

# Equilibrium, Thermodynamic, and Density Functional Theory Modeling Studies for the Removal of Dichromate Ions from Wastewater Using Calix[4]arene Modified Silica Resin

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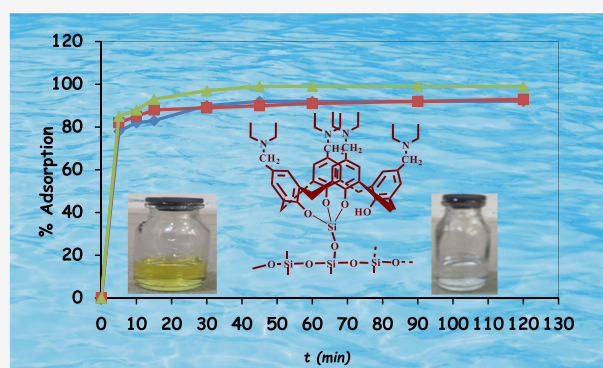


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Supporting Information

**ABSTRACT:** Water is contaminated by different toxicants such as anions, cations, and organic waste products. In this regard, this study reveals the removal of  $\text{Cr}_2\text{O}_7$  ions from water using calix[4]arene modified silica (CMS) resin under the optimized conditions of concentration, pH, resin dosage, and effects of temperature. During the experiments, it was noticed that the adsorption of  $\text{Cr}_2\text{O}_7$  ions onto CMS resin is highly pH-dependent and has high adsorption capacity using only 25 mg of resin. The adsorption equilibrium data have been subjected to different isotherm models such as Langmuir, Freundlich, and Dubinin–Radushkevich (D-R). From the results, it has been observed that the Freundlich model is the best fit for an adsorption phenomenon as compared to the Langmuir model, while the D-R model demonstrates that the adsorption is an ion exchange type according to the values of  $E$  (kJ/mol). The thermodynamic study reveals that the values of  $\Delta H$ ,  $\Delta G$ , and  $\Delta S$  show that the adsorption process is endothermic and spontaneous. Dichromic acid ( $\text{H}_2\text{Cr}_2\text{O}_7$ ) and its conjugated base ( $\text{Cr}_2\text{O}_7^{2-}$  anion) were optimized at the B3LYP/LANL2DZ/6-311++G(d,p) level by using G09W software to analyze the adsorbate-adsorbent interaction mechanism. The efficiency and adsorption capacity of CMS resin have also been checked on real wastewater collected samples.



## 1. INTRODUCTION

Wastewater might be contaminated by different toxicants such as inorganic ions, organic dyes, and pesticides that may produce several diseases in humans.<sup>1–3</sup> Among different inorganic ions, chromium is one of the highly toxic metal ions and known as a major water pollutant due to its uses in the electroplating process, metal finishing, leather tanning, and chromate synthesis.<sup>4–7</sup> Chromium exists in two forms in water Cr(VI) and Cr(III). Cr(VI) is present in acidic media while Cr(III) in basic media.<sup>8,9</sup> Cr(VI) is highly soluble in water, and its oxidation potential shows hazardous properties.<sup>10</sup> According to the EPA and WHO, the maximum discharge limit of  $\text{Cr}^{+6}$  from industrial effluents is less than 1 mg/L and in potable is 0.05 mg/L.<sup>11</sup> Therefore, chromium contamination in wastewater should be monitored very carefully.

Due to the various toxic effects of chromium, it is very crucial to remove it from wastewater using an efficient method that is low-cost along with a better % recovery. Previously, precipitation, electrolytic reduction, ion exchange, adsorption, and membrane separation techniques were utilized for decontamination of chromium from wastewater.<sup>12–14</sup> Among all other techniques, adsorption is convenient for the removal of chromium from wastewater because it is a simple setup,

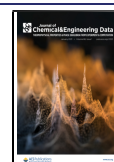
economical, and easy to operate.<sup>15–18</sup> Different adsorbent materials such as zeolite, clay, magnetic nanoparticles, and some natural cheaper adsorbents have been used, but they have low adsorption capacities and less selectivity.<sup>19–21</sup> Therefore, adsorbent materials with high capacity, selectivity, and reusability are known as desired adsorbent materials for adsorption.<sup>22,23</sup>

Silica gel is a very stable adsorbent and has good mechanical as well as thermal stabilities. The silanol groups are present on the silica surface, which are weak ion exchangers. In an acidic medium, these groups are protonated, which reduces their adsorption capacity up to zero. In basic pH, hydrolysis of OH groups takes place. Therefore, the surface of silica has been formed to get solid adsorbents with higher adsorption capacity as well as selectivity. Therefore, organic moieties are loaded

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onto silica gel, affording a higher adsorption capacity, stability, and selectivity. In this regard, supramolecular chemistry has introduced new paths for the preparation of synthetic materials that act as a host for different toxic metals, anions, drugs, and dyes for their recognition.<sup>24</sup> Among all the supramolecular hosts, calixarenes have gotten more attention due to their ease of functionalization, size of the cavity, and simple large-scale synthesis.<sup>25,26</sup> The calixarenes are cyclic oligomers comprising phenol and methylene units. Calixarenes are very attractive and excellent cavities that may provide a platform for chemical bonding of different functional groups to introduce a host molecule for the selective attraction of cationic/anionic and organic species. Calixarenes have lower and upper rims that can be modified by different organic moieties and polymeric matrices for the preparation of selective, thermally stable, and regenerable adsorbents [1–10]. Previously, different researchers have modified the silica surface with calix[4]arene moieties. *p*-*tert*-Butylcalix[4]arene was chemically immobilized onto silica and used for the removal of dye-contaminated wastewater.<sup>27</sup> Similarly, *p*-*tert*-butylcalix[8]arene-based silica resin was used for the adsorption of azo dyes from wastewater samples.<sup>28</sup> *p*-Morpholinomethylcalix[4]arene-based silica resin was prepared and used for extraction of copper metal ions by selective online solid-phase extraction of copper.<sup>29</sup> The calix[4]arene-based compounds have been applied onto many other polymeric matrices such as Amberlite XAD-4, Merrifield resin, etc. as to prepare selective and regenerable adsorbents. *p*-Tetrathioarecalix[4]arene has been synthesized and appended onto Merrifield resin for the removal of Pb metal ions from water samples.<sup>30</sup> Similarly, piperidine-functionalized calix[4]arene was appended onto Merrifield resin for the removal of perchlorate ions from water. In addition to this, the two novel polymeric materials, namely, 25,27-bis(*n*-octyloxy)calix[4]arene-crown-6 (BnOCalix[4]-C6)/SiO<sub>2</sub>-P and 25,27-bis(*i*-octyloxy)calix[4]arene-crown-6 (BiOCalix[4]C6)/SiO<sub>2</sub>-P, were synthesized and applied for the adsorption of Na, K, Rb, Cs, Sr, Ba, La, Y, Pd, Ru, Zr, and Mo ions.<sup>31</sup> Another study was performed using a novel macro porous silica-calix[4]arene-crown polymeric composite for the adsorption of alkali and alkaline metal ions.<sup>32</sup> Moreover, the *p*-piperidinomethylcalix[4]arene-attached silica resin was used for the removal of Cu and Pb metal ions from water.<sup>33</sup> In this study, diethylamine-functionalized calix[4]arene was synthesized and attached onto silica resin. The synthesized resin was applied for the treatment of chromium-contaminated water through an adsorption procedure. The synthesized resin has high adsorption capabilities due to the presence of active moieties onto the surface and has high stability due to the polymeric silica gel support.

