

## Amberlite IRC-718 ion chelating resin extraction of hazardous metal Cr (VI) from aqueous solutions: equilibrium and theoretical modeling

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### ABSTRACT

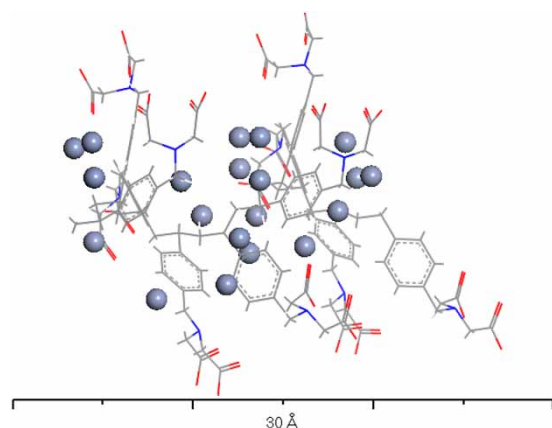
Under varied conditions, the IRC 718 ion-exchange resin is used to extract chromium (VI) ions from aqueous solutions. On chromium (VI) removal effectiveness, the effects of adsorption dosage, contact time, beginning metal concentration, and pH were examined. The batch ion exchange process reached equilibrium after around 90 minutes of interaction. With an initial chromium (VI) concentration of 0.5 mg/dm<sup>3</sup>, the pH-dependent ion-exchange mechanism revealed maximal removal in the pH 2.0–10 range. The adsorption mechanism occurs between Cr (VI) determined as the electron acceptor, and IRC 718 determined as the electron donor. The equilibrium ion-exchange potential and ion transfer quantities for Amberlite IRC 718 were calculated using the Langmuir adsorption isotherm model. The overall ion exchange capacity of the resin was determined to be 187.72 mg of chromium (VI)/g of resin at an ideal pH of 6.0.

**Key words:** adsorption isotherm, chromium (VI), ion exchange, IRC 718

### HIGHLIGHTS

- Amberlite IRC 718 is efficient at extracting and recovering chromium from wastewaters.
- Chelating resin could remove Cr (VI) from a single aqueous solution containing initial metal ion concentrations ranging from  $0.162 \times 10^{-3}$  to  $10.3 \times 10^{-3}$  M at room temperature.
- Chelating sorption closely matched the Langmuir model isotherm.
- The monolayer adsorption capacities of these ion metals at the interface were 187.72 mg/g of resin.

### GRAPHICAL ABSTRACT



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## 1. INTRODUCTION

Heavy metals including Cr, Cu, Pb, Mn, Hg, and Cd are prevalent contaminants in soil and water. Chromium (Cr) is a very hazardous element employed in various sectors, including electroplating, tanning, mining, metal and dye production, and so on (Babel & Opiso 2007; Mustafa *et al.* 2008; Prasad *et al.* 2021). Liquid chromium in wastewater poses a health danger to all plants and animals as either the trivalent form (Cr (III)) or the hexavalent form (Cr (VI)) due to its toxicity and carcinogenic effects. Nonetheless, it has been discovered that some species require trivalent chromium in their diet. On the other hand, Cr (VI) is 300 times more poisonous than Cr (III) (Gatto *et al.* 2010). Because it affects chromosomes by breaking DNA strands, producing DNA-protein crosslinks, and changing the DNA transcription pathway, hexavalent chromium is a probable carcinogen. Long-term exposure to this metal is harmful to humans. Stomach ulcers, nausea, diarrhea, liver and kidney damage, and dermatitis are all possible side effects (Nickens *et al.* 2010; Rambabu *et al.* 2019). It can potentially lead to cancers of the esophagus and lungs. The most prevalent routes of chromium toxicity to living beings are inhalation, oral absorption, and skin contact. In potable water, inland surface water, and industrial wastewater, the maximum allowed amounts of Cr (VI) are 0.05, 0.1, and 0.25 mg L<sup>-1</sup>, respectively (World Health Organization 1988; Wilbur *et al.* 2012). As a result, effluent containing Cr (VI) must be treated before disposal.

