

Ultrasound-Assisted Synthesis of MXene-Grafted Coconut Husk Activated Carbon for Enhanced Adsorption of Carbamazepine: Batch Study and Optimization

Sampad Sarkar

sarkarsampad300@gmail.com

Jadavpur University

Suryanshu Mukherjee

Jadavpur University

Papita Das

Jadavpur University

Avijit Bhowal

Jadavpur University

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Abstract

The presence of multiple pharmaceuticals in the water bodies as waste causes several hazardous environmental effects for both aquatic and terrestrial animals. The present study investigates the potential of novel MXene nanosheet grafted coconut husk-derived activated carbon (AcC/MXene) on the uptake of a pharmaceutical, i.e., carbamazepine, from the experimental solutions. MXene nanosheet was synthesized from the MAX phase. Coconut husk was pyrolysed at a higher temperature and in an inert atmosphere to synthesise activated carbon, and MXene nano-sheet was grafted on the activated carbon using ultrasonication and hydrothermal reaction. The highest adsorption capacity of 427.47 mg.g^{-1} of the nanocomposite was calculated from the batch adsorption study. The detailed investigation of the physicochemical characteristics of the nanocomposite displayed micropores, a high surface area, with several functional groups responsible for the high uptake of the adsorbate molecule from the experimental solutions. The adsorption process was optimized using response surface methodology (RSM), in which 99.2515% of carbamazepine removal by the AcC/MXene nanocomposite was estimated in optimized conditions. Furthermore, the kinetic analysis and the isotherm analysis of the adsorption process were performed. The thermodynamic analysis revealed that the adsorption process was spontaneous at a negative ΔG value, and the adsorption process was endothermic, as concluded from the positive ΔH value of $59.47836 \text{ kJ. mol}^{-1}$. In the 7th cycle of the reusability study, 51.018% of the carbamazepine removed from the experimental solutions demonstrated the economic applications in wastewater treatment.

1 Introduction

Wastewater management has become a pressing global issue due to rapid urbanization, industrialization, and population growth. In many regions, ageing infrastructure, insufficient treatment capacity and the presence of emerging contaminants such as dyes, pharmaceuticals (Patel et al., 2019), microplastics (Samir et al., 2021) and heavy metals (Pal et al., 2023) pose significant challenges. Pharmaceutical residues can enter water bodies through various pathways, including excretion, inappropriate disposal of manufacturing plant effluents and unused pharmaceuticals. These contaminants can remain in the environment, leading to accumulation in aquatic ecosystems.

Carbamazepine ($\text{C}_{15}\text{H}_{12}\text{N}_2\text{O}$) is an antiepileptic medication used to treat epilepsy, trigeminal neuralgia, and bipolar disorder. Carbamazepine is a stable molecular structure, which makes it difficult for it to biodegrade, especially at low concentrations found in wastewater. The majority of the wastewater treatment plants employ traditional biological treatment techniques; however, carbamazepine is resistant to them. Membrane filtration technologies, including nanofiltration (NF) and reverse osmosis (RO), offer high rejection rates for small pharmaceutical molecules but face challenges such as membrane fouling and concentrate disposal. Biological treatments like membrane bioreactors (MBRs) and moving bed biofilm reactors (MBBRs) improve pharmaceutical removal by combining microbial degradation with physical filtration, allowing for higher biomass retention and longer treatment times (Kato & Kansha, 2024). Adsorption techniques using activated carbon, both powdered (PAC) and granular (GAC), are also widely employed due to their strong affinity for organic compounds, though the regeneration of spent carbon remains a concern (Gadipelly et al., 2014). It highlights the need to develop and implement more advanced, selective, and high-capacity adsorbents for effective and sustainable wastewater treatment.