## 2. EXPERIMENTAL SECTION

**2.1. Materials and Methods.** The pH of the K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub> solution has been adjusted using 0.1 M solution of HCl/NaOH and determined on a pH meter (781-pH/Ion meter, Metrohm, Herisau, Switzerland) having a glass electrode and an internal reference electrode. The equilibrium concentration of K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub> solution was analyzed by a UV–Vis spectrophotometer (Agilent Cary 100). All the reagents used (Table 1) in experiments were of GR grade. Stock standard solution (0.1 M) was prepared using K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub> (Sigma-Aldrich). All glasswares were washed with water, and for further decontamination, they were saturated in 1 M HNO<sub>3</sub> and finally rinsed with deionized water.

**Table 1. List of Chemicals**

name of chemical/reagent	supplier	% purity
K <sub>2</sub> Cr <sub>2</sub> O <sub>7</sub>	Fluka: CAS no. 60200	99.0%
dichloromethane	Supelco: CAS no. 0000075092	99.8%
chloroform	SAFC: CAS no. 0000067663	99.8%
4- <i>tert</i> -butylphenol	Sigma: CAS no. 0000098544	99%
formaldehyde (37%) solution	SAFC: CAS no. 0000050000	5–10% stabilizers
sodium hydroxide	Sigma: CAS no. 0001310732	99%
toluene	Merck: CAS no. 0000108883	99.8%

**2.2. Synthesis.** All the compounds shown in Figure 1 were synthesized by following reported methods.<sup>34–36</sup> The synthesized compounds were characterized by FTIR, SEM, TGA, and BET techniques, and results are given in Figures S1–S4, respectively.<sup>36</sup>

**2.3. Adsorption Study.** The batch methodology was performed for the adsorption of Cr<sub>2</sub>O<sub>7</sub><sup>2-</sup> on CMS resin. K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub> solution (10 mL) (2.5 × 10<sup>-5</sup> mol/L) was poured into a 25 mL flask and added with a fixed amount of CMS resin. The reaction mixture was equilibrated for 60 min onto the mechanical shaker and then filtered through filter paper. The remaining concentration of K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub> solution was analyzed by a UV–Visible spectrophotometer using eq 1, while the adsorption capacity (*q<sub>e</sub>*) of CMS resin was calculated by eq 2. During the adsorption process, the effects of pH, CMS resin dosage, and temperature were optimized. All experiments were conducted in triplicate with average results reported, and the measured adsorption data (including uncertainties) are listed in the Supporting Information (Tables S1–S7).

$$\% \text{adsorption} = \frac{C_i - C_f}{C_i} \times 100 \quad (1)$$

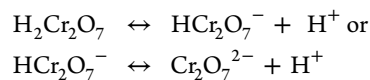
$$q_e = \frac{(C_i - C_e)V}{m} \quad (2)$$

In eq 1, *C<sub>i</sub>* and *C<sub>f</sub>* (mol/L) show the initial and final concentrations of K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub> solution. In eq 2, *C<sub>e</sub>* is the equilibrium concentration. The real wastewater samples were collected from the local industrial zone, and the total chromium was determined through an EPA standard method.

## 3. RESULTS AND DISCUSSION

### 3.1. pH Effect on the Adsorption of Dichromate Ions.

The pH has a very important role for adsorption of dichromate ions on CMS resin as it is concerned with the binding site interaction phenomenon. It is clear in Figure 2 that the adsorption of dichromate is higher at acidic pH because at this stage, K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub> is converted into H<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub>, and after its ionization in water, its form is changed as shown in the following chemical equation<sup>24</sup> (Table S1).



**3.2. Effect of Adsorbent Dosage.** Adsorbent dosage is a very important parameter that is concerned with the ability and capacity of any adsorbent material. Thus, the effect of

