

Article

Sustainable Valorization of Coal Gasification Slag via Low-Temperature Alkaline Activation for Efficient Cd²⁺ Removal: Performance, Mechanism, and Life Cycle Assessment

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Abstract

Coal gasification slag (CGS), a massive industrial solid waste, possesses inherent adsorptive potential that remains underutilized due to pore blockage by amorphous siliceous phases. Conventional modification strategies typically rely on energy-intensive high-temperature processes. Herein, we report a facile, low-temperature alkaline activation approach to transform CGS into a high-efficiency adsorbent (denoted NCGS) for Cd²⁺ removal. Sodium hydroxide (NaOH) solution was employed under mild conditions (90 °C) to selectively etch siliceous species, thereby generating a porous architecture and enriching surface oxygen-containing functionalities. Orthogonal experimental design identified optimal synthesis parameters (1 mol/L NaOH, solid–liquid ratio of 1:30 g/mL, 12 h), yielding NCGS with significantly enhanced textural properties. The adsorption isotherm was well described by the Langmuir model, with a maximum capacity of 87.06 mg/g at pH 6.0, while kinetic studies indicated the adsorption process could be described by pseudo-second-order kinetic model. Comprehensive characterization via SEM-EDS, FTIR, and XPS elucidated a multi-mechanistic adsorption pathway mainly involving ion exchange (Na⁺/Cd²⁺) and coordination complexation. Life cycle assessment analysis revealed that NCGS production generates 11.23 kg CO₂ eq emissions, with transportation accounting for 88%. This study presents an energy-saving and environmentally friendly strategy to unlock the adsorptive potential of CGS, providing a highly promising waste-based adsorption material for the remediation of Cd²⁺-contaminated water.

Keywords: coal gasification slag; NaOH modification; orthogonal experiment; cadmium adsorption; life cycle assessment



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1. Introduction

Global population growth and intensified industrialization have led to the substantial release of cadmium (Cd) into aquatic environments, often resulting in concentrations that exceed the World Health Organization (WHO) safety limit of 0.003 mg/L [1]. As a non-essential and highly toxic heavy metal, Cd poses severe threats to plants, animals, and human health [2,3]. Long-term intake of trace amounts of Cd can lead to the accumulation of Cd in the human body, causing chronic diseases such as cancer, osteoarthritis, and renal tubular necrosis [4,5]. Industrial wastewater remains the primary source of Cd pollution, which subsequently enters the ecosystem through runoff, irrigation, and sedimentation [6]. Once in the food chain, Cd undergoes biomagnification, posing a persistent risk to public

health [7]. Consequently, developing efficient removal technologies is imperative. Among various physicochemical treatments—including ion exchange [8], chemical precipitation [9], and adsorption [10,11]. Among them, adsorption is considered particularly promising due to its high efficiency, operational simplicity, cost-effectiveness, and environmental safety. Carbon-based materials, such as biochar and activated carbon, have demonstrated significant potential for the remediation of Cd-contaminated water [12,13].

Coal gasification slag (CGS) is a predominant solid byproduct of the coal gasification industry, with annual production in China reaching approximately 33 million tons [14]. Currently, the primary disposal methods remain landfilling and open stockpiling, owing to low resource utilization rates and high treatment costs [15]. These practices not only consume vast land resources but also cause severe soil and groundwater degradation [16]. Therefore, transforming CGS into high-value resources is a pressing environmental priority. CGS is mainly composed of SiO_2 , Al_2O_3 , CaO , Fe_2O_3 and residual carbon, and its composition is affected by the type of raw coal and gasification process [17]. Given its large specific surface area, well-developed pore structure, and relatively high carbon content [18,19], CGS serves as an ideal precursor for the synthesis of low-cost adsorbents [20,21].

However, the adsorption capacity of raw CGS is limited by its high silicon (Si) content, which exists mainly as amorphous silicon–oxygen tetrahedra. These amorphous structures tend to block the primary pores and fissures, thereby reducing the available active sites for pollutant capture [22,23]. To address this, two main strategies have been developed: (1) synthesizing zeolite-based composites by combining the silicon in CGS with aluminum-rich wastes [24], and (2) removing silicon to enrich the carbon matrix. For instance, Luoyang et al. utilized sequential acid and alkali leaching to etch SiO_2 , creating a hierarchical porous structure (CSM) that enhanced pollutant diffusion and adsorption [25]. Similarly, Xuan et al. prepared carbon-based materials via acid leaching followed by alkali activation for ammonia nitrogen removal [26]. Despite these advancements, conventional modification routes often rely on complex acid-base combinations and high-temperature pyrolysis (up to 800 °C), resulting in high energy consumption and limited economic efficiency. Furthermore, research specifically focused on the simplified modification of CGS using only alkali treatment remains scarce.

Sodium hydroxide (NaOH), a strong alkali, can react with silicon dioxide (SiO_2) under relatively mild temperatures. In this study, a one-step NaOH modification approach was employed to achieve efficient silicon dissolution and the synthesis of a carbon-based adsorbent (NCGS) for Cd^{2+} removal from aqueous solutions. The influence of critical modification parameters was systematically evaluated, and the underlying adsorption mechanisms were elucidated through batch experiments and comprehensive material characterization. This strategy avoids repeated acid leaching and high-temperature calcination inherent to traditional treatments, substantially cutting energy and chemical inputs to yield a more economical and eco-friendly modification scheme. Meanwhile, this work provides a sustainable strategy for the resource valorization of industrial solid waste and the management of heavy metal pollution in aquatic systems, and further advances the technical system of CGS-based adsorbent preparation.

2. Materials and Methods

2.1. Materials

The stock solution of Cd was prepared from the dissolution of CdCl_2 (>98%, Shanghai Aladdin Reagent Co., Ltd., Shanghai, China). NaOH (AR, Shanghai Aladdin Reagent Co., Ltd.) is used in the synthesis of NaOH-modified CGS (NCGS). All chemicals were prepared using deionized water (18.2 M). The CGS used for composite synthesis was sourced from Yulin City, Shaanxi Province, China. The chemical composition characterized by X-ray

fluorescence (XRF) was summarized in Figure 1, with all data reported as equivalent oxides. The results indicated that SiO_2 is the predominant oxide, constituting 45.528% by mass, with Al_2O_3 , CaO , and Fe_2O_3 being the subsequent major components.

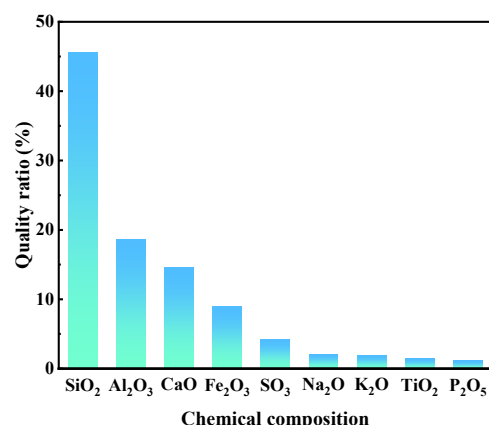


Figure 1. Chemical composition of gasification slag.

2.2. Synthesis of Modified Coal Gasification Slag

The synthesis procedure for NCGS is illustrated in Figure 2. In a typical process, 3.0 g of raw CGS was mixed with a NaOH solution in a 250 mL conical flask at a specific ratio. The mixture was then heated in a water bath at a constant temperature of 90 °C. Following the reaction, the resulting solid–liquid mixture was repeatedly washed with deionized (DI) water until the filtrate reached a neutral pH. The obtained samples were then dried in an oven at 60 °C until a constant weight was achieved. To optimize the modification conditions, the effects of various parameters—including modification time, NaOH concentration, and solid–liquid ratio—on the Cd^{2+} adsorption performance of NCGS were systematically investigated.