For the separation and detection of Cr (VI) ions, techniques such as solvent extraction, coprecipitation, solid-phase extraction, and ion exchange have been reported (Ramnani & Sabharwal 2006; Hosseini *et al.* 2009; Sharma *et al.* 2017). One of the heavy metal removal technologies that has received far more attention than the others is the ion exchange method on chelating resin (Bajpai *et al.* 2012). For removing different heavy metals in a high-volume treatment solution, this procedure is quick and affordable. It is economically significant due to its reusability and relatively safe and energy-efficient nature (Ramnani & Sabharwal 2006). Chelating resins are ion exchangers with different functional groups, such as iminodiacetic acid (IDA), often utilized in heavy metal adsorption and recovery studies (Sharma & Forster 1994; Ramnani & Sabharwal 2006; Rafique *et al.* 2021). In the IDA chelating resins, transition metals have been shown to be more selective than alkali metals. Aside from the exchange phenomenon, this group will provide divalent metals with electron pairs in order to create a stable coordination bond. As a result, it can be considered a powerful instrument for removing metal ions from metal combinations (Sharma & Forster 1994; Ramnani & Sabharwal 2006). pH, contact time, temperature, metal ion concentration, and adsorbent dosage were utilized at varied operative circumstances in the adsorption and removal of metals from industrial effluents. Iminodiacetic acid functional adsorbents include styrene-divinylbenzene (Chelex 100, amberlite 718, and Lewatit TP 207 and 208) (Fernández *et al.* 2005; Lin & Juang 2005; Agrawal & Sahu 2006; Pehlivan & Altun 2007; Dinu *et al.* 2009; Dragan *et al.* 2009; Yu *et al.* 2009; Zainol & Nicol 2009; Ling *et al.* 2010; Rudnicki *et al.* 2014), magnetic glycidyl methacrylate (GMA) styrene-divinylbenzene (Chen *et al.* 2006), polyurethane foam (El-Shahat *et al.* 2008), and aminomethyl polystyrene (AMPS) (Liu *et al.* 2011).

In this work, we propose the application of ion exchangers as an interesting solution to remove Cr (VI) from aqueous solution.

Among these ion exchangers, the amberlite IRC 718 from Na<sup>+</sup> can be qualified as a means of removing heavy metals due to its selectivity, a macroporous low cation resin, durability, high adsorption capacity and the ease of the removal protocol in the industry.

The adsorption approach was conducted in batch by using synthetic aqueous solutions at different contact times, starting concentrations, adsorbent dosages and pH.

The current study examines the removal of Cr (VI) from aqueous solutions using Amberlite IRC-718, a macroporous low cation resin, under various laboratory settings such as starting concentration, adsorbent dosage, contact time, and pH. It should be mentioned that ion exchange for heavy metal removal is always done in batches.

## 2. MATERIALS AND METHODS

The majority of the chemicals utilized in this experiment were of analytical quality. To make potassium dichromate [K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub>] solutions acquired from PROLABO, dilutions of double deionized water (Milli-Q) are utilized (France). Rohm and Haas provided Amberlite IRC 748, a macroporous cationic exchanger chelating resin functionalized by iminodiacetic acid groups (IDA) in the hydrogen form (USA). The macro reticular composition of this resin ensures its stability in a hostile environment. Its adaptability enables it to be utilized for targeted adsorption and the removal of heavy metals from waste effluents in a wide pH range while retaining a high flow rate.

The content of metal solutions was determined using a Perkin-Elmer AAnalyst 100 (Canada) AAA type atomic absorption spectrophotometer (AAS) with an air acetylene flame. A glass electrode was used to determine the pH (Fisher Scientific Dual

Channel AR25 Canada). A batch technique was used to investigate Cr (VI) adsorption on Amberlite IRC 718. The impacts of essential parameters on removal efficiency, such as pH, Cr (VI), and resin dosage, have been investigated. The adsorption efficiency was calculated at room temperature.

## 2.1. Adsorption isotherms

Before being used to extract potential organic and inorganic pollutants or synthesis impurities, the chelating adsorbent beads were washed with 1 M NaOH, 1 M HCl, and n-hexane. It was then thoroughly rinsed three times with deionized water (ENPEC, National Company of Electrochemical Products, Algeria) before being converted to Na<sup>+</sup> by a 12-hour column flushing with 1 M NaCl (Eccles & Greenwood 1992). The resin was then rewashed in deionized water and dried at 60 °C in a vacuum oven until it was ready to use.

The solution (resin in presence of Cr(VI) solution) was agitated for a period of time at a constant temperature in batch ion exchange testing. In a beaker, batch studies were conducted using a dry resin fixed weight (0.5 g) at 25 °C, 30 ml, 19.231 mol/L Cr(VI), and 120 rpm stirring until equilibrium was established. To determine the adsorbed content of metal ions into the resin, the difference between the initial and residual concentrations of metal solution before and after the adsorption process was used. The results represent the averages of all the trials, which were conducted in pairs.

The sum of metal ions sorbed at time  $t$ ,  $Q_e$ , was calculated using the mass balance equation:

$$Q_e = \frac{(C_0 - C_e) V}{m} \quad (1)$$

Various starting metal concentrations ranging from 0.162 to 10.3 mmol/L were utilized to determine sorption isotherms at room temperature. For ion exchange studies, the resin quantity in the batch vessel was raised from 0.2 to 1 g. The shaker was set to 120 rpm to keep the resin particles in suspension. The pH was adjusted until the resin and solution were in balance. The resin was filtered to determine the Cr (VI) content after normalizing and equilibrating the pH of the solutions.