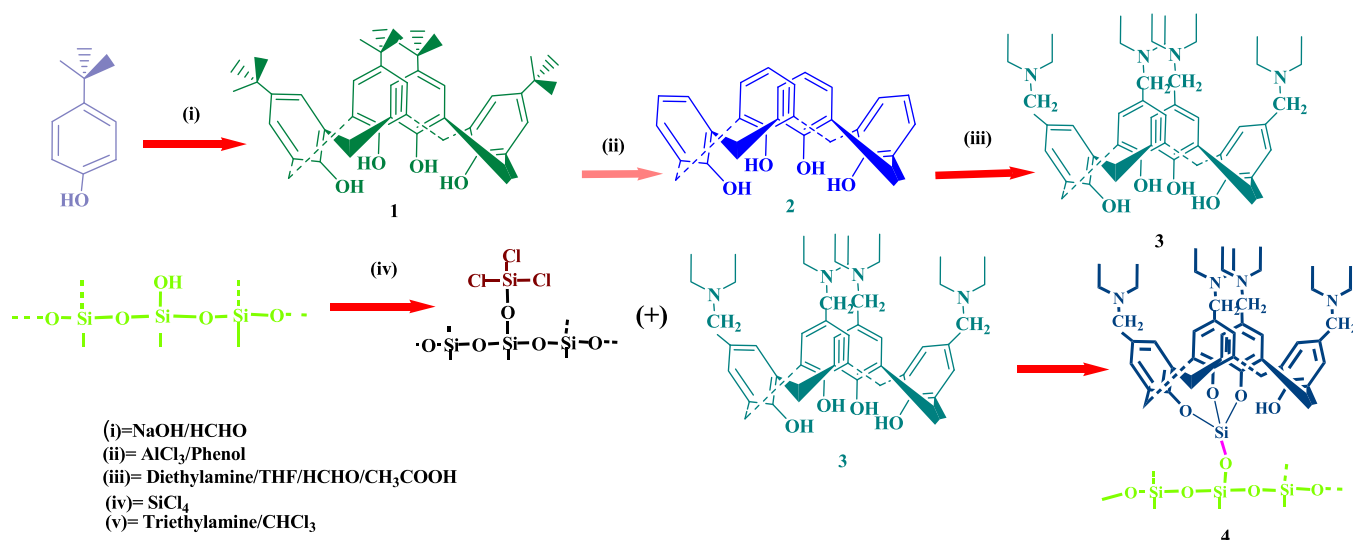


Figure 1. Synthesis route of CMS resin.

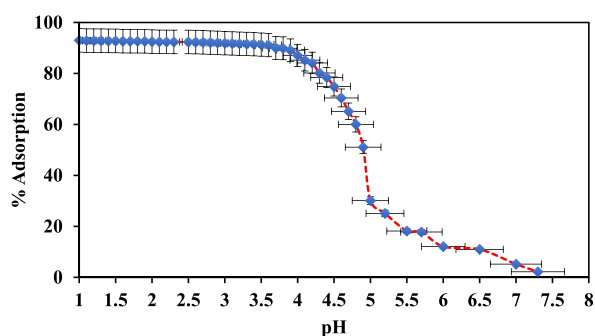


Figure 2. Effect of pH on the adsorption of dichromate ions (25 mg of CMS resin in 10 mL of dichromate solution with a concentration of  $2.5 \times 10^{-5}$  mol/L, 60 min contact time, and 298 K).

adsorbent dosage on the adsorption of dichromate ions from water samples is shown in Figure 3, in which the adsorption percentage increases with increasing CMS resin dosage due to more surface area with more binding sites with chromate ions. Hence, maximum adsorption percentage (99.13%) was achieved at 25 mg of CMS resin, further increasing CMS resin dosage has no significant effect on adsorption percentage due to the complete saturation of binding sites with

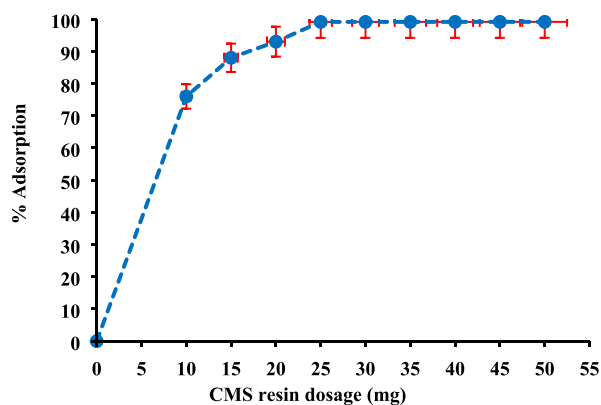


Figure 3. Effect of CMS resin dosage on % adsorption of dichromate ions from water (10 mL of dichromate solution with a concentration of  $2.5 \times 10^{-5}$  mol/L, 60 min contact time, 2.0 pH, and 298 K).

dichromate ions, and there is no further concentration of dichromate ions in solution; so, that is why further addition of adsorbents does not affect adsorption percentage. Previously, 94.42% chromate ions were removed from water using 100 mg of 25,27-bis-(*N,N*-dimethyl-2-aminoethyl)carbonyl-methoxy-26,28-dihydroxycalix[4]arene-based XAD-4 resin.<sup>37</sup> Another study has been performed for the adsorption of dichromate ions using calix[4]arene-attached XAD-4 resin, and the maximum 97.12% dichromate ions have been removed from water using 75 mg of resin.<sup>24</sup> Herein, the maximum 99.13% adsorption was achieved using only 25 mg of CMS resin; therefore, all further experiments were processed using 25 mg of CMS resin (Table S2).

**3.3. Adsorption Isotherms.** The adsorption isotherm defines the behavior of an adsorbate during an adsorption phenomenon. Therefore, the adsorption equilibrium data was subjected to the Langmuir, Freundlich, and D-R adsorption isotherm models to validate the equilibrium data.

The Langmuir adsorption isotherm (eq 3) assumes monolayer surface adsorption, all adsorption is on equivalent sites, and only one molecule thickness.

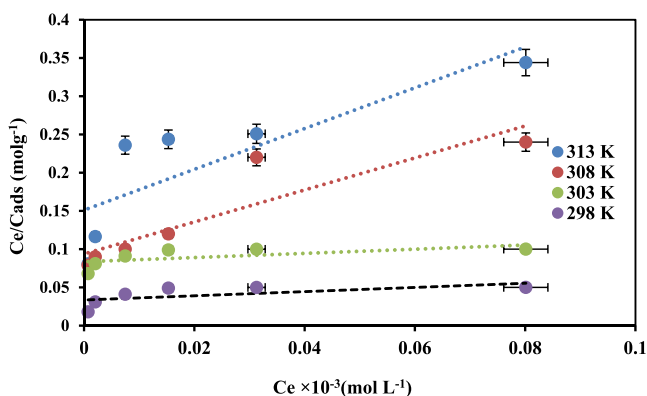
$$\left(\frac{C_e}{C_{\text{ads}}}\right) = \left(\frac{1}{Qb}\right) + \left(\frac{C_e}{Q}\right) \quad (3)$$

In eq 3,  $C_{\text{ads}}$  is the adsorbed concentration of dichromate ions (mol/g), while  $C_e$  is the equilibrium concentration.  $Q$  is the maximum amount of adsorbed dichromate ions, which imply the monolayer formation on the adsorbent surface, and  $b$  is a Langmuir constant, which defines the binding energy of the solute.