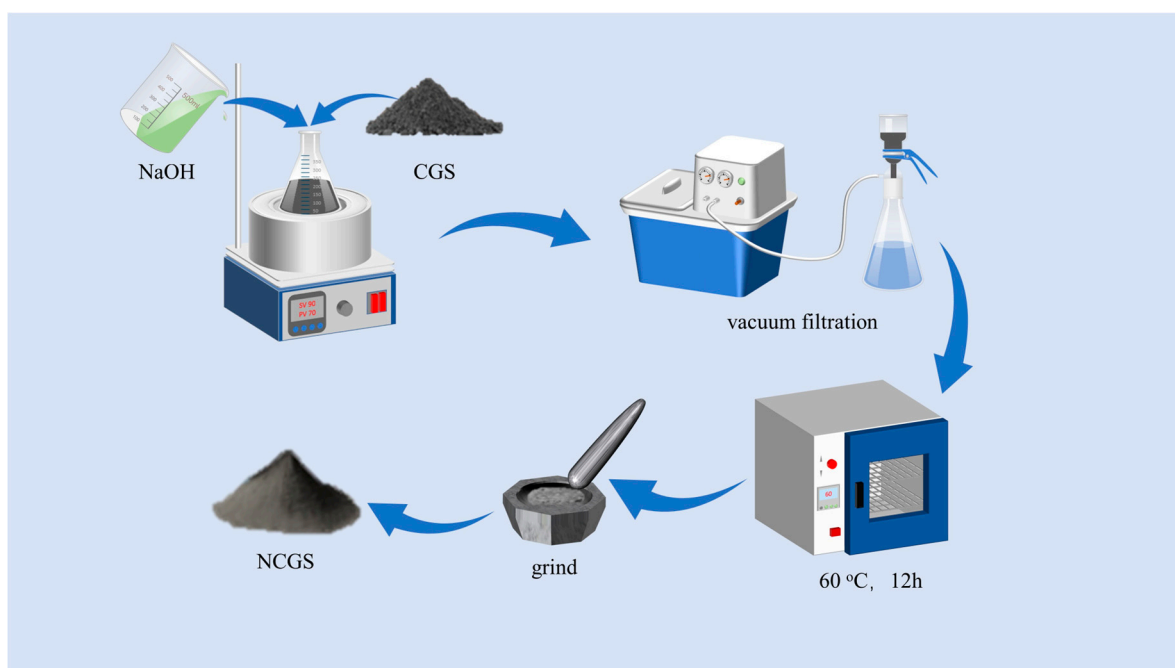


Figure 2. The schematic diagram of NCGS preparation.

2.3. Design of Orthogonal Experiment Table

Based on the actual operation process of the modification experiment, three factors—NaOH concentration, modification time, and solid–liquid ratio—and their levels were selected. The $L^9(3^3)$ orthogonal table was used for the experimental design, with a total of 9 groups of treatments. In this study, the concentrations of NaOH were taken as 0.25, 0.5, and 1 mol/L, the modification times were taken as 3, 6, and 12 h, and the solid–liquid ratios were taken as 1:10, 1:30, and 1:50 g/mL for the pre-experiment.

2.4. Adsorption Experiments

In this experiment, 0.05 g of CGS and NCGS under different modification conditions were weighed separately into 50 mL centrifuge tubes, then 30 mL of 50 mg·L^{−1} Cd solution was added to each tube, and the tubes were placed in a shaker (25 °C, 180 r·min^{−1}). At the 12th hour, water samples were collected, filtered through a 0.22 µm filter membrane, and then the Cd concentration was determined. With the goal of maximizing the adsorption capacity of Cd, the optimal modification conditions were explored.

After the optimal modification conditions were determined, 30 mL of Cd ion solutions of different concentrations (30–200 mg/L) were mixed with 0.05 g of adsorbent and shaken at room temperature for different times (5 min–24 h). The relative adsorption rate (P%) and adsorption capacity (q_e) of the adsorbents were obtained by Equations (1) and (2) [27].

$$P\% = \frac{(C_0 - C_e)}{C_0} \times 100\% \quad (1)$$

$$q_e = \frac{(C_0 - C_e)V}{m} \quad (2)$$

where C_0 (mg/L) is the initial mass concentration of Cd²⁺ in the solution; C_e (mg/L) is the equilibrium mass concentration of Cd²⁺ in the solution; V (L) is the volume of the solution; and m (g) is the mass of the adsorbent.

2.5. Characterization

The micro-structure and surface element distribution of gasification slag were investigated by field scanning electron microscopy (FSEM, M0AIA3, LMH, TESCAN, Brno, Czech Republic) combined with energy dispersive spectrometer (EDS, Oxford Instruments, Oxfordshire, UK). The porosity and specific surface area were quantified utilizing the Brunauer–Emmett–Teller analysis (BET, Autosorb-iQ, Quantachrome Instruments, Boynton Beach, FL, USA). The surface functional groups were analyzed using Fourier transform infrared spectrum (FTIR, VERTEX80V, Bruker, Karlsruhe, Germany). Spectral data were collected at a resolution of 4 cm^{−1} over 4000–400 cm^{−1}, and each spectrum represented an average of 32 scans. X-ray photoelectron spectroscopy (XPS, ESCALAB 250Xi, Thermo Fisher Scientific, Waltham, MA, USA) was used to determine the elemental composition under a monochromatic Al Kα (1486.6 eV) source at 110 W. A wide-range spectrum (0–1200 eV) was scanned with a pass energy of 150 eV, while narrow-range high-resolution scans were collected at a pass energy of 20 eV. The binding energy scale was calibrated by referencing the adventitious carbon C 1 s peak to 284.8 eV. Inductively coupled plasma optical emission spectrometry (ICP-OES, Thermo Fisher iCAP PRO, Waltham, MA, USA) was applied to determine the concentration of Cd²⁺ in aqueous solutions.

2.6. Environmental Impact Based on Life Cycle Assessment

To evaluate the environmental sustainability of NCGS synthesis, a life cycle assessment (LCA) was conducted using openLCA software (2024), following the ISO 14044 guidelines [28]. A “cradle-to-gate” system boundary was defined (Figure 3), which encompasses raw material

acquisition, transportation, and all stages of NCGS production. Based on representative logistics in China, the transportation distance for raw materials was modeled at an average of 181 km [29]. This work does not take into account the use and end-of-life phases, following the assumption that there is not environmental impact in use phase and the end-of-life phase does not require disposal [29]. The functional unit for the analysis was set as the production of 1 kg of NCGS. Detailed inventory data, allocation procedures, and the comprehensive Life Cycle Inventory (LCI) are provided in Text S1 and Table S1, respectively.

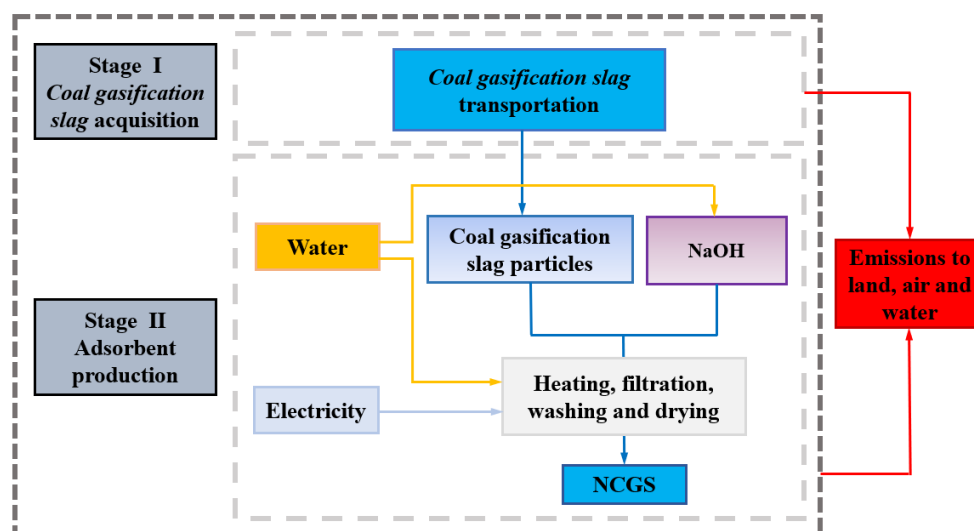


Figure 3. System boundary consideration for producing NCGS.

3. Results and Discussion

3.1. Optimization of Modification Parameters and ANOVA Analysis

In this study, the adsorption capacity of Cd^{2+} by NCGS under different modification conditions was investigated, and the optimal conditions for CGS modification were determined through orthogonal experiments with the goal of maximum adsorption capacity (Table 1), where the number 0 represents the adsorption capacity of the original CGS. The results showed that NaOH modification can effectively increase the adsorption capacity of CGS. Moreover, under the conditions of NaOH concentration of 1.0 mol/L, a solid–liquid ratio of 1:30 g/mL, modification temperature of 90 °C, and modification time of 12 h, the adsorption capacity of NCGS for Cd^{2+} reached the maximum value (29.83), indicating that the prepared NCGS exhibits promising adsorption capacities and is suitable for the subsequent heavy metal adsorption process.