Sorption isotherms are plotted as Cr(VI) uptake vs. the amount of adsorbate left in the final equilibrium concentration of the solution. Using a Langmuir ion exchange model to compare a single sorption metal in different settings, the Cr (VI) ion capacity of resins was evaluated at 25 °C. Using 0.1 N HCl or diluted NaOH, the pH of the sample solutions was changed from 2.0 to 10. The pH of the solution was measured once equilibrium had been established.

The Cr (VI) recovery factor (%R) was calculated using the following equation:

$$\%R = \frac{(C_0 - C_e)}{C_0} \times 100 \quad (2)$$

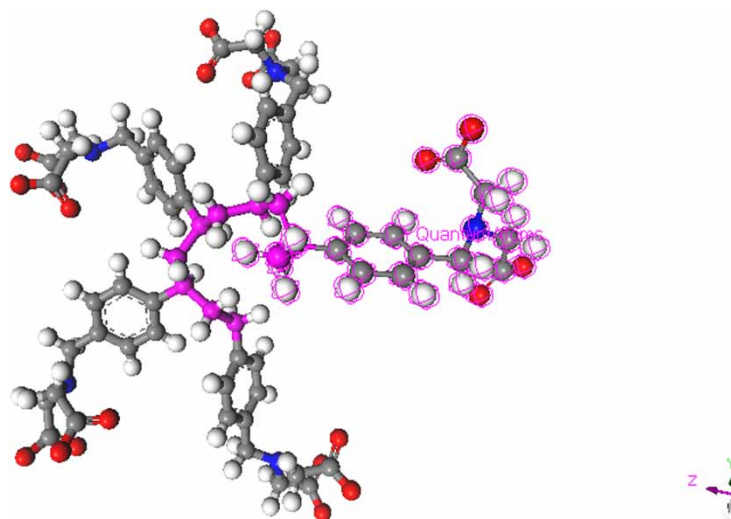
$C_0$  and  $C_e$ , in mmol L<sup>-1</sup> or mg L<sup>-1</sup>, are the initial and equilibrium metal ion concentrations in an aqueous solution;  $m$  is the weight or density of the chelating resin in grams, and  $V$  is the volume of the solution in milliliters.

The batch approach is used to record metal ion tests, which use Cr (VI) mmol per g of ion exchanger. With 0.5 g dry resin, a beaker of 50 cm<sup>3</sup> Cr(VI) ions of various concentrations was applied. The contents of the beaker were shaken for 90 minutes at room temperature to achieve balance. After filtering the solution, the Cr (VI) concentration was determined. On the ion exchanger, the isotherms were used to calculate Cr (VI) adsorbed ion levels.

## 2.2. Computational details

The QMERA module in Materials Studio<sup>®</sup> was used to perform the hybrid QM/MM calculations. This module can be used with the ChemShell (Sherwood *et al.* 2003) environment to perform integrated quantum mechanical (QM) and molecular mechanics (MM) calculations. Because QMERA combines the precision of quantum mechanics with the speed of a force field measurement, it can do accurate computations on very large systems in a short amount of time. The DMol3 (Delley 1990) force field engine is used to define the QM region, whereas the GULP (Gale 2005) force field engine is used to characterize the MM region. In all cases, hydrogen connection atoms were utilized to cap the QM region, and the total energy of the system was measured using a subtractive expression (see Figure 1):

$$E_{tot\ subtractive} = E_{QM\ (Quantum\ atoms)} + E_{MM\ (all\ atoms)} - E_{MM\ (Quantum\ atoms)} \quad (3)$$



**Figure 1** | Mechanical subtractive QM/MM scheme used in the simulations.

In this type of embedding strategy, known as subtractive mechanical, the polarization of the QM region owing to the MM region, which is not thought to be important in the system under discussion, is ignored. In this approach, the van der Waals interactions are managed using the force field method. The QM field was described in all cases using the BP exchange-correlation functional (Perdew *et al.* 1996) and a DNP basis set. In the MM region, the DREIDING (Mayo *et al.* 1990) force field was employed. The charges in the QM regions were set to be equal to (2-).