Applying Langmuir model eq 3, the graph has been plotted between  $C_e/C_{\text{ads}}$  versus  $C_e$ , as shown in Figure 4 (Table S3); from the slope and intercept values,  $Q$  and  $b$  were obtained and are given in Table 2.

The  $R_L$  is the characteristic of the Langmuir isotherm model, which is a separation factor, describing the type of Langmuir isotherm. The  $R_L$  is a dimensionless constant that can be calculated using eq 4.

$$R_L = \frac{1}{(1 + bc_i)} \quad (4)$$



**Figure 4.** Langmuir isotherm (conc. of  $2 \times 10^{-7}$  to  $2.5 \times 10^{-5}$  mol/L, 25 mg of CMS resin per 10 mL of adsorbate with 60 min shaking time, 2.0 pH, and 298–313 K).

**Table 2.** Langmuir Isotherm Parameters

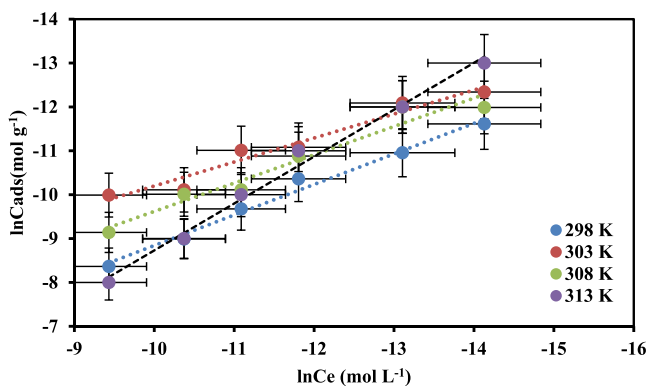
temperature	$Q$ (mmol/g)	$b$	$R_L$	$R^2$
298	366	17.26	0.81–0.99	0.862
303	375	18.34	0.89–0.99	0.813
308	477	18.91	0.87–0.99	0.881
313	510	91.99	0.88–0.99	0.878

In this equation,  $b$  is the Langmuir constant, and  $C_i$  is the initial concentration of dichromate ions. Therefore, the  $R_L$  value calculated for dichromate ions was between 0.812 and 0.980, which indicates favorability ( $0 < R_L < 1$ ) of the Langmuir isotherm.

The Freundlich adsorption isotherm mentioned in eq 5 below describes the multilayer formation on the adsorbent surface. This adsorption isotherm deals with the adsorption sites that are distributed exponentially with respect to the heat of adsorption.

$$\log C_{\text{ads}} = \log A + \left(\frac{1}{n}\right) \log C_e \quad (5)$$

In this equation,  $A$  and  $1/n$  describe the Freundlich constants representing the adsorption capacity and adsorption intensity, obtained from the slope and intercept of the graph  $\ln C_{\text{ads}}$  versus  $\ln C_e$  (Figure 5) given in Table 3. The values of  $1/n < 1$  are mentioned in Table 3 showing that the dichromate ions were favorably adsorbed, while the value of  $A$  at lower



**Figure 5.** Freundlich isotherm (conc. of  $2 \times 10^{-7}$  to  $2.5 \times 10^{-5}$  mol/L, 25 mg of CMS resin per 10 mL of adsorbate with 60 min shaking time, and 2.0 pH at 298–313 K).

**Table 3.** Freundlich Isotherm Parameters

temperature	$A$ (mg g <sup>-1</sup> )	$1/n$	$R^2$
298	13.45	0.545	0.985
303	14.21	0.643	0.959
308	14.71	0.681	0.978
313	15.17	0.74	0.989

concentration suggests that CMS resin has high uptake of dichromate ions (Table S4).

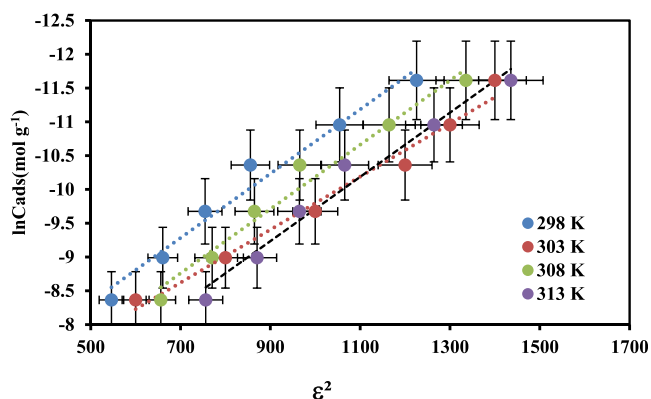
The Dubinin–Radushkevich (D-R) model given in eq 6 describes the Polanyi potential theory. The Polanyi potential equation demonstrates the mechanism of adsorption in micropores through pore filling rather than layer-by-layer surface exposure.

$$\ln C_{\text{ads}} = \ln X_m - \beta \varepsilon^2 \quad (6)$$

where  $\varepsilon = RT \ln(1 + 1/C_e)$ ,  $C_{\text{ads}}$  shows the amount of dichromate adsorbed, and  $C_e$  is the equilibrium concentration (Table S5).  $X_m$  and  $\beta$  are D-R model constants given in Table 4 obtained from the values of Figure 6. The D-R model can

**Table 4.** D-R Isotherm Parameters

temperature	$X_m$ (mmol/g)	$E$ (kJ/mol)	$R^2$
298	2.66	10.20	0.972
303	3.87	10.54	0.974
308	4.19	11.32	0.981
313	5.09	11.87	0.987



**Figure 6.** D-R isotherm (conc. of  $2 \times 10^{-7}$  to  $2.5 \times 10^{-5}$  mol/L, 25 mg of CMS resin per 10 mL of adsorbate with 60 min shaking time, and 2.0 pH at 298–313 K).

also provide information of the mean free energy  $E$  (kJ/mol) of adsorption per molecule when the adsorbate molecule is moved to the surface of the adsorbent. The mean energy  $E$  (kJ/mol) can be calculated using eq 7.

$$E = \frac{1}{\sqrt{-2\beta}} \quad (7)$$

The abovementioned parameter provides knowledge that the adsorption mechanism is chemical, ion exchange, or physical depending upon the values of  $E$ , such that if the value of  $E$  is 0–8 or 8–16, then the adsorption is physical or chemical adsorption, respectively. In our present data, the value of  $E$  is between 8 and 16 kJ/mol and assumes that the process is chemical ion exchange.