Table 1. Orthogonal experiment of modified conditions.

Number	NaOH Concentration (mol/L)	Time (h)	Solid–Liquid Ratio (g/mL)	Adsorption Capacity (mg/g)
0	0	0	0	4.76
1	0.25	3	1:10	8.20
2	0.25	6	1:30	8.77
3	0.25	12	1:50	13.43
4	0.5	3	1:30	11.70
5	0.5	6	1:50	13.93
6	0.5	12	1:10	24.00
7	1.0	3	1:50	17.48
8	1.0	6	1:10	28.88
9	1.0	12	1:30	29.83

To determine the significance of the influence of the three modification parameters on the NCGS preparation process, we conducted an analysis of variance (ANOVA) on the experimental data using the SPSSAU system and obtained the results shown in Table 2. According to the analysis results, the class III sum of squares of NaOH concentration is the largest (352.44), and the F value (146.85) and *p* value ($0.0008 < 0.01$) show extremely significant influence, indicating that it has the strongest independent contribution to the adsorption capacity and is positioned as the most influential factor. The modification time also demonstrates significance at the 0.05 level ($F = 62.05, p = 0.0024 < 0.05$), and the liquid–solid ratio is also significant at the 0.05 level ($F = 18.97, p = 0.0123 < 0.05$), but its class III sum of squares is the smallest, belonging to a relatively weak factor. Therefore, the order of influence of modification conditions on the preparation process is as follows: NaOH concentration > modification time > solid–liquid ratio.

Table 2. ANOVA on the influence of modification conditions on NCGS.

Conditions	Class III Sum of Squares	Degrees of Freedom	Mean Square	F	<i>p</i>
NaOH concentration	352.44	2	176.22	146.85	0.0008
Time	148.92	2	74.46	62.05	0.0024
Solid–liquid ratio	45.53	2	22.76	18.97	0.0123
Residual	2.4	2	1.2	-	-

This results indicates that the concentration of the alkaline solution is the most crucial parameter for regulating the surface chemical properties and pore structure of NCGS. As a strong alkali, NaOH determines the etching intensity of the aluminosilicate framework on the CGS surface [30]. At a low concentration, NaOH treatment only results in mild surface cleaning and the activation of a limited number of functional groups. As the concentration increases, the enhanced corrosive effect of OH[−] ions on the mineral lattice effectively dissolves amorphous silica and alumina. This process exposes more active adsorption sites, expands the specific surface area, and introduces abundant oxygen-containing functional groups, thereby significantly enhancing the adsorption capacity for Cd²⁺. Regarding the modification time, the alkali etching effect becomes more thorough as the reaction progresses, leading to increased surface roughness and higher active site density. However, beyond a certain threshold, the etching reaction approaches equilibrium, and further extension of time yields diminishing returns. The solid–liquid ratio primarily influences mass transfer efficiency and alkali utilization [31]. Its relatively low significance implies that within the tested range, mass transfer limitations were minimal, and the contact between the liquid and solid phases was sufficient to meet modification requirements. In summary, the optimal preparation conditions for Cd(II) removal were identified as 1.0 mol/L NaOH, a 12 h modification time, and a solid–liquid ratio of 1:30 g/mL.

3.2. Characterization of Adsorbents

3.2.1. SEM-EDS Analysis

The morphology and microstructure of the three samples were characterized by scanning electron microscopy (SEM). As shown in Figure 4a, the pristine CGS predominantly comprises vitreous silicate particles exhibiting smooth, unblemished surfaces devoid of any surface accretions or adhered phases—morphological features consistent with observations documented in prior studies [32]. The surface of NCGS is rougher than that of CGS. Under the action of alkaline chemical corrosion, etching pits are formed on the particle surface, presenting a honeycomb-like structure and obvious cracks (Figure 4b). This rough surface not only increases the effective contact area but also provides more adsorption

sites for the subsequent loading of Cd^{2+} . Furthermore, the EDS analysis (Figure 4d,e) further corroborates these structural transformations, demonstrating a marked depletion of surface Si and Al species concomitant with substantial Na enrichment. These compositional changes confirm that the alkaline treatment facilitates the dissolution of crystalline aluminosilicate phases, with subsequent formation of soluble sodium aluminosilicate species (e.g., NaAlSiO_4) that are leached into the alkaline medium [33].

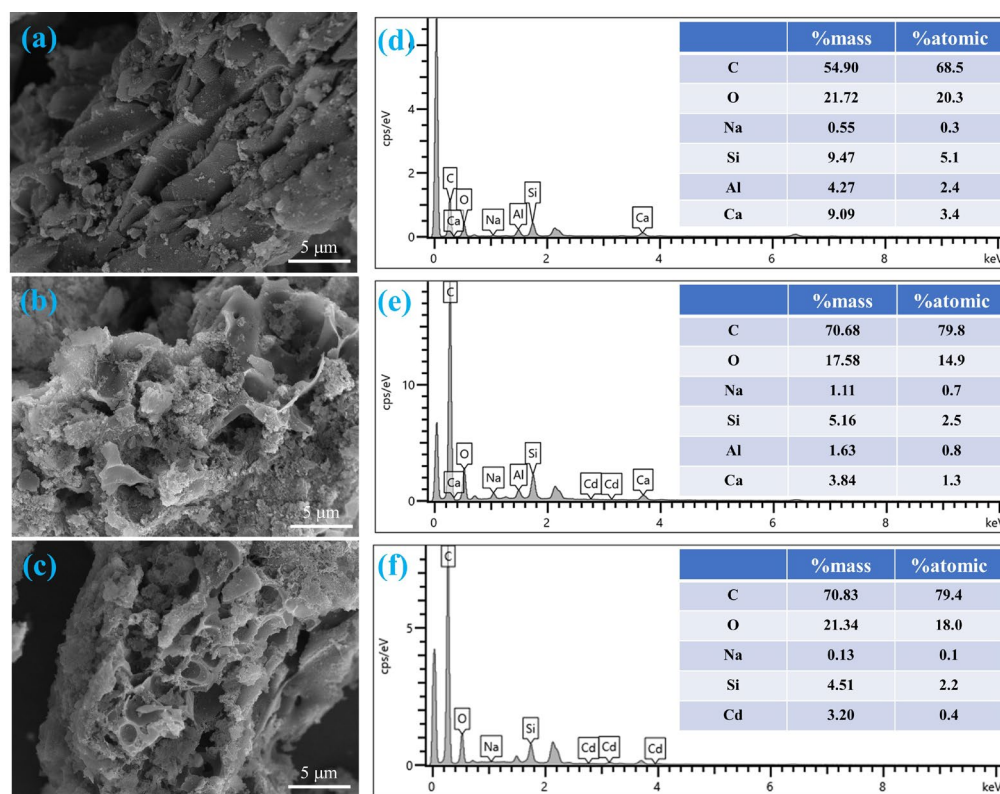


Figure 4. (a) The SEM of CGS. (b) The SEM of NCGS. (c) The SEM of NCGS-Cd. (d) The SEM-EDS of CGS. (e) The SEM-EDS of NCGS. (f) The SEM-EDS of NCGS-Cd.

3.2.2. BET Analysis

The N_2 adsorption–desorption isotherms of NCGS and CGS are shown in Figure 5a. Both of these materials exhibit typical type IV isotherms, and both hysteresis loops belong to type H4 ($0.4 < P/P_0 < 1$), which is usually associated with capillary condensation in mesopore structures [34,35]. Combined with the pore size distribution of NCGS and CGS (Figure 5b), it can be found that mesoporous pores are mainly concentrated between 2 nm and 4 nm. Subsequently, a plateau is reached, indicating the absence of further multilayer adsorption. Furthermore, N_2 sorption isotherms reveal significantly enhanced uptake for NCGS relative to pristine CGS, confirming that alkaline modification promotes extensive dissolution of mineral phases, consequently creating a well-developed porous network with increased specific surface area and pore volume. Additionally, the re-precipitation of dissolved aluminosilicate species under local supersaturation conditions contributes to the formation of an open mesoporous framework, offering facilitated diffusion pathways for adsorbate transport and active site accessibility [36]. According to the BET calculation, the specific surface area of NCGS increased from $225 \text{ m}^2/\text{g}$ to $279 \text{ m}^2/\text{g}$ after modification, and both the average pore diameter and pore volume increased accordingly (Table 3).