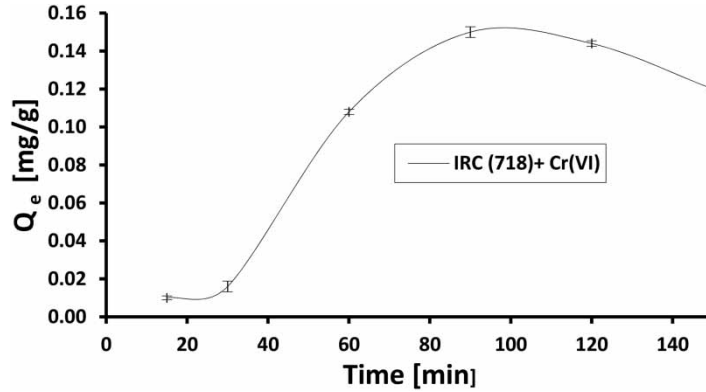
Cr(VI) adsorption on Amberlite IRC-718 was investigated using Materials Studio's Adsorption Locator tool. As the temperature is steadily decreased, the Adsorption Locator module discovers possible adsorption configurations by running Monte Carlo searches of the substrate-adsorbate system's configurational space (Simulated Annealing). To locate more local energy minima, this technique is performed numerous times. The Universal force field was utilized since Adsorption Locator offers a variety of force fields. To achieve good statistics, the calculations were carried out at the ultra-fine level, which meant that 10 Simulated Annealing cycles were performed, lowering the temperature from 10,000 to 100 K (a total of 100,000 steps per cycle).

### 3. RESULTS AND DISCUSSION

#### 3.1. Effect of time on the removal of chromium (VI)

The chelating resin Amberlite IRC 748 was examined in Cr (VI) adsorption in a non-competitive or single device using a constant resin concentration and altering the contact time at pH (6.0) and ambient temperature. As the equilibration time increased, the effect of contact time on the adsorbed ion metal content or concentration on the chelating resin increased, as shown in Figure 2. Several research articles have found a chromium adsorption capacity ( $Q_e$ ) of 0.150 mg/g within 90 minutes of the saturated plateau value (Gode & Pehlivan 2003). The sorption mechanism was unaffected by an increase in contact time, and the potential for Cr(VI) slowly grew before equilibrium was reached. As a result, in the following research, the contact interval of 90 minutes is utilized to assess the equilibrium of metal absorption at the interface. The equilibrium period was kept at 90 minutes in all future investigations since it was assumed to be sufficient for Cr (VI) ion removal by resin (Cortina *et al.* 1996; Namasivayam & Senthilkumar 1999; Namasivayam & Yamuna 1999; Bayat 2002; Dakiky *et al.* 2002; Yu *et al.* 2003).

The absorption capability of Amberlite IRC 748 against Cr (VI) ion is comparable to that of other commercially available materials such as strongly acidic polystyrene sulphonic cation exchanger and strongly simple anion exchanger (Dudzińska 1988), Amberlite IR-120 Na, Amberlite IRA-420, Lewatit MP-500A, Lewatit S 100, Pmc, YK, and MP 62 (Gode & Moral 2008). The absorption capability of Amberlite IRC 748 against Cr (VI) ion is comparable to that of other commercially available materials such as strongly acidic polystyrene sulphonic cation exchanger and strongly simple anion exchanger



**Figure 2** | Effect of contact time on Cr(VI) adsorption on the Na-form chelating resin at pH = 6 and ambient temperature (each point represents a mean of two tests).

(Dudzińska 1988), Amberlite IR-120 Na, Amberlite IRA-420, Lewatit MP-500A, Lewatit S 100, Pmc, YK, and MP 62 (Gode & Moral 2008).

### 3.2. Effect of pH

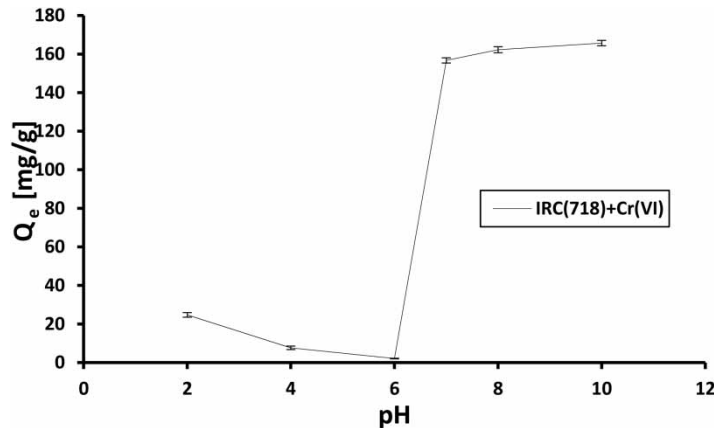
Figure 3 shows how the pH of the medium affects the uptake of Cr (VI) metal ions. As the pH rises, the dissociation of the hydroxyl group  $\text{Cr}(\text{OH})_6$ , which is suitable for cooperation with metal ions, enhances metal ion absorption.  $K_c$  can be used to compare the performance of different exchangers because experimental circumstances such as pH have a significant impact on the equilibrium constant. Metal interactions with Amberlite IRC 748 resin are expected to be dominated by adsorption and ion exchange at the same time. The ion exchange system adsorbed metal ions due to their dependence. The effect of pH on Cr (VI) ion-exchange was studied at room temperature with pH ranging from 2.0 to 10 and a metal solution concentration of 19,231 mmol/l.

