 10 | Rice husk ash-polyacrylamide-Cd-N2(4) | 81.5 |
| Rice husk ash-polyacrylamide-Cd-O1(1) | 65 | Rice husk ash-polyacrylamide-Cd-N2(5) | 73 |

| | | | |
|---|---|---|---|
| Rice husk ash-polyacrylamide-Cd-O1(2) | 65 | Rice husk ash-polyacrylamide-Cd-N2(6) | 77 |
| Rice husk ash-polyacrylamide-Cd-O1(3) | 66 | Rice husk ash-polyacrylamide-Cd-N2(7) | 80 |
| Rice husk ash-polyacrylamide-Cd-O1(4) | 66 | Rice husk ash-polyacrylamide-Cd-N2(8) | 98 |
| Rice husk ash-polyacrylamide-Cd-O2(1) | 67 | Rice husk ash-polyacrylamide-Cd-N2(9) | 95 |
| Rice husk ash-polyacrylamide-Cd-O2(3) | 70 | Rice husk ash-polyacrylamide-Cd-N2(10) | 75 |
| Rice husk ash-polyacrylamide-Cd-O2(4) | 74 | Rice husk ash-polyacrylamide-Cd-N2(11) | 70 |
| Rice husk ash-polyacrylamide-Cd-O2(2) | 70 | Rice husk ash-polyacrylamide-Cd-N2(12) | 64 |
| Rice husk ash-polyacrylamide-Cd-N1(1) | 64 | Rice husk ash-polyacrylamide-Cd-N4(1) | 155 |
| Rice husk ash-polyacrylamide-Cd-N1(2) | 64 | Rice husk ash-polyacrylamide-Cd-N4(2) | 128 |
| Rice husk ash-polyacrylamide-Cd-N1(3) | 63 | Rice husk ash-polyacrylamide-Cd-N4(3) | 128 |
| Rice husk ash-polyacrylamide-Cd-N1(4) | 66 | Rice husk ash-polyacrylamide-Cd-N4(4) | 140 |
| Rice husk ash-polyacrylamide-Cd-N1(5) | 64 | Rice husk ash-polyacrylamide-Cd-N4-O2(1) | 352 |
| Rice husk ash-polyacrylamide-Cd-N1(6) | 65 | Rice husk ash-polyacrylamide-Cd-N4-O2(2) | 329 |
| Rice husk ash-polyacrylamide-Cd-N1(7) | 65 | Rice husk ash-polyacrylamide-Cd-N4-O2(3) | 354 |
| Rice husk ash-polyacrylamide-Cd-N1(8) | 65 | Rice husk ash-polyacrylamide-Cd-N4-O2(4) | 325 |

**Table 2**. Continue..

Figure 4 is provided based on the calculated optimization energies as an outcome of the geometry optimization which is provided in Table 2. As we mentioned above, the structure that requires the least amount of optimization energy would be the most stable. We can infer from Figure 4 that the structure “Rice husk ash- polyacrylamide-Cd-N1(3)” has the minimum optimization energy and the most stable structure. These steps enable the identification of the region where Cd binds to the structure. Additionally, the structures in which the Cd ion forms single bonds have lower optimization energies. In this instance, it can be claimed that the structures are more stable when the Cd ion takes the H ions from the O and N ions.

Furthermore, there are a few structures (such as "rice husk ash- polyacrylamide-Cd-N1(5)") whose optimization energies are comparable to those of "rice husk ash- polyacrylamide-Cd-N1(3)" and may be classified as stable. Figure 5 provides this structure's optimization energies, which are single-bonding Cd ion configurations.