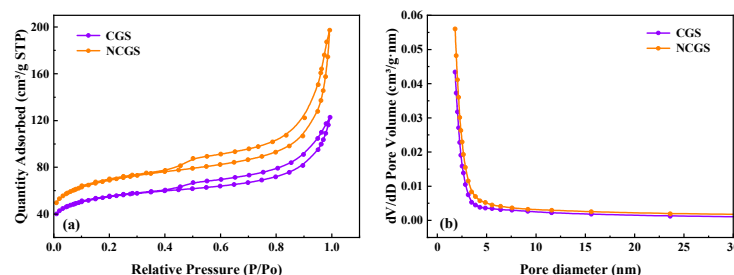


Figure 5. Nitrogen adsorption–desorption isotherms of CGS and NCGS (a) and pore size distribution curves (b) of CGS and NCGS.

Table 3. The textural properties of CGS and NCGS.

Sample	Surface Area (m ² /g)	Average Pore Width (nm)	Pore Volume (cm ³ /g)
CGS	225.34	3.2464	0.0955
NCGS	279.24	3.4630	0.1190

3.2.3. FTIR Analysis

FTIR spectroscopy was employed to elucidate the surface chemical transformations induced by alkaline modification (Figure 6). The retention of comparable spectral features between CGS and NCGS indicates preservation of the fundamental surface chemistry, while quantitative differences reveal specific structural modifications. The broad band at $\sim 3435\text{ cm}^{-1}$ (O–H stretching) [19] and the composite bands at $1300\text{--}1600\text{ cm}^{-1}$ (O–C=O and –OH bending) exhibit increased intensity in NCGS, corroborating the introduction of oxygen-rich functionalities [37]. Concurrently, the disappearance of the 1064 cm^{-1} and 873 cm^{-1} bands (Si–O–Si and Si–O–Al symmetric stretching) and the concomitant appearance of the 998 cm^{-1} band (Si–OH stretching) were observed. This feature may stem from the process of framework depolymerization via hydroxide-mediated cleavage of bridging oxygen bonds, generating soluble silicate/aluminate species and exposing undercoordinated surface sites. Furthermore, the shift in the 466 cm^{-1} band (Si–O stretching in SiO_4 tetrahedra [38]) reflects alkali-induced modification of the Si–O bond electronic structure and enhanced lattice polarization [39].

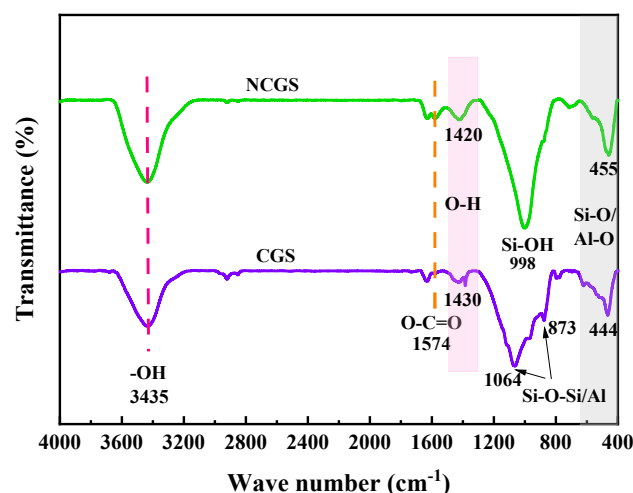


Figure 6. FTIR spectra before and after CGS modification.

3.2.4. XPS Analysis

XPS was employed to investigate the surface chemical composition and bonding environments of CGS and NCGS (Figure 7). The survey spectra reveal the emergence of a Na 1s peak in NCGS (Figure S1), confirming the successful incorporation of sodium species, consistent with the EDS elemental analysis. High-resolution O 1s spectra were deconvoluted into four distinct components centered at 530.64, 531.91, 532.67, and 533.65 eV (Figure 7c), corresponding to C–O, O–H, Si–O, and O–C=O moieties, respectively [40]. Notably, the O–C=O and O–H peaks in NCGS exhibit positive binding energy shifts and significantly enhanced intensities relative to pristine CGS (Figure 7d), corroborating the FTIR findings and confirming the enrichment of carboxyl and hydroxyl functionalities on the modified surface [41]. Additionally, the Si–O peak intensity decreases modestly in NCGS compared to CGS (Figure 7d). This attenuation is mainly attributed to the alkaline hydrolysis of Si–O–Si bridging bonds, resulting in the partial solubilization of silicon species from the solid matrix. Although this process diminishes the overall Si–O signal, it simultaneously promotes the extensive generation of silanol (Si–OH) groups on the material surface, which effectively offsets the reduction in bulk Si–O signal intensity.

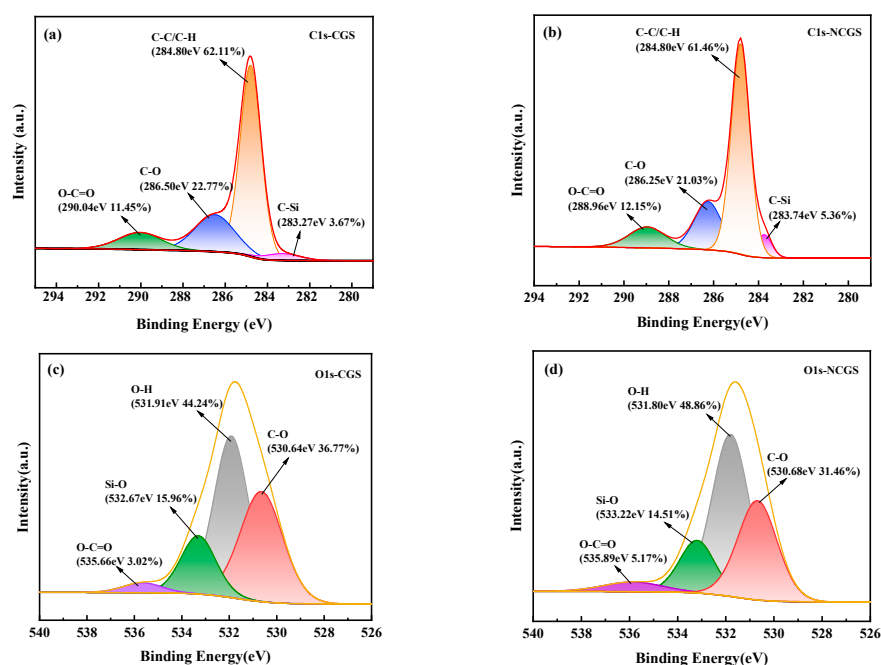


Figure 7. Spectra of CGS before and after modification. (a) C1s spectrum of CGS; (b) C1s spectrum of NCGS; (c) O1s spectrum of CGS; (d) O1s spectrum of NCGS.

Comprehensive characterization via SEM-EDS, FTIR, and XPS elucidates that the modification of CGS by NaOH treatment proceeds through a tripartite synergistic mechanism encompassing alkali-mediated desilication, pore generation, and active site functionalization. Under highly alkaline conditions, NaOH selectively leaches siliceous and aluminous species from the CGS matrix, generating soluble polysilicate and aluminate ions. This dissolution process induces extensive surface pitting and creates a well-developed microporous network, substantially enhancing the textural properties and generating accessible void spaces conducive to adsorption. Concomitantly, alkaline treatment promotes the surface oxidation and hydroxylation of carbonaceous moieties, enriching oxygen-containing functional groups (particularly –OH and –COOH). This augmentation of active sites significantly amplifies the material’s affinity for Cd²⁺ coordination and immobilization.