Depending on the pH, the iminodiacetic acid group chelating ion exchanger exhibits significant complexing capabilities, creating heterocyclic chromium(IV)-ion chelates (Namasivayam & Senthilkumar 1999; Kotaś & Stasicka 2000).

### 3.3. Metal concentration effect on sorption isotherm

The equilibrium isotherm, also known as the relationship between the equilibrium exchanged amount ( $Q_e$ ) and the equilibrium concentration in the aqueous phase ( $C_e$ ), must be established to understand how the solutes interact with the resin, and so maximize their use (Lacour *et al.* 2001).

$C_0 = 19,231$  mmol/l and ambient temperature (each point represents a mean of two tests).



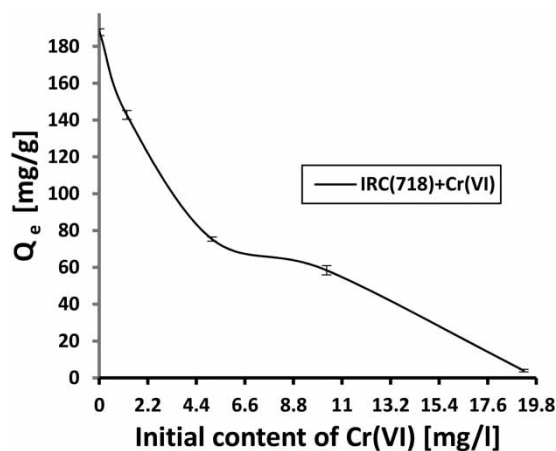
**Figure 3** | pH effect of on Cr (VI) ion exchange with chelating resin Na-form.

Plotting the initial metal content (mg/L) (mmol/L) and the metal ion adsorbed per gram of adsorbent (mmol/g) (mg/g) at equilibrium state yielded the chromium metal ion's adsorption isotherms onto the sodium type chelating resin (Figure 4). In a single non-competitive mode, the profile isotherms of Cr (VI) show a continuous decrease in the sorption of these metals at the interface. Their initial medium concentrations declined until Cr (VI) reached or exceeded 5.11 mmol/L. This figure represents the saturation of IDA functional, open groups on the resin vs. the metals of interest at the interface. The overall adsorption potential for chromium per gram of resin was 187.72 mg, with 99.64 percent metal ion recovery.

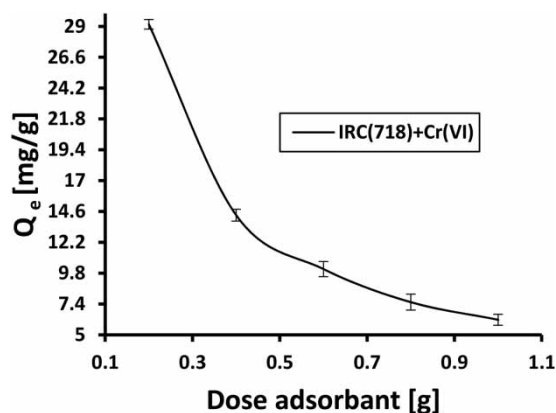
### 3.4. Effect of resin dosage

In a single non-competitive mode, Cr (VI) profile isotherms show a steady decrease in sorption of these metals at the interface. Their initial medium concentrations fell until Cr reached or exceeded 5.11 mmol L<sup>-1</sup> (VI). This value represents the saturation of IDA functional, free groups on the resin versus the metals of interest at the contact. The overall adsorption capacity per gram of resin for chromium was 187.72 mg, with 99.64 percent metal ion recovery. Increasing the adsorbent dosage enhances removal performance while lowering the ion exchange density, as can be determined. The decrease in ion-exchange density is attributable to the fact that not all ion-exchange sites are saturated throughout the sorption process. As a result, as the number of these sites grows, so does removal efficiency (Cortina *et al.* 1996).

Due to increased surface area or ion-exchange sites for a given initial solute concentration, the equilibrium concentration for a given initial Cr(VI) concentration falls with adsorbent dosages (Pradhan *et al.* 1999; Yu *et al.* 2003). A minimum resin dosage of 0.8 g of iminodiacetic resin is required for the quantitative removal of 19.231 mmol/L Cr(VI) in 30 ml.