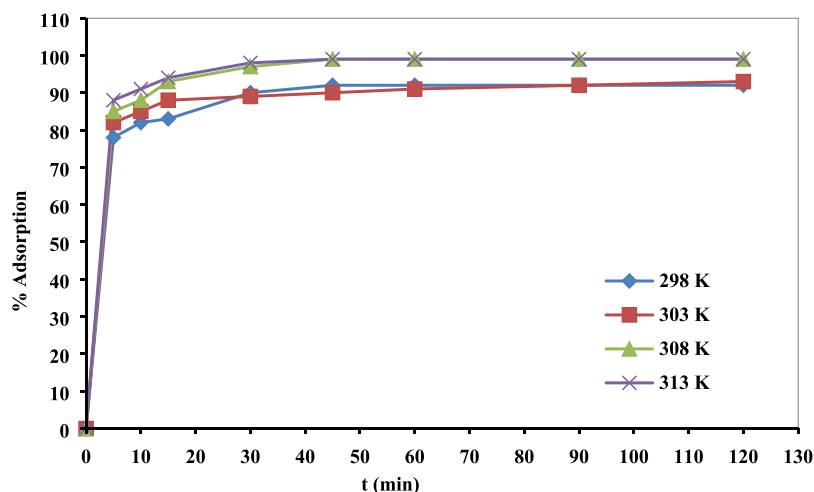


Figure 7. Adsorption of dichromate on CMS resin as a function of time at varying conditions of temperature.

**3.4. Thermodynamic Study.** Adsorption of dichromate ions onto CMS resin was checked at varying conditions of temperatures and time given in Figure 7 (Table S6), which shows that the adsorption percentage increases with increasing the temperature.

From the plot of  $\ln k_c$  versus  $1/T$  (Figure 8), the values of  $\Delta H$  (kJ/mol),  $\Delta S$  (kJ/mol/K), and  $\Delta G$  (kJ/mol) were obtained by applying eqs 8 and 9.

$$\ln k_c = \frac{-\Delta H}{RT} + \frac{\Delta S}{R} \quad (8)$$

$$\Delta G = -RT \ln k_c \quad (9)$$

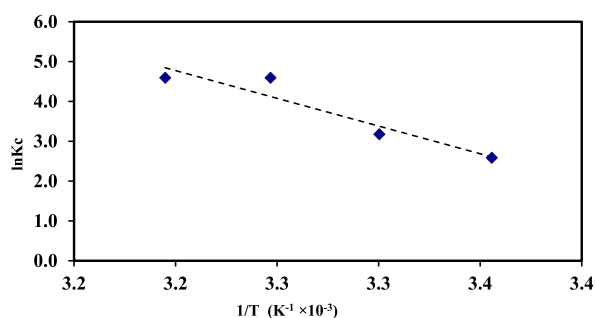


Figure 8. Arrhenius plot of the adsorption of dichromate on CMS resin.

The calculated thermodynamic parameters such as  $\Delta H$  (kJ/mol),  $\Delta S$  (kJ/mol/K), and  $\Delta G$  (kJ/mol) are given in Table 5. The obtained values of  $\Delta G$  describe the feasibility and spontaneity of the adsorption process, the values of  $\Delta H$  show the endothermic process, and  $\Delta S$  reveals that there is good affinity of dichromate ions toward CMS resin.

**3.5. Kinetics Study.** The adsorption of dichromate ions onto CMS resin was studied in terms of the kinetic model. In

this regard, the pseudo first and second order kinetic models were applied to check the adsorption mechanism. The pseudo first order kinetic model is given in eq 10 and was applied onto equilibrium data.

$$\ln(q_e - q_t) = \ln q_e - k_1 t \quad (10)$$

where  $q_t$  and  $q_e$  (mol g<sup>-1</sup>) show the adsorbed quantity of dichromate ions at time  $t$  and equilibrium, while  $k_1$  (min<sup>-1</sup>) is the pseudo first order rate constant. Applying eq 10, the graph has been plotted between  $\ln(q_e - q_t)$  vs  $t$  given in Figure S5; from the slope and intercept, the values of  $q_e$  and  $k_1$  have been calculated and are given in Table 6.

The pseudo second order kinetic model (eq 11) was applied, and the graph is plotted between  $t/q_t$  (mol/g) and time in Figure S6. From the slope and intercept, the values of  $q_e$  and  $k_2$  were obtained and are mentioned in Table 6. It is noticed that experimental data follows the pseudo second order kinetic model very well as compared to the pseudo first order kinetic model.

$$\frac{t}{q_t} = \left( \frac{t}{k_2 q_e^2} \right) + \left( \frac{1}{q_e} \right) \quad (11)$$

**3.6. Reusability Experiment of CMS Resin.** The reusability of CMS resin was checked in order to realize the economic benefits as well as its stability. Therefore, the recycling experiments have been performed as shown in Figure 9 that a total of 10 cycles of adsorption were carried out by washing CMS resin with 25 mL of 0.01 M solution of NaOH and then deionized water. Results show that the reusability of CMS resin remains almost the same, which indicates that CMS resin is suitable for cyclic adsorption of chromium ions. After recycling, CMS resin has been characterized by FTIR to check the stability of CMS resin given in Figure S7 in which the spectrum (a) before usage and the spectrum (b) after using 10 cycles are shown.