3.3. Adsorption Performance

3.3.1. Effect of Adsorbent Dosage

The effects of NCGS dosage on Cd^{2+} removal efficiency and equilibrium adsorption capacity (q_e) are shown in Figure 8a. As the NCGS dosage increased from 0.33 to 1.67 g/L, the Cd^{2+} removal rate ($P\%$) exhibited a rapid initial ascent, followed by a gradual plateau. Conversely, q_e remained relatively stable at approximately 28 mg/g within the 0.33–1.67 g/L range, but declined markedly at higher dosages. This divergent trend can be rationalized that increasing the adsorbent dosage enhances the total number of available binding sites, thereby improving the probability of Cd^{2+} -adsorbent encounters and elevating the overall removal efficiency. However, once the adsorption equilibrium is established under a fixed initial Cd^{2+} concentration, further increasing the NCGS dosage introduces excess unoccupied sites relative to the finite amount of Cd^{2+} ions. Consequently, the adsorbent utilization efficiency decreases, manifesting as a reduction in the unit adsorption capacity [42]. Considering both removal efficiency and adsorption capacity, an optimal NCGS dosage of 1.67 g/L was selected for subsequent experiments, as this condition achieves near-complete Cd^{2+} removal while maintaining a high q_e value without excessive adsorbent consumption.

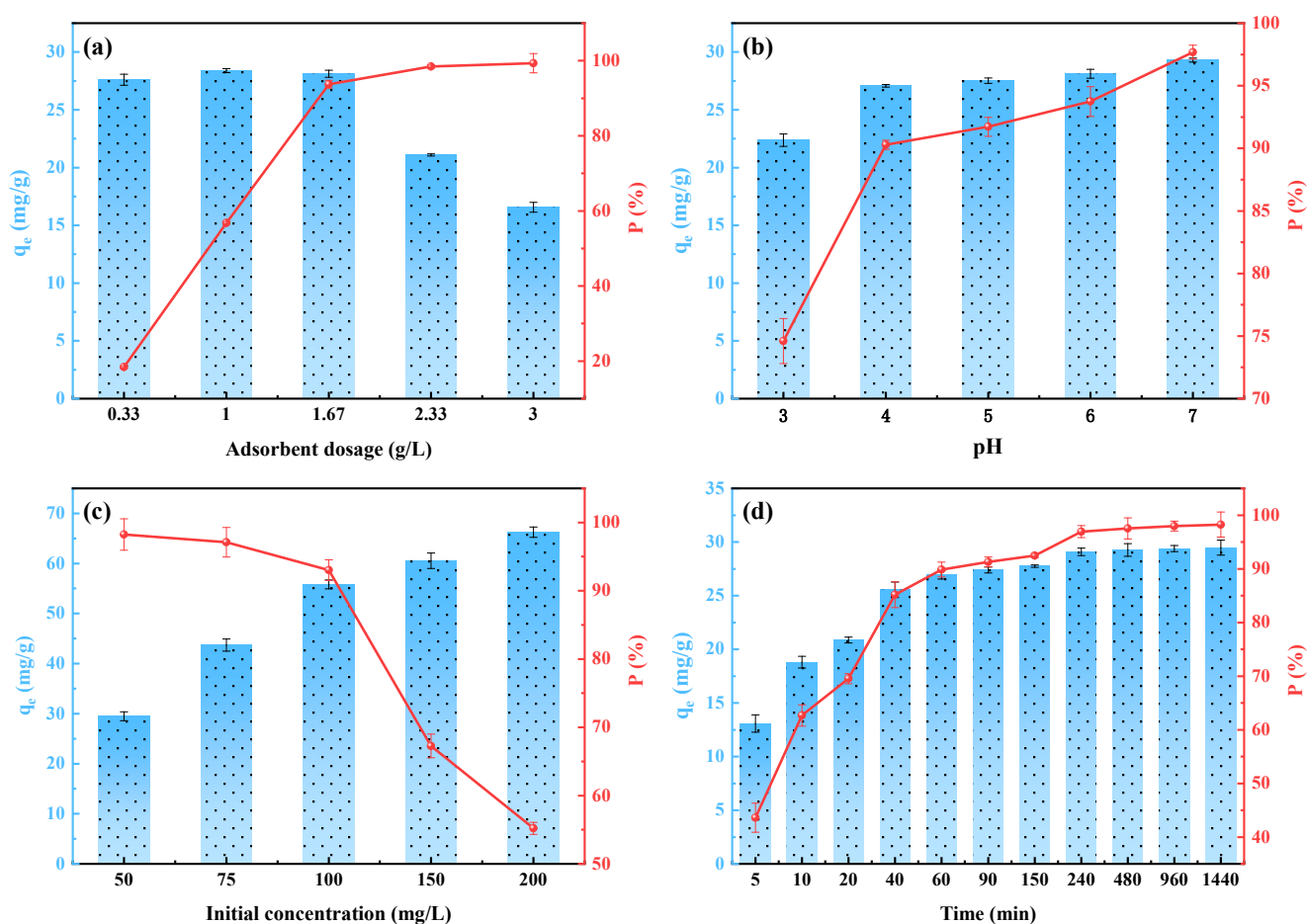


Figure 8. The effects of (a) adsorbent dosage, (b) solution pH, (c) initial concentration and (d) adsorption time on the adsorption efficiency.

3.3.2. Effect of Solution pH

Solution pH represents a critical parameter governing Cd^{2+} speciation and, consequently, its adsorptive behavior. Accordingly, the influence of pH on Cd^{2+} removal efficiency was systematically investigated at a fixed NCGS dosage of 1.67 g/L. Visual MINTEQ geochemical modeling reveals that Cd^{2+} speciation is strongly pH-dependent

(Figure S2). At $\text{pH} < 7$, free Cd^{2+} cations predominate in solution, while the monohydroxy complex CdOH^+ becomes increasingly prevalent within the pH 8–12 range. Precipitation of amorphous $\text{Cd}(\text{OH})_2(\text{s})$ commences at $\text{pH} \sim 9$ and persists through pH 13, whereas anionic hydroxyl complexes $[\text{Cd}(\text{OH})_3]^-$ and $[\text{Cd}(\text{OH})_4]^{2-}$ emerge at $\text{pH} > 12$. To preclude the confounding effects of precipitation and ensure exclusive evaluation of adsorption mechanisms, all batch experiments were conducted within the pH window of 1–7.

As illustrated in Figure 8b, both Cd^{2+} removal efficiency and adsorption capacity exhibit a pronounced positive correlation with pH over the range 3–7. Under strongly acidic conditions ($\text{pH} < 3$), elevated proton concentrations result in competitive occupation of surface binding sites via protonation, thereby electrostatically hindering Cd^{2+} accessibility and diminishing removal performance. With increasing pH , the progressive deprotonation of surface functional groups enhances the negative surface charge density, facilitating Cd^{2+} coordination and ion exchange [43]. However, approaching pH 7 risks the incipient hydrolysis and precipitation of Cd^{2+} species, potentially conflating adsorption with surface precipitation mechanisms. Therefore, to ensure unambiguous attribution of Cd removal to adsorption processes, subsequent experiments were conducted at an optimal initial pH of 6.0.

3.3.3. Effect of Initial Concentration

Subsequently, the initial pH of the solution was adjusted to 6, and the NCGS dosage was maintained at 1.67 g/L, the effects of initial concentration on the adsorption performance of the adsorbent were investigated. As shown in Figure 8c, more than 90% of the Cd^{2+} was removed when the initial concentration was within the scope of 50–100 mg/L, while the removal rate descended gradually from 93.02% to 55.02% when the concentration of Cd^{2+} increased from 100 mg/L to 200 mg/L. This phenomenon can be attributed to the limited number of reactive binding sites on the adsorbent; there were enough adsorption sites for the cadmium ions to occupy the solution with a lower concentration of Cd^{2+} . When the initial concentration of Cd^{2+} was greater than 100 mg/L, the surface adsorption sites of NCGS were saturated, and further removal of Cd^{2+} could not be achieved, generating a decrease in the diffusion of Cd from the aqueous to the NCGS surface. However, the adsorption capacity of NCGS for Cd increased with the increase in the initial concentration. When the Cd concentration increased from 50 mg/L to 200 mg/L, q_e increased sharply from 29.47 mg/g to 66.24 mg/g. This is due to the increase in the driving force provided by the increase in Cd concentration, which could overcome the resistance of adsorbates mass transfer [44].

3.4. Adsorption Behavior

3.4.1. Adsorption Isotherm

To evaluate the adsorption characteristics of Cd^{2+} by NCGS, the Freundlich, Langmuir, and Temkin models were used to fit the adsorption of Cd^{2+} on the surface of NCGS in this study. The Freundlich model is applicable to multilayer adsorption on heterogeneous surfaces with uneven energy distribution [45] and the Langmuir model describes monolayer adsorption on uniform surfaces with finite identical binding sites [46], while the Temkin model is applicable to scenarios where monolayer adsorption occurs and the adsorption heat has a linear relationship with coverage [47]. The adsorption isotherm fitting results of Cd^{2+} by NCGS are shown in Figure 9a and Table 4.