**Figure 4** | Chelating resin sorption isotherm vs. initial Cr (VI) concentration ( $0.162 \times 10^{-3}$  to  $10.3 \times 10^{-3}$  M) at pH = 6. 0.2 g of resin, and ambient temperature (each point represents a mean of two tests).



**Figure 5** | Effect of sorbent dosage on sorption capacity of Cr(VI) (pH = 7.0; t = 90 min; T = 25 °C, C<sub>0</sub> = 19.231 mmol L<sup>-1</sup>).

#### 4. EQUILIBRIUM ADSORPTION ISOTHERMS

The thermodynamic parameters were obtained after the adsorption results fit the Langmuir isotherm equation. The Langmuir isotherm (Gode & Pehlivan 2003) describes adsorption on an utterly homogenous surface with little interaction between adsorbed molecules. According to the Langmuir phase, maximum adsorption is proportional to the saturation frequency of an adsorbate monolayer on the adsorbent surface. There is no adsorbate molecule transmigration in the surface plane, and the adsorption energy is constant (Cooney 1999).

The Langmuir isotherm is defined by the equation below.

$$\frac{C_e}{Q_e} = \frac{1}{K_L Q_{max}} + \frac{C_e}{Q_{max}} \quad (4)$$

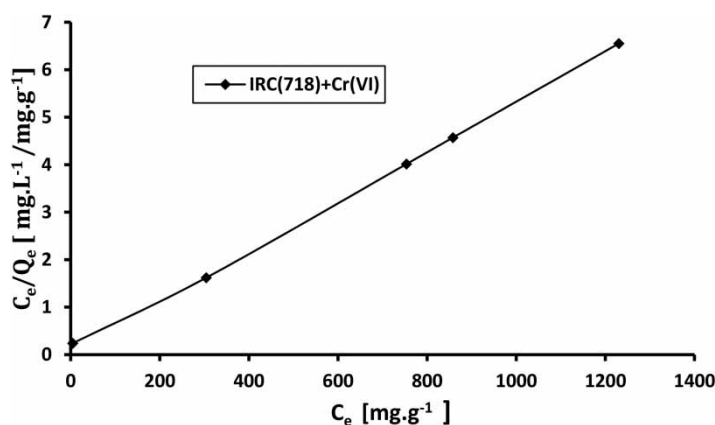
At equilibrium, the concentration of residual Cr(VI) ions in the solution is  $C_e$  ( $\text{mg L}^{-1}$ ).  $Q_e$  ( $\text{mg g}^{-1}$ ) is the mass of adsorbed chromium, while  $Q_{max}$  is the maximum adsorption capacity ( $\text{mg g}^{-1}$ ). The Langmuir constant is  $K_L$  ( $\text{L mg}^{-1}$ ).

The linear regression equation derived is  $C_e/Q_e = 0.0053 C_e + 0.018$ , with a regression coefficient ( $R^2$ ) of 0.987 (see Figure 6). The  $Q_{max}$  and  $K_L$  isotherm parameters for this equation are  $187.61 \text{ mg g}^{-1}$  and  $0.0723 \text{ Lmg}^{-1}$ , respectively.

#### 5. COMPUTATIONAL RESULTS

The highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) in a molecule are used to study chemical reactivity and kinetic stability. Electronic absorption, or the transition from the ground to the first excited state, is best demonstrated by one-electron excitation from HOMO to LUMO. As the HOMO-LUMO gap increases, the mechanism's kinetic stability improves. As a result, moving electrons from the ground state (HOMO) to the excited state (LUMO) necessitates a certain amount of energy. Table 1 shows the measured orbital energies as well as chemical characteristics for each molecule.