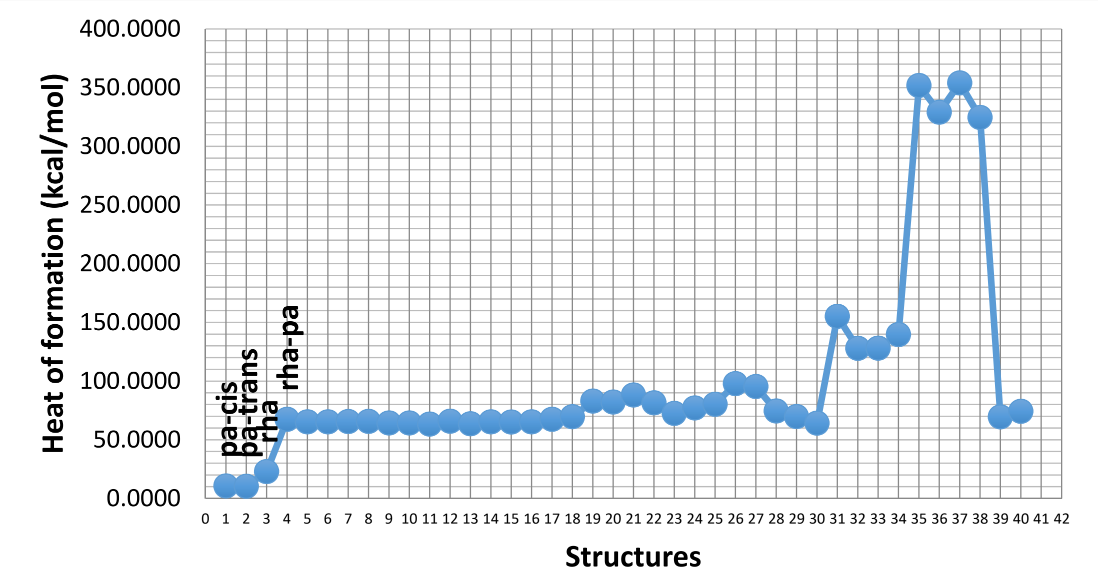

**Figure 4.** Adsorbent, polyacrylamide, rice husk ash, and all potential Cd-bound molecules.

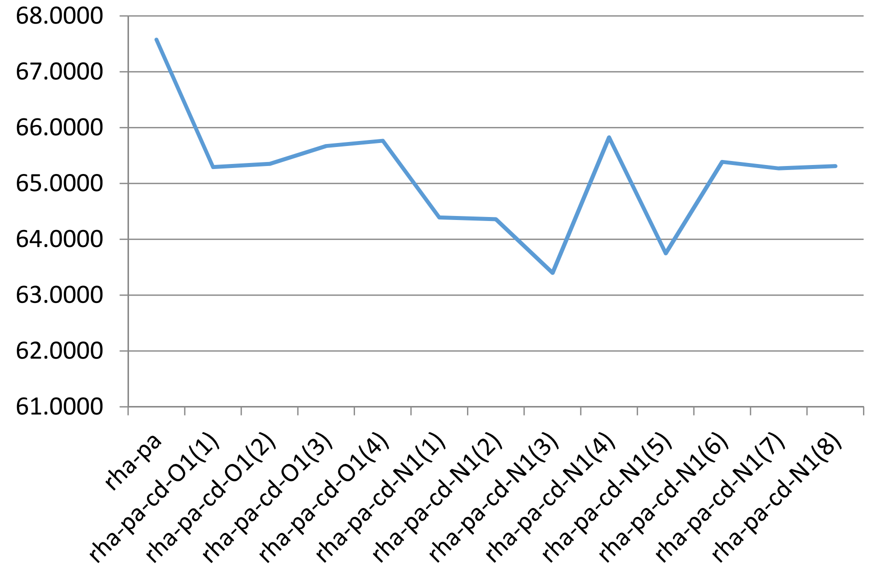

**Figure 5.** Structure-specific optimization energies for single-bonding Cd ion configurations.

### *5.2. Results of the Adsorption Simulation*

According to research by Sharma and colleagues [35], polymer-coated rice husk is a powerful and affordable adsorbent for removing $Cd^{2+}$ ions from aqueous solutions. In 3 hours at a pH of 9, in the concentration range of 30–300 mg/L, 85% of $Cd^{2+}$ ions can be absorbed. According to recent studies, rice husk has an adsorption capacity of 21.36 mg/g, according to a study by Roy et al. [38], 0.16 mg/g by Munaf and Zein [39], and 7 mg/g when modified with NaOH solution by Tarley et al. [40].