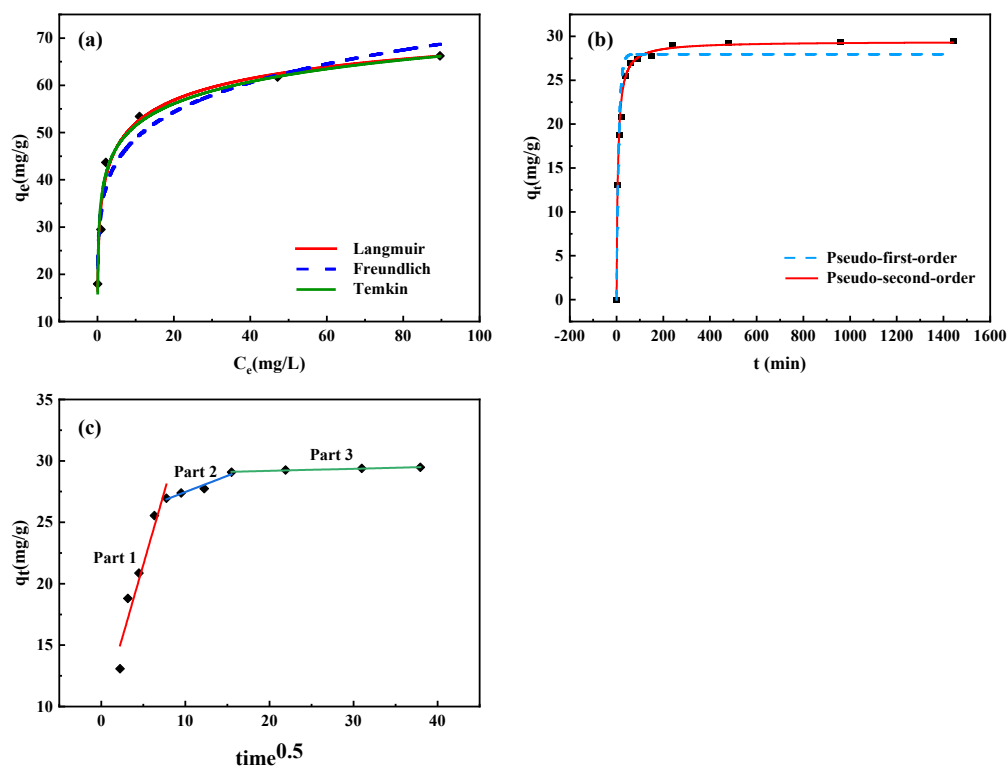


Figure 9. (a) Adsorption isotherms of Cd by NCGS. (b) Adsorption kinetics of Cd by NCGS; (c) Intra-particle diffusion of Cd by NCGS.

Table 4. Parameters of Cd adsorption isotherm and kinetics on NCGS.

Type	Model	Constants	
Langmuir	$q_e = \frac{q_m K_L C_w}{1 + K_L C_e}$	q_m (mg/g)	87.0653
		K_L (L/mg)	0.6655
		R^2	0.9817
Freundlich	$q_e = K_F C_e^{\frac{1}{n}}$	K_F ($\text{mg}^{(1-1/n)} \text{L}^{1/n}/\text{g}^{-1}$)	34.0574
		n	6.4070
		R^2	0.9573
Temkin	$q_e = \frac{RT}{b_T} \ln(A_T C_e)$	A_T	0.0688
		b_T	26.3579
		R^2	0.9749
Pseudo-first-order	$q_t = q_e (1 - e^{-k_1 t})$	q_e (mg/g)	27.9722
		k_1 (min^{-1})	0.1053
		R^2	0.9636
Pseudo-second-order	$q_t = \frac{tk_2 q_e^2}{1 + tk_2 q_e}$	q_e (mg/g)	29.4185
		k_2 ($\text{mg}/\text{g} \cdot \text{min}$)	0.0056
		R^2	0.9933
Intra-particle diffusion	$q_t = k_i t^{\frac{1}{2}} + C$	C_1 (mg/g)	9.6603
		k_{d1} ($\text{mg}/\text{g} \cdot \text{min}^{1/2}$)	2.3785
		R^2	0.9311
		C_2 (mg/g)	24.8317
		k_{d2} ($\text{mg}/\text{g} \cdot \text{min}^{1/2}$)	0.2634
		R^2	0.9453
		C_3 (mg/g)	28.8490
		k_{d3} ($\text{mg}/\text{g} \cdot \text{min}^{1/2}$)	0.0028
		R^2	0.9508

As presented in Table 4, the fitting correlation coefficient of the Langmuir model ($R^2 = 0.9817$) is greater than that of the Temkin model and the Freundlich model ($R^2 = 0.9573, 0.9743$), indicating that it is a uniform monolayer adsorption on the surface with a theoretical maximum adsorption capacity of 87.06 mg/g. To further evaluate the adsorption performance of the prepared material, the adsorption capacities toward Cd^{2+} of various reported adsorbents and NCGS were comprehensively compared. As shown in Table 5, the adsorption capacity of NCGS for Cd^{2+} was significantly higher than that of some previously reported adsorbents, including safflower leaf biochar(MnFeB), cadmium ion-imprinted polymers (IA-IIIP), magadiite (Na-magadiite/Cyanex-272), polymeric microsphere adsorbents (TEVS-EGDMA-CRM), and $\text{Fe}_3\text{O}_4/\text{MnO}_2$ magnetic composite (nano-PFM). Although it was not the highest adsorption capacity among all the adsorbents, the aim of this study was to utilize the coal gasification slag from industrial solid waste to prepare an efficient adsorbent, achieving the dual goals of waste treatment and pollution control. Therefore, the preparation of adsorbents from coal gasification slag for the remediation of heavy metal-contaminated water bodies has broad application prospects.

Table 5. Comparison of Cd adsorption capacity of different adsorbents.

Adsorbents	q_m (mg/g)	Initial Concentration (mg/L)	pH	Dosage (g/L)	References
MnFeB	34.25	100	6.0	2.5	[48]
MBC	59.60	50	5.5	1	[49]
IA-IIIP	50.54	50	7.0	2	[50]
Na-magadiite/Cyanex-272	64.06	50	6.0	1	[51]
TEVS-EGDMA-CRM	64.26	50	6.63	1	[52]
nano-PFM	39.05	50	6.0	1.6	[53]
APR@Sam	103.5	50	5.0	0.1	[54]
FeCa-Bc	92.16	100	6.0	1	[55]
NCGS	87.06	50	6.0	1.67	This paper

3.4.2. Adsorption Kinetic

The influence of adsorption contact time on adsorption performance is shown in Figure 8d. The experimental data indicate that within the first 40 min, the removal rate of Cd^{2+} increased sharply. This is attributed to the abundant available binding sites on the NCGS surface, which enables rapid adsorption of Cd^{2+} [56]. However, as the adsorption process continued, the available adsorption sites gradually decreased, and the mass transfer momentum gradually reduced, resulting in a slower increase in the removal rate. When the adsorption time reached 240 min, the removal rate gradually stabilized.

The adsorption process of Cd^{2+} by NCGS was analyzed by using pseudo-first-order kinetic model, pseudo-second-order kinetic model and intra-particle diffusion model. As shown in Figure 9b, the Cd adsorption capacity increased sharply in the first 40 min, while the adsorption rate increased more slowly as time went on. When the adsorption time reached 240 min, the adsorption gradually approached equilibrium. As can be seen from Table 4, the correlation coefficient of the pseudo-second-order kinetic model ($R^2 = 0.9933$) is larger than that of the pseudo-first-order kinetic model ($R^2 = 0.9636$), and the measured value of its equilibrium adsorption capacity is highly consistent with the simulated value. It indicates that the pseudo-second-order model can better explain the kinetic rate, and the rate-limiting step might be chemical adsorption.