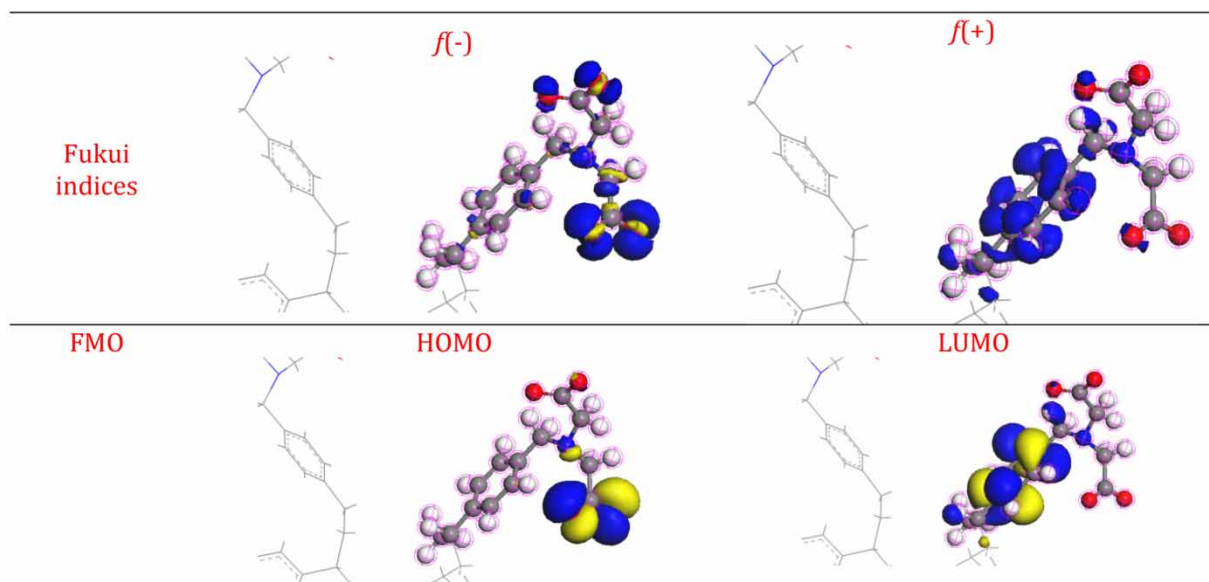
Adsorbent reactivity can be seen in the HOMO-LUMO gap (1,992 eV) and hardness (0,99 eV). The global electrophilicity index ( $\omega$ ) was established by Parr *et al.* (Parr & Pearson 1983; Parr *et al.* 1999) using thermodynamic properties to calculate the favorable change in energy when a chemical system reaches saturation by adding electrons. It is the loss of energy caused by electrons flowing from the donor (HOMO) to the acceptor (LUMO). It's also essential in determining a system's chemical



**Figure 6** | Langmuir isotherm for Cr(VI) adsorption on IRC 718 (pH = 6; t = 90 min; dosage = 0.2 g; and ambient temperature).

**Table 1** | DFT global reactivity for IRC 718

	$E_{\text{HOMO}}(\text{eV})$	$E_{\text{LUMO}}(\text{eV})$	$E_{\text{gap}}(\text{eV})$	$\mu(\text{eV})$	$\eta(\text{eV})$	$\omega(\text{eV})$
IRC 718	3.129	5.121	1.992	4.125	0.996	8.541
Cr(VI)	-151.939	-103.889	48.05	-126.914	24.05	334.868



**Figure 7** | Fukui indices with frontier molecular orbitals for the IRC 718.

**Table 2** | MCS adsorption energies ( $\text{kcal mol}^{-1}$ ) results

Total energy	Adsorption energy	Rigid adsorption energy	Deformation energy	Cr + 6 :dEad/dNI
-12.037	-12.037	-12.037	0.000	-0.421

reactivity:

$$\omega = \mu^2 / 2\eta \quad (5)$$

$$\mu = \frac{E_{HOMO} + E_{LUMO}}{2} \quad (6)$$

$$\eta = \frac{E_{LUMO} - E_{HOMO}}{2} \quad (7)$$

The high  $E_{HOMO}$  value of the molecules suggests that they have a predisposition for donating electrons to low  $E_{HOMO}$  acceptor molecules. Cr(VI) is determined to be the electron acceptor, while IRC 718 is determined to be the electron donor. The HOMO of the IRC 718 indicates a significant contribution of the two  $\text{COO}^-$  groups, as shown in Figure 7. This could be due to the IRC 718's chelating properties.

### 5.1. Adsorption

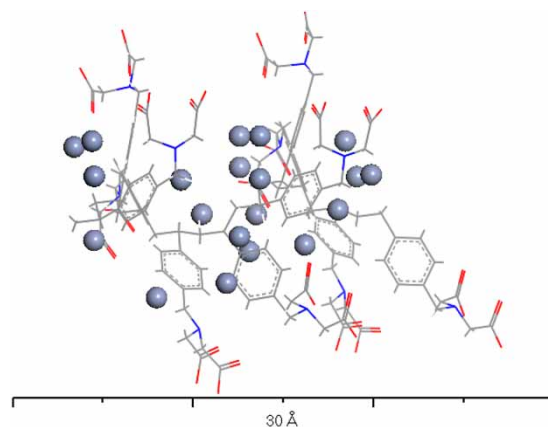
The MCS analysis (Table 2) demonstrates that IC has higher negative adsorption energy than MB, corroborating the findings as mentioned earlier. It's possible that IC molecules can adsorb preferentially and forcefully on the A-CNF/DT surface, allowing them to expel water molecules successfully.