Adsorption is widely regarded as a superior technique for removing carbamazepine from water bodies due to its simplicity, cost-effectiveness, and high efficiency. Compared to methods like membrane filtration, advanced oxidation processes, and biological treatments, which often involve complex operations, higher energy consumption, and potential formation of harmful by-products, adsorption offers a more straightforward and environmentally friendly approach. It operates effectively under ambient conditions without the need for extensive infrastructure or chemical inputs. Alternative low-cost adsorbents derived from agricultural waste, like coconut husk, peanut shell, orange peel, rice husk, rice straw, sugarcane bagasse, corn cobs and many more have been explored for their effectiveness in adsorbing pharmaceuticals (Ahmed et al., 2021; Akinhanmi et al., 2020; Sarkar, Chakraborty, et al., 2025; Shamsollahi & Partovinia, 2019; Verma et al., 2021). Activated carbon made from coconut husk has a larger surface area, porosity, and micropore volume than many other adsorbents made from agricultural waste. Despite their potential, these materials often exhibit lower adsorption capacities and may require surface modifications to enhance performance. These challenges necessitate careful selection and optimization of adsorbents for effective pharmaceutical removal from wastewater (Satyam & Patra, 2024). Studies have demonstrated that MXene-activated carbon composites exhibit enhanced adsorption capacities and faster kinetics for various contaminants. The improved performance is due to the increased active sites and the facilitation of electron transfer processes, enhancing interactions with pharmaceutical molecules (Keneshbekova et al., 2024). Moreover, the composite's structural stability and reusability make it a viable option for the treatment of wastewater in a sustainable manner. To the best of our knowledge, the synergistic combination of sustainable, biomass-derived activated carbon with 2D MXene nanosheets has not been previously reported for carbamazepine removal.

The present study introduces the development of a novel coconut husk-derived activated carbon/MXene composite material for the effective removal of carbamazepine from aqueous solution. After analyzing the necessary characterization for the AcC/MXene nano-composite, a batch study was conducted to analyze the effect of each parameter on the adsorption efficiency and the capacity of the nano-composite. Further, three parameters were taken into consideration to optimize, and the interaction between the parameters was determined by using Design Expert software by the Response Surface Methodology (RSM).

2 Materials and Methods

2.1 Materials

Raw materials for the development of activated carbon were coconut husk, which was collected from the waste at a local shop in Jadavpur, Kolkata, India. Other materials required for the synthesis of activated carbon, MXene, and the nanocomposite were sodium hydroxide (NaOH), potassium hydroxide (KOH), MAX phase (Ti_3AlC_2), hydrochloric acid (HCl, 37%), sulfuric acid (H_2SO_4 , 98%) were purchased from Merck and absolute ethanol from Sigma-Aldrich and distilled water.

2.2 Preparation of Nanocomposite

To prepare activated carbon from the coconut husk, the collected coconut husk was cleaned with water and cut into pieces before being ground in a mixer grinder. After being grounded, the husk part was dried in a hot air oven at 333 K and ground again to reduce the size of the husk. Then the sample was carbonized at 723 K for 4 hours. Next, the char was treated with 0.05 M H₂SO₄ for 3 hours and neutralized by washing it with distilled water. Now, 4 g of the acid-treated char was impregnated with 8g of sodium hydroxide pellet with a ratio of 1:2 and pyrolyzed at 973 K for 3 hours with a constant N₂ flow rate. The chemically and thermally treated activated product was rinsed with distilled water to eliminate the NaOH present in the char, and finally, the pH was adjusted with 0.1 M HCl and 0.1 M NaOH solutions. The final product was the activated carbon derived from coconut husk, was named AcC.

The synthesis of functionalized MXene was discussed in our previously reported original research article (Sarkar, Mukherjee, et al., 2025). Briefly, the synthesis of MXene nanosheets involved 2g of MAX phase, with 6 g of KOH, of 50 ml of water solution mixed in a beaker at 350 rpm for 6 hours. The solution was transferred into the hydrothermal reactor for 8h at 423 K. After that, the solution was sonicated for two hours, and the final solution's pH was adjusted to 7 by washing and finally dried at 353 K in a vacuum drier to obtain dry functionalized MXene nanosheets.