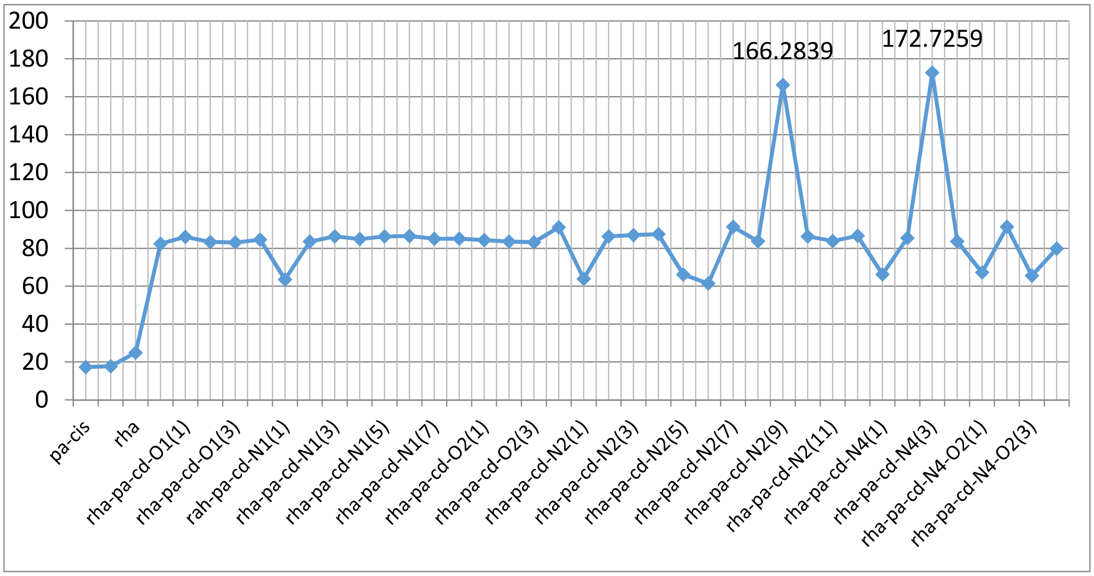

**Figure 6.** Energy levels of all potential configurations for adsorption

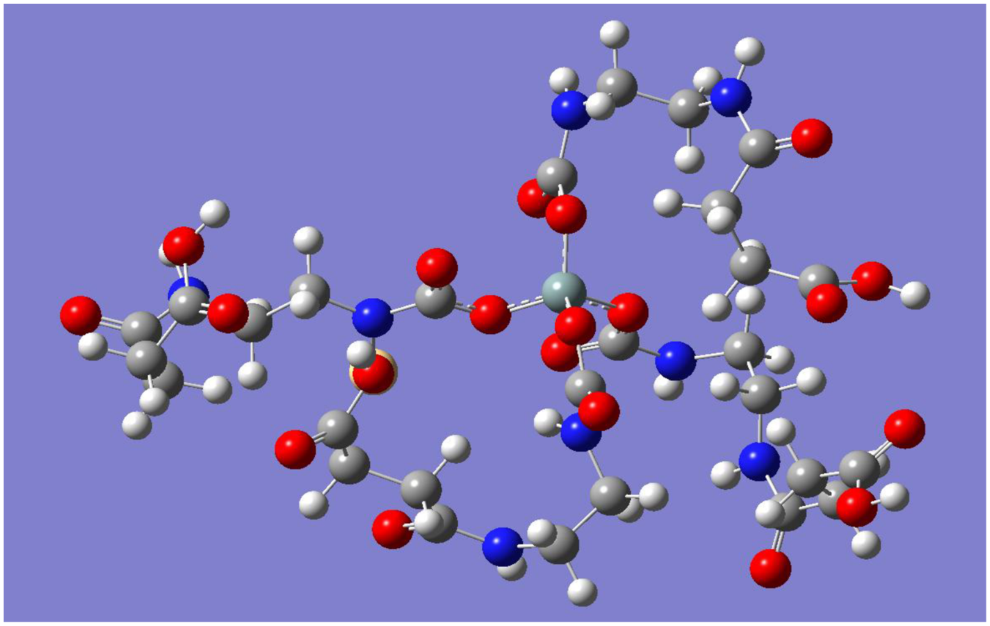

**Figure 7.** Molecular visualization of the optimized rice husk ash-polyacrylamide-Cd-N1(3) structure.

In this study, we demonstrated the adsorptive property of rice husks using computer programming. The adsorption energies of configurations bound to Cd have been computed. The adsorption energy of potential geometrically optimized structures after Cd ion bonding is displayed in Figure 6. Results indicate that the “rice husk ash-polyacrylamide-Cd-N4(3)” structure has the maximum adsorption capacity when all of the structures are taken into consideration. Additionally, we can infer from Figure 6 that the adsorption energy of rice husk is 44.9287 before polymer treatment and 82.4124 after polymer treatment. This finding suggests that polymer treatment increases the rice husk's adsorption capacity. Figure 7 demonstrates the molecular visualization of the optimized rice husk ash-polyacrylamide-Cd-N1(3) structure.

## 5. Conclusions

Due to high production rates, rice husk storage is a problem that can be solved by using them for adsorption. Additionally, using rice husks for adsorption is a more affordable way to remove heavy metals from industrial effluent. In our research, we looked at the rice husk's capacity for adsorptive action. Our study is the first in the literature to provide a computer-based strategy for optimizing the binding mechanism of rice husk through the use of geometry optimization and absorption simulation techniques. Additionally, the mechanism of $Cd^{2+}$ adsorption from industrial effluent by rice husk was investigated.

Initially, the molecular visualizations of the polyacrylamide, rice husk, their composite structure, and the expected structures that will arise once Cd has been adsorbed in the medium were sketched and optimized. The region of the structure where Cd binds was identified. Evaluating and contrasting the structures' optimization energies reveals that those in which the Cd ion forms single bonds have fewer optimization energies. Throughout this situation, it may be argued that the structures with the highest degree of stability are those in which the Cd ion accepts the H ions rather than the O and N ions. For these geometry optimizations, we employed the software from the Gaussian® 0.9 package.