To explore the main limitations of Cd^{2+} adsorption on the NCGS surface, the obtained data were fitted with the intraparticle diffusion model. As shown in Figure 9c, the adsorp-

tion of Cd^{2+} onto NCGS exhibited a multilinear increase, suggesting that the process can be divided into three stages: external surface diffusion, internal particle diffusion, and final equilibrium [54]. In the first stage, Cd^{2+} diffuses from the solution to the outer surface of the adsorbent. Notably, the fitted line at this stage does not pass through the origin, indicating that the mass-transfer rate is not the dominant rate-limiting factor. The second stage is gradual adsorption. Since the line in the second part does not cross the origin, intraparticle diffusion is not the only rate-limiting factor, other factors also influence the adsorption process [57]. The third stage is related to the final equilibrium. Specifically, once equilibrium is reached within the pores, some adsorbates will immediately transfer to the active sites where chemical reactions occur. These results indicate that after the metal ions diffuse onto the surface of the adsorbent, the active sites on the NCGS are likely to guide the adsorption process through chemical adsorption.

3.4.3. Adsorption Thermodynamics

The thermodynamic study of the adsorption process of Cd^{2+} on NCGS was carried out at 288 K, 298 K and 308 K. Relevant parameters such as free energy changes (ΔG° , kJ/mol), enthalpy changes (ΔH° , kJ/mol) and entropy changes (ΔS° , J/mol/K) were calculated using the following equations [58]:

$$\Delta G = -RT \ln \frac{q_e}{c_e} \quad (3)$$

$$G = \Delta H - T\Delta S \quad (4)$$

$$\ln \frac{q_e}{c_e} = \frac{\Delta S}{R} - \frac{\Delta H}{RT} \quad (5)$$

where q_e (mg/g) is the specific equilibrium quantity of the adsorbate, c_e (mg/L) is the equilibrium concentration, R is the perfect gas constant (8.314 J/mol/K), and T (K) is the absolute temperature.

The calculation results of thermodynamic parameters are shown in Table 6. The value range of ΔG° is -4.76 to -8.41 kJ/mol, the negative value of ΔG° indicated that the adsorption was spontaneous, which was thermodynamically favorable. The positive ΔH° indicated that the adsorption process was endothermic, and increasing the temperature was conducive to the reaction [59]. The positive ΔS° indicated that the interaction between Cd^{2+} and NCGS was an entropy increase at the solid/liquid interface, suggesting that the adsorbate has a high affinity for the adsorbent [52].

Table 6. Thermodynamic parameter values of Cd^{2+} adsorption by NCGS (adsorbent dosage = 1.67 g/L, pH = 6, and initial concentration = 50 mg/L).

Adsorbates	ΔH° (kJ/mol)	ΔS° (J/mol/K)	ΔG° (kJ/mol)		
Cd^{2+}	47.80	182.50	288 K −4.76	298 K −6.59	308 K −8.41

3.5. Adsorption Mechanism

The adsorption of Cd^{2+} by NCGS is mainly governed by two key mechanisms: (1) physical adsorption, derived from the well-developed mesoporous structure of NCGS that accelerates pollutant diffusion and supplies abundant adsorption sites [60]; and (2) chemical adsorption, characterized by active surface groups and ion exchange processes on NCGS [61]. Herein, the adsorption of Cd^{2+} on NCGS is predominantly dominated by the chemical adsorption mechanism. Accordingly, this section focuses on dissecting the chemical adsorption mechanism of Cd^{2+} onto NCGS.

Post-adsorption SEM analysis reveals that the surface morphology of NCGS-Cd remains largely unaltered compared to pristine NCGS (Figure 4c). However, EDS elemental mapping (Figure 4f) indicates a substantial decrease in surface Na atomic concentration from 0.7% to 0.1%, concomitant with the emergence of Cd characteristic emission. This compositional change provides direct evidence for an ion exchange mechanism, whereby Na^+ ions are displaced by Cd^{2+} at surface binding sites.

FTIR spectroscopic analysis further elucidates the adsorption mechanism (Figure 10). While most absorption bands exhibit minor intensity variations, two critical regions display significant perturbations. Specifically, the bands at 3435 cm^{-1} (O–H stretching) and 1574 cm^{-1} (O–C=O asymmetric stretching) demonstrate marked intensity attenuation following Cd^{2+} uptake, accompanied by a distinct shift in the 1420 cm^{-1} band. These spectral modifications suggest the possible formation of coordination complexes between Cd^{2+} and surface hydroxyl/carboxyl functionalities [62].

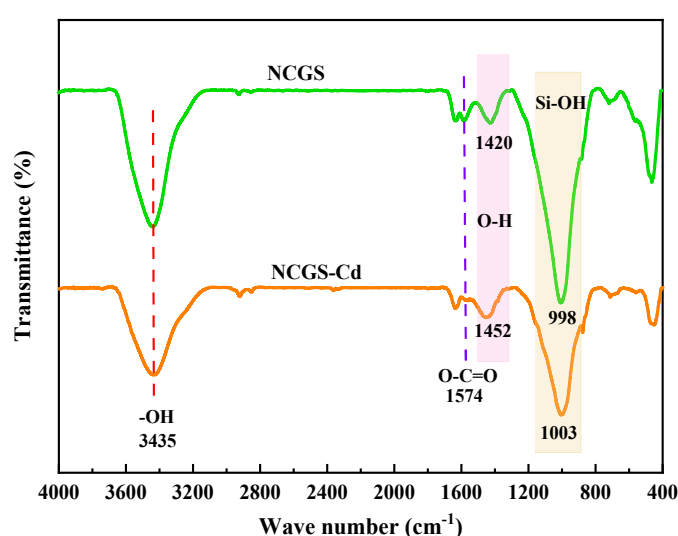


Figure 10. FTIR spectra of NCGS before and after Cd adsorption.

XPS analysis provides definitive confirmation of the adsorption mechanism and chemical speciation (Figure 11). The appearance of the Cd 3d core level spectrum (Figure 11a) substantiates successful Cd immobilization on the NCGS surface. Notably, substantial attenuation of the Na 1s peak at 1072 eV corroborates the ion exchange process between Na^+ and Cd^{2+} during adsorption. High-resolution O1s deconvolution (Figure 11d) reveals significant changes in oxygen bonding environments. For instance, the relative contributions of O–H and O–C=O moieties decrease from 48.86% to 29.56% and from 5.17% to 3.33%, respectively, while a new component emerges at 532.7 eV (31.25% contribution) corresponding to Cd–O bonding [63]. This confirms the direct involvement of hydroxyl and carboxyl groups in Cd complexation. Furthermore, the high-resolution Cd 3d spectrum exhibits spin–orbit doublet peaks at 412.53 eV ($3d_{3/2}$) and 405.78 eV ($3d_{5/2}$), characteristic of Cd–O and Cd–OH surface species [64,65], consistent with the formation of inner-sphere surface complexes.

Collectively, the aforementioned characterization results elucidate that Cd^{2+} sequestration by NCGS proceeds via a multi-mechanistic pathway encompassing (Figure 12): (i) ion exchange involving the displacement of exchangeable Na^+ by Cd^{2+} ; (ii) coordination complexation with surface oxygen-containing functional groups (particularly carboxyl and hydroxyl moieties); and (iii) physical adsorption within pores.

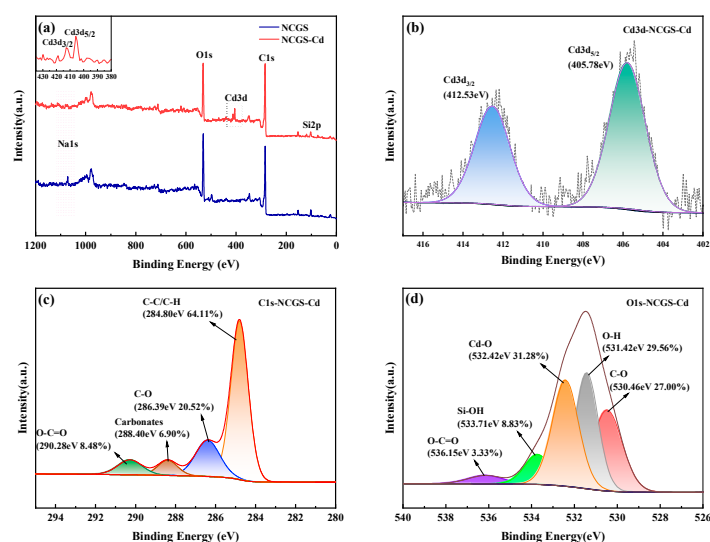


Figure 11. (a) XPS spectra before and after NCGS adsorbed Cd; (b) Cd3d spectrum of NCGS-Cd; (c) C1s spectrum of NCGS-Cd; (d) O1s spectrum of NCGS-Cd.