Table 5. Thermodynamic Parameters for Adsorption of Chromate Ions onto CMS Resin

$\Delta H$ (kJ/mol)	$\Delta S$ (kJ/mol/K)	$\Delta G$ (kJ/mol)			
		298 K	303 K	308 K	313 K
0.152	0.531	-6.41	-8.00	-11.76	11.95
		$\ln k_c = 2.6$	$\ln k_c = 3.2$	$\ln k_c = 4.6$	$\ln k_c = 4.6$

Table 6. Comparison of Pseudo First and Second Order Kinetic Models

T (K)	pseudo first order kinetic model			pseudo second order kinetic model		
	$K_1$ (min <sup>-1</sup> )	$q_e$ (mol g <sup>-1</sup> )	$R^2$	$K_2$ (g mol <sup>-1</sup> min <sup>-1</sup> )	$q_e$ (mol g <sup>-1</sup> )	$R^2$
298	0.0501	0.078	0.221	60.11	0.337	0.998
303	0.0450	0.085	0.273	185.91	0.677	0.997
308	0.0231	0.036	0.136	223.73	0.772	0.989
313	0.0550	0.045	0.232	281.91	0.829	0.991

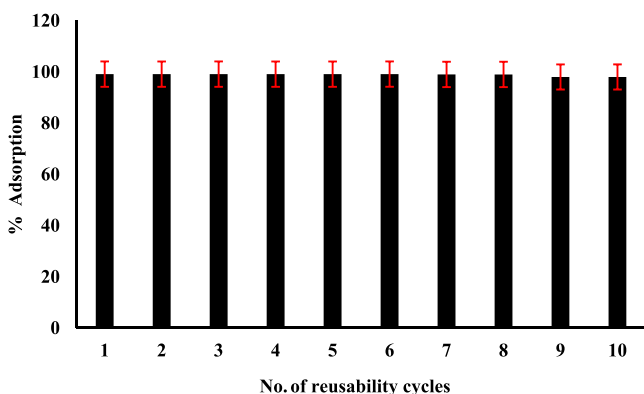


Figure 9. Reusability of CMS resin.

**3.7. Wastewater Samples.** The efficiency of CMS resin was checked by applying real wastewater samples from industrial effluents. The wastewater samples were collected from leather industries of Karachi, Sindh, Pakistan. Results show that the 25 mg of CMS resin is enough to remove above 90% dichromate ions from wastewater samples shown in Table 7.

Table 7. The % Removal of Dichromate Ions from Wastewater Samples

sample	concentration mol/L before adsorption	concentration mol/L after adsorption	% adsorption
1	$3.14 \times 10^{-7}$	$3.10 \times 10^{-8}$	90.12
2	$4.08 \times 10^{-7}$	$1.10 \times 10^{-7}$	73.03
3	$5.10 \times 10^{-7}$	$4.10 \times 10^{-8}$	91.96

#### 4. DFT CALCULATIONS

Dichromic acid ( $\text{H}_2\text{Cr}_2\text{O}_7$ ) and its conjugated base ( $\text{Cr}_2\text{O}_7^{2-}$  anion) were optimized at the B3LYP/LANL2DZ/6-311++G(d,p) level<sup>38,39</sup> by using G09W<sup>40</sup> software. In addition, the physicochemical quantities and reactivity tendencies were evaluated after the structure verification of both compounds. Based on the Koopmans theorem,<sup>41</sup> the HOMO and LUMO energies were used for predicting of the ionization energy and proton affinity as given below

$$I = -E_{\text{HOMO}}$$

$$A = -E_{\text{LUMO}}$$

In addition, the DFT-based reactivity identifiers<sup>42–46</sup> were calculated by using eqs 12–15 as follows

$$\chi = -\frac{I + A}{2} \quad (12)$$

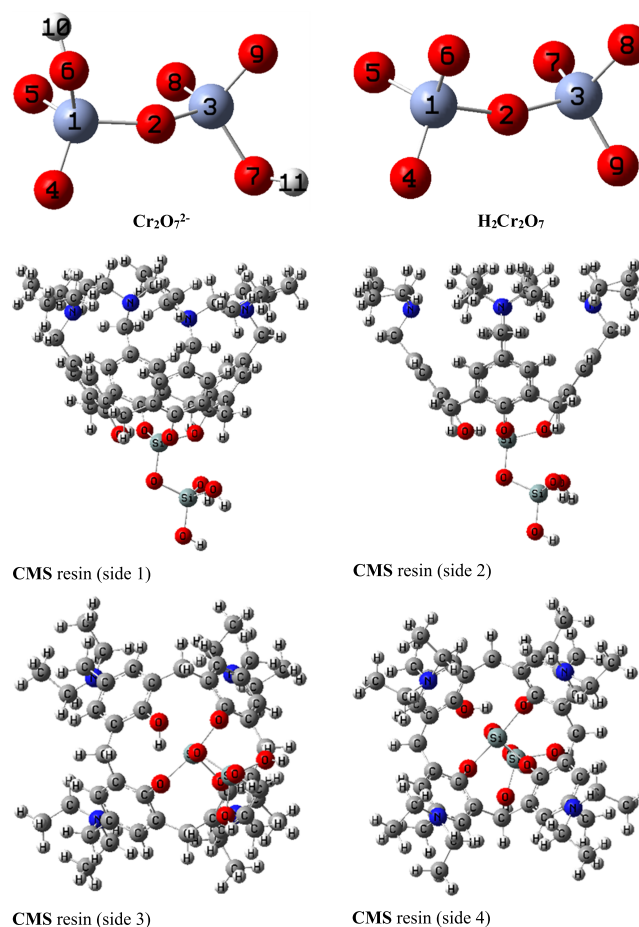
$$\eta = \frac{I - A}{2} \quad (13)$$

$$\omega = \frac{\mu^2}{2\eta} \quad (14)$$

$$\Delta N_{\text{max}} = \frac{I + A}{2(I - A)} \quad (15)$$

Here,  $\chi$  is the electronic chemical potential,  $\eta$  is global hardness,  $\omega$  is the electrophilicity index, and  $\Delta N$  is the maximum charge transfer index.