The Cr(VI) adsorption on the IRC 718 is shown in Figure 8. Table 2 summarizes the interaction data, confirming that Cr(VI) is spontaneously adsorbed on the adsorbent. With  $-12.036 \text{ kcal mol}^{-1}$ , the interaction was found to be of the Van der Waals type (see Figure 9).

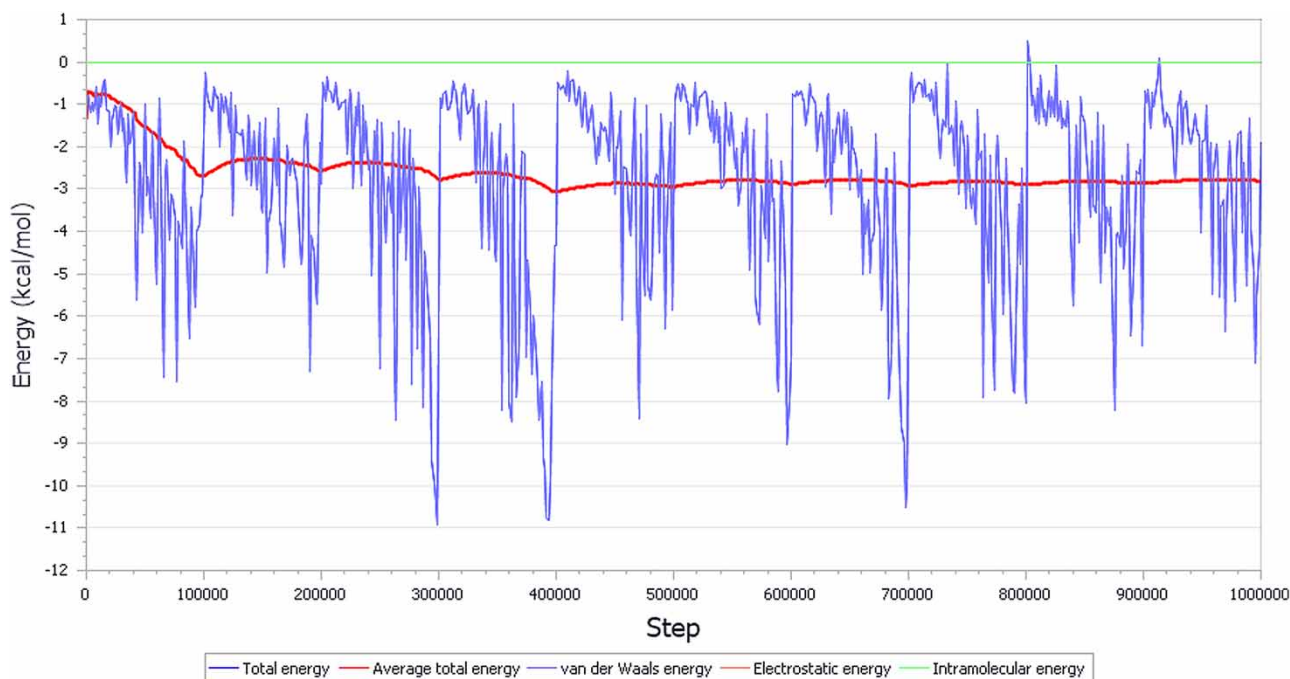
## CONCLUSION

This study aimed to investigate the sorption of chromium metal ions from artificial solutions employing a chelating polystyrene adsorbent with iminodiacetic acid groups in sodium form (Amberlite IRC 718). At ambient temperature and pH 6, the chelating resin was found to be capable of removing Cr (VI) from a single aqueous solution bearing initial metal ion





**Figure 8** | A presentation of the Cr(VI) adsorption on IRC 718.



**Figure 9** | Annealing cycles during the Monte Carlo simulations.

concentrations ranging from  $0.162 \cdot 10^{-3}$  to  $10.3 \cdot 10^{-3}$  M. With correlation coefficients of 0.987, the experimentally collected Cr(VI) adsorption findings on the chelating sorbent closely fit the Langmuir model isotherm, which gave a strong approximation of the equilibrium. According to their respective isotherm profiles, the monolayer adsorption capabilities of these ion metals at the interface were 187.72 mg/g of resin. These results demonstrated that the adsorbent is effective in extracting and recovering chromium from wastewaters. According to the theoretical investigation, the HUMO-LUMO gap (1.992 eV) and hardness (0.99 eV) demonstrate that the adsorbent is highly reactive. The electrophile index ( $\omega$ ) demonstrates that Cr(VI) is an electron acceptor, while IRC 718 is an electron giver. The MCS analysis supports Cr(VI) adsorption on IRC 718 as a strong Van Der Waals preferential adsorption and efficiently expels water molecules.

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## DATA AVAILABILITY STATEMENT

All relevant data are included in the paper or its Supplementary Information.

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