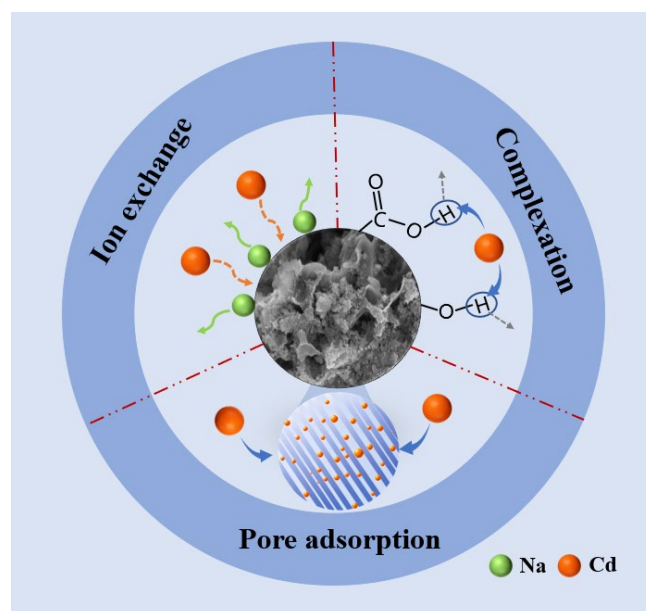


Figure 12. Main mechanisms of adsorption of Cd^{2+} by NCGS.

3.6. Environment Effects of NCGS Synthesis Based on LCA

To evaluate the industrial application potential and environmental impacts of NCGS, a cradle-to-gate LCA was conducted to quantify the environmental burden of producing 1 kg of this adsorbent (Table S2), with a further comparison against other conventional adsorbents.

Quantitative analysis identified distinct environmental footprints across eight impact categories: Global Warming Potential (GWP: 11.23 kg CO_2 eq), Stratospheric Ozone Depletion Potential (SODP: 5.97×10^{-6} kg CFC11 eq), Ionizing Radiation Potential (IRP: 0.63 kBq Co-60 eq), Ozone Formation Human Health Potential (OFHP: 0.08 kg NO_x eq), Ozone Formation Terrestrial Ecosystems Potential (OFTP: 0.08 kg NO_x eq), Marine Eutrophication Potential (MEP: 6.6×10^{-4} kg N eq), Fossil Resource Scarcity Potential (FRSP: 5.73 kg oil eq) and Freshwater Eutrophication Potential (FEP: 2.7×10^{-3} kg N eq). To develop a more sustainable comprehensive strategy, a detailed analysis of each component contributions was conducted. As shown in Figure 13a, transportation emerged as the dominant contributor across multiple impact categories, accounting for 88% (GWP), 72%

(SODP), 27% (IRP), 64% (OFHP), 60% (OFTP), 77% (MEP), 85% (FRSP) and 47% (FEP). This dominance is attributed to the substantial emissions of greenhouse gases, particulate matter, and aromatic hydrocarbons resulting from diesel combustion during logistics. Sodium hydroxide, the primary reagent for NCGS synthesis, was the second-largest contributor, significantly impacting IRP (68%), FEP (30%), and SODP (25%). Additionally, the impact of electricity consumption was noteworthy. Given that coal-fired thermal power remains the predominant source of electricity in China, this finding underscores the necessity of transition to cleaner energy configurations to further mitigate the environmental burden of adsorbent production.

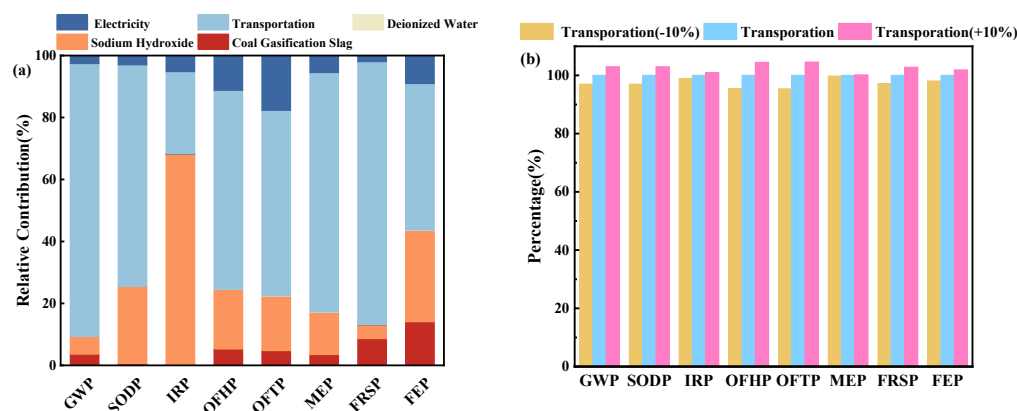


Figure 13. (a) Relative contribution of environmental impact indicators for NCGS. (b) Transportation sensitivity analysis.

Transportation constitutes the dominant contributor to overall environmental impacts; thus, a data sensitivity analysis focusing on this stage was performed. Transportation distances were adjusted by $\pm 10\%$, while the contribution values of original environmental impact categories were set as the baseline (100%), to quantify the resulting variation magnitudes of each environmental indicator. As illustrated in Figure 13b, a 10% increase in transportation distance leads to elevated values across all 18 impact categories, with variation rates ranging from 0.20% to 4.61%. This phenomenon is mainly driven by diesel consumption during transportation, as fluctuations in diesel usage directly alter the associated environmental burdens. Among all categories, Ozone Formation Terrestrial Ecosystem Potential (OFTP) exhibits the most pronounced sensitivity. Such sensitivity analysis enables the identification of key parameters that induce substantial fluctuations in specific environmental impact categories, providing a critical reference for subsequent environmental monitoring and the tracing of abnormal indicator values.

Despite these environmental impacts, the global warming potential (GWP), a key climate change indicator, was calculated to be 11.23 kg CO₂ eq per kilogram of NCGS. This value is lower than those of alternative materials, such as sodium alginate-functionalized electrolytic manganese residue (S-EMR: 12.36 kg CO₂ eq) [66] and Amidoxime functionalized silica aerogel (ASA-X: 58.07 kg CO₂ eq) [67]. This comparative analysis confirms that NCGS imposes a relatively low environmental burden, demonstrating significant potential for sustainable, large-scale application in heavy metal wastewater treatment.

4. Conclusions

In this study, a novel adsorbent (NCGS) was successfully synthesized from coal gasification slag (CGS) via a facile low-temperature alkaline activation method for Cd²⁺ removal. The main findings are as follows:

- (1) Under the optimal synthesis conditions of 1 mol/L NaOH, solid–liquid ratio 1:30 g/mL, and water bath at 90 °C for 12 h, the material modification follows a ternary synergistic mechanism of alkali-mediated desilication, pore structure development and active site functionalization.
- (2) The adsorption behavior fits well with the Langmuir isotherm and pseudo-second-order kinetic models, FTIR and XPS analyses further reveal that Cd²⁺ removal proceeds via a synergistic mechanism including ion exchange (Na⁺/Cd²⁺), coordination complexation with hydroxyl and carboxyl groups, and physical adsorption within pores.
- (3) Life cycle assessment revealed that the production of 1 kg of NCGS generates 11.23 kg CO₂ eq of emissions. Although transportation is the primary environmental contributor (accounting for 88% of the GWP), NCGS maintains a significantly lower environmental burden compared to many conventional and functionalized adsorbents.

Overall, this work demonstrates that alkali-modified CGS is a cost-effective and environmentally friendly candidate for the remediation of Cd-contaminated water, providing a viable pathway for the high-value resource utilization of industrial solid waste.

Supplementary Materials: The following supporting information can be downloaded at <https://www.mdpi.com/article/10.3390/separations13070198/s1>. Figure S1. XPS spectra before and after modification of gasification slag. Figure S2. Distribution of cadmium species under different pH solution values. Table S1. Inventory data for conducting LCA to production 1kg of NCGS. Table S2. The environmental impacts for producing 1 kg of NCGS.

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