The optimized structures of both  $\text{H}_2\text{Cr}_2\text{O}_7$  and  $\text{Cr}_2\text{O}_7^{2-}$  are shown in Figure 10, and the calculated physicochemical and

Figure 10. Optimized structures of  $\text{Cr}_2\text{O}_7^{2-}$ ,  $\text{H}_2\text{Cr}_2\text{O}_7$ , and CMS resin at the B3LYP/LANL2DZ/6-311++G(d,p) level.

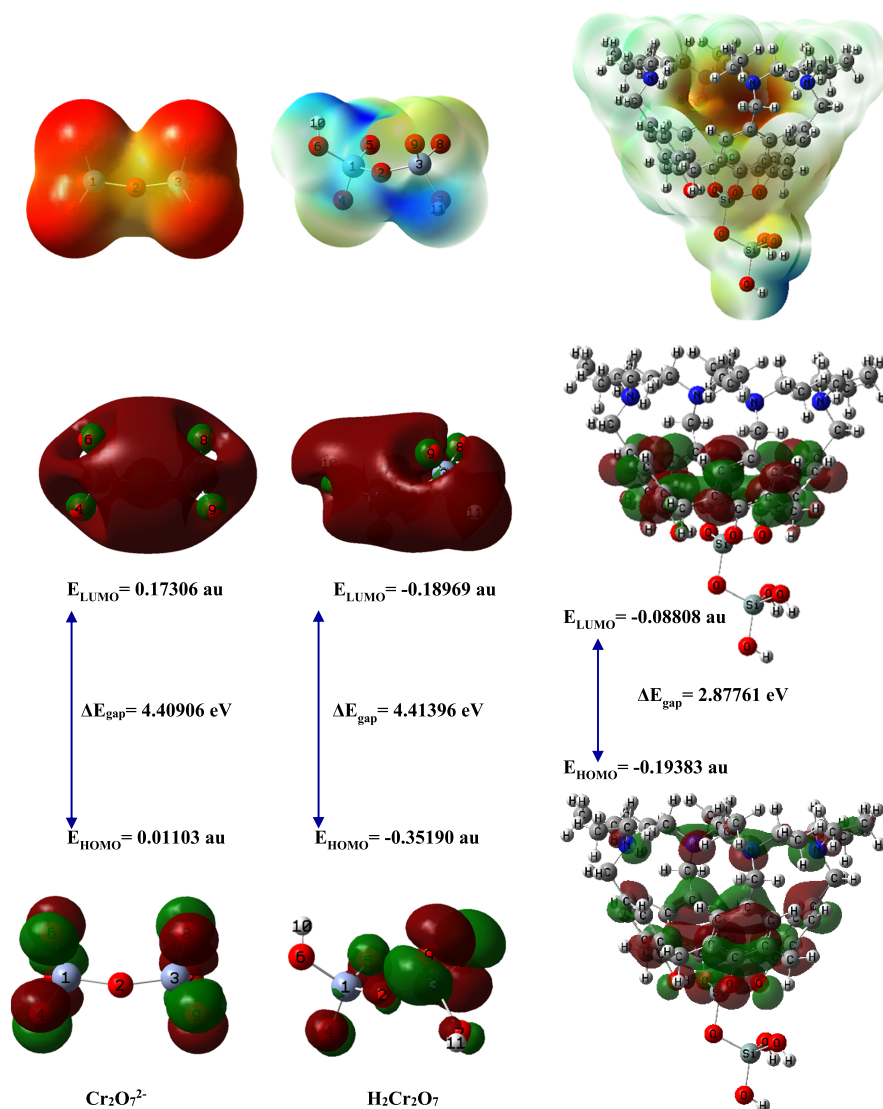
quantum chemical values are given in Table 8. Accordingly, the thermal energies of  $\text{Cr}_2\text{O}_7^{2-}$  and  $\text{H}_2\text{Cr}_2\text{O}_7$  compounds were calculated to be 21.271 and 35.956 kcal/mol, respectively. As expected, the heat capacity and entropy quantities (cal/mol/K) of  $\text{Cr}_2\text{O}_7^{2-}$  and  $\text{H}_2\text{Cr}_2\text{O}_7$  compounds were calculated in the tendency of  $32.391 < 37.390$  and of  $106.547 < 109.646$ , which should be noted that the heat capacity and entropy of the

**Table 8. The Physicochemical and Quantum Chemical Quantities of  $\text{Cr}_2\text{O}_7^{2-}$ ,  $\text{H}_2\text{Cr}_2\text{O}_7$ , and Calix[4]arene Compounds at the B3LYP/LANL2DZ/6-311++G(d,p) Level**

	$\text{Cr}_2\text{O}_7^{2-}$	$\text{H}_2\text{Cr}_2\text{O}_7$	CMS resin
$H$ (-I)	0.01103	-0.35190	-0.19383
$L$ (-A)	0.17306	-0.18969	-0.08808
$\Delta E$ (L-H)	4.40906	4.41396	2.87761
$\mu$	2.50467	-7.36871	-3.83558
$\eta$	2.20453	2.20698	1.43880
$\omega$	1.42284	12.30140	5.11248
$\Delta N_{\text{max}}$	-1.13615	3.33882	2.66582
DM (debye)	0.16541	2.14206	4.39571
$\alpha$ (au)	111.06700	96.80467	
$\Delta E$ (au)	-699.451187	-700.549773	-3270.492317
$\Delta H$ (au)	-699.440225	-700.537633	
$\Delta G$ (au)	-699.490849	-700.589729	
$\Delta E_{\text{thermal}}$ (kcal/mol)	21.271	35.956	
$C_v$ (kcal/mol/K)	32.391	37.390	
$S$ (kcal/mol/K)	106.547	109.646	

acidic form ( $\text{H}_2\text{Cr}_2\text{O}_7$ ) are calculated higher than those of the base form ( $\text{Cr}_2\text{O}_7^{2-}$ ). From Table 6, the electron delocalization possibility of  $\text{Cr}_2\text{O}_7^{2-}$  ions is higher than that of the  $\text{H}_2\text{Cr}_2\text{O}_7$  molecule because of the ordering of  $\Delta E$  as  $\text{Cr}_2\text{O}_7^{2-}$  (4.40906 eV) <  $\text{H}_2\text{Cr}_2\text{O}_7$  (4.41396 eV). As expected, the electronic chemical potential of  $\text{H}_2\text{Cr}_2\text{O}_7$  (-7.36871 eV) is lower than that of  $\text{Cr}_2\text{O}_7^{2-}$  (2.50467 eV), which demonstrates that the acidic compound is more stable than its conjugated base form. It is clear that  $\text{Cr}_2\text{O}_7^{2-}$  (2.20453 eV) is softer than  $\text{H}_2\text{Cr}_2\text{O}_7$  (2.20698 eV). Also, it can be said that  $\text{Cr}_2\text{O}_7^{2-}$  is a better nucleophile than the counterpart acidic structure because of both the calculated electrophilicity index and charge transfer values.