The Material Studio® 6.1 software was then used to demonstrate the adsorptive characteristics of rice husk. The adsorption energies of Cd-bounded structures have been computed and contrasted. In this instance, the structure with the highest energy value was chosen. As a result, the ability of the rice husk to behave as an adsorptive substance was investigated using geometry optimization and absorption simulation approaches.

An important finding of our study is that expensive materials like active carbon may be replaced with rice husks as adsorbents. And the use of inexpensive and abundant adsorbent rice husk ash for removing cadmium ions is a promising alternative for application in wastewater treatment, which is a difficult task. Moreover, this finding proves that polymer treatment increases the rice husk's adsorption capacity. All these findings are compatible with the results of studies in the literature.

Furthermore, all of the research in the literature concentrated on experimentally assessing the RHA-based absorbents' ability to remove heavy metals based on a number of factors, including adsorbent dosage, pH, pollutant concentration, and interaction time. They also carried out experimental research on the adsorption kinetics of this procedure. In our study, we used computer programming to show the adsorptive feature of rice husks. This is the first study in the literature to provide a computer-based strategy for optimizing the binding mechanism of rice husk through the use of geometry optimization and using absorption simulation techniques for modeling $Cd^{2+}$

adsorption from industrial effluent by rice husk. Comparing the proposed procedure to experimental ones, it is demonstrated that the proposed method is quicker and less expensive in many aspects (such as workload, used materials, and labor skills).

As we mentioned above, there are several advantages to using a computer program in adsorption calculation studies rather than an experimental study, including cost and time savings, the ability to develop new materials more quickly than through experimentation, a decrease in researcher workload, an increase in productivity, etc. The computational method used in adsorption calculations is crucial in terms of providing a basis for extensive experimental studies. These studies make it easier to determine the starting points of experimental studies and direct the study. Despite this, more research is still required to determine whether using the method in substantial wastewater treatment plants is both technically and economically feasible, which is in the scope of our future research plan.

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