In addition, the HOMO is localized on the ionic surface except for the Cr and O atoms, while for the acidic structure ( $\text{H}_2\text{Cr}_2\text{O}_7$ ), it is expanded on the molecular surface except for the Cr and hydroxyl group (-O6-H10). From Figure 11, the LUMO for both compounds is localized on the whole ionic and neutral molecular surface. Also,  $\text{Cr}_2\text{O}_7^{2-}$  looks like the almost red color that indicates the abundance of the electron density, while the  $\text{H}_2\text{Cr}_2\text{O}_7$  molecule promises the possibility



**Figure 11.** HOMO and LUMO (isoval, 0.02) and MEP (isoval, 0.0004) plots of  $\text{Cr}_2\text{O}_7^{2-}$ ,  $\text{H}_2\text{Cr}_2\text{O}_7$ , and CMS resin at the B3LYP/LANL2DZ/6-311++G(d,p) level.

Table 9. The Comparative Study for the Removal of Dichromate Ions from Water

adsorbent	adsorbate	adsorption efficiency	reference
$\beta$ -cyclodextrin modified magnetic graphene oxide ( $\beta$ -CD/MGO) composite calix[4]arene-based polysiloxane resin (CBPSR)	dichromate ions	49.95 mg/g	5
	metal ions and dichromate anions	87–91%	49
N-methylglucamine derivative of calix[4]arene immobilized onto poly[(phenyl glycidyl ether)- <i>co</i> -formaldehyde]	arsenate and dichromate anions	As 90% and Cr <sub>2</sub> O <sub>7</sub> <sup>2-</sup> 30%	50
silica gel immobilized calix[4]arene graphene oxide/silica nanosheets	dichromate anions	86.61%	51
	Cr(VI)	92.2510 mg/g	52
calix[4]arene appended Amberlite XAD-4 resin	dichromate anions	91%	24
CMS resin	dichromate ions	99.13% (380.6178 mg g <sup>-1</sup> )	this study

of both the nucleophilic (blue color) and electrophilic attack (red color) reactions. Namely, the red color is densified over the central oxygen atom, which is a bridge between the Cr atoms, and the blue color is positioned over the hydrogen atoms belonging to the hydroxyl group, as expected. Chromate salts are known well as an oxidizing agent being important in living bodies. In this context, Figure 10 clearly represents the reactive sites and types of both compounds.

As is known, chemical hardness and electronegativity are charge-dependent properties. Chemical hardness, a simple method for the calculation of lattice energies of inorganic ionic crystals based on the chemical hardness,<sup>47</sup> is defined as the resistance toward electron cloud polarization or deformation of chemical species. On the other hand, electronegativity is known as the electron withdrawal power of compounds. According to Sanderson's electronegativity equalization principle, when two chemical species with different electronegativities interact with each other, electron transfer between them continue until their electronegativities become equal, which is known as equilibrium state. The fraction of electron transfer ( $\Delta N$ ) between two chemical species (A and B) and binding energy ( $\Delta\psi$ ) are calculated using the following equations (eqs 16 and 17). Absolute hardness is a companion parameter to absolute electronegativity.<sup>48</sup>

$$\Delta N = \frac{\chi_A - \chi_B}{2(\eta_A + \eta_B)} \quad (16)$$

$$\Delta\psi = -\frac{(\chi_A - \chi_B)^2}{4(\eta_A + \eta_B)} \quad (17)$$

It can be understood from the equations given, the fraction of electron transfer ( $\Delta N$ ) between two chemical species (A and B) and binding energy ( $\Delta\psi$ ) can be calculated considering absolute hardness and absolute electronegativity values reported for the mentioned species. It is important to note that the equations given above have been derived in light of the electronegativity equalization principle and hardness equalization principle.  $\Delta N$  and  $\Delta\psi$  values calculated for the interaction between dichromate ions and calix[4]arene using the data given in Table 8 are 0.87011 and -2.7583 eV, respectively. These values obtained show that the interaction between dichromate ions and calix[4]arene is very strong. Theoretical data support the experimental observations.

## 5. COMPARATIVE STUDY

The adsorption efficiency of CMS resin has been checked by different adsorbents already reported and is shown in Table 9. The result indicated that in comparison to other materials,

CMS resin shows better efficiency for the removal of dichromate ions.

## 6. CONCLUSION

In this study, CMS resin has been found as an effective material for the removal of dichromate ions from wastewater. The maximum adsorption percentage was obtained at acidic pH 2.0. To validate the equilibrium data, different modes were applied, but the Freundlich model was the best fit with a good correlation coefficient as compared to the Langmuir model. The energy  $E$  (kJ/mol) was calculated with the help of the D-R model, which suggests that the adsorption is ion exchange in nature. The thermodynamic parameters show that the adsorption of dichromate is endothermic and spontaneous and follows pseudo second order kinetics. The CMS resin reusability potential has been checked, which shows that the material is efficient and can be used many times without any change in % adsorption and very efficient to treat wastewater effluents. The DFT calculations are very helpful to understand the interaction phenomenon.

## ■ ASSOCIATED CONTENT


### SI Supporting Information

The Supporting Information is available free of charge at <https://pubs.acs.org/doi/10.1021/acs.jced.0c00735>.

Removal of dichromate ions from water samples performed under the optimized conditions (the optimized parameters are given in details) (PDF)

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## Notes

The authors declare no competing financial interest.

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