For the making of the composite of coconut shell-derived activated carbon and MXene nanosheets, 0.2 g of MXene nanosheets and 2 g of AcC were dispersed in 20 ml of ethanol and 50 ml of deionized water, respectively. Both mixtures were ultrasonicated for an hour, and after that, mixed in a separate beaker at 350 rpm for 2 hours. Now, the final mixed solution was transferred to a hydrothermal reactor and heated for 10 hours at 393 K. The excess amount of water was then removed and dehydrated in a vacuum oven for 6 hours. The final product was kept in an airtight container, and the making of MXene-coated activated carbon (AcC/MXene) was completed. A schematic illustration of the synthesis process for AcC/MXene composite is demonstrated in Fig. 1.

The techniques and the instruments used for the physicochemical characteristics of the AcC/MXene nanocomposite have been mentioned in the supplementary section.

2.3 Batch Adsorption Study

To investigate the impact of the experimental parameters on the adsorption capacity and the removal % of AcC/MXene for carbamazepine, three hours of batch study were carried out. There were several different independent parameters, including the amount of the composite (0.1 to 0.3 g. L⁻¹), the concentration of adsorbate (100 to 300 mg. L⁻¹), pH (2 to 10) of the experimental solution, temperature (293 to 308 K) and agitation speed (70 rpm to 160 rpm) of the incubator shaker. Other factors remain unchanged to examine the impact of every adsorption parameter of carbamazepine by the nano-composite. Each experiment used a 100 ml Erlenmeyer flask to test 50 ml of carbamazepine solution aqueously. 0.1M NaOH and 0.1M HCl solutions were used to modify the pH of the experimental solution. Carbamazepine was added in an aqueous solution containing 2% ethanol. To measure the residual concentration of the experimental solution, 1 ml of the experimental solution was taken at predetermined periods and further examined using a UV-VIS Spectrophotometer, and the maximum adsorption peak($\lambda_{\max}$) for carbamazepine was found at 284 nm. The following formula was used to estimate the amount of absorbed carbamazepine at each time point (mg.g⁻¹):

$$q_t = (C_0 - C_t) \times \frac{v}{w}$$

1

Where, the capacity of carbamazepine adsorption at a specific time t (min) is denoted by q_t (mg. g⁻¹), The initial carbamazepine's concentration is indicated by C_0 (mg. L⁻¹), the residual concentration of carbamazepine at a specific time t (min) by C_t (mg. L⁻¹), the volume and the adsorbent weight of the experimental solution were denoted by v (L) and w (g) respectively. The percentage of carbamazepine removal was estimated using the formula below:

$$\text{Removal efficiency (\%)} = \frac{C_0 - C_t}{C_0} \times 100$$

2

where C_0 and C_t stand for the initial and final carbamazepine concentrations at specific times t (min), respectively (Ji et al., 2024).

Every experiment was carried out in three separate batches, and the present study reports the average values that were achieved. The standard deviation of all average values was computed in order to statistically represent the data, and the results are shown in the figures as standard deviation bars.

Details of formulas for kinetics, isotherms, and thermodynamics have been given in the supplementary material.

2.4 Response Surface Methodology (RSM) Optimization

The RSM is an essential statistical and mathematical method for the systematic design and analysis of experiments. To create a link between the importance of various experimental parameters on the adsorption investigation, RSM was utilized for further optimization. The 3-level 3-factor Box-Behnken Design (BBD) of RSM in Design Expert version 7.0.0 was used to optimize this adsorption process. A statistical analysis of the interactions within parameters is used to anticipate the outcomes based on optimization of the experimental data. Process While pH 6, 308 K, and agitation speed of 130 rpm were kept

constant as input parameters, optimization was examined in terms of experimental parameters such as adsorbent dosage (g.L^{-1}), carbamazepine concentration (mg.L^{-1}), and treatment duration (min). The factors' levels were categorized as follows: +1 indicates high, 0 indicates middle or central, and -1 indicates low (Tripathi et al., 2009). The procedure was optimized according to the number of trials (call runs) that the software suggested. Table 1 shows the three independent variable ranges.

To evaluate the impact of three primary independent parameters on the effectiveness of carbamazepine removal, this study comprised a total of 17 tests. Pareto analysis of variance (ANOVA), statistical and response plots, and the coefficient of determination (R^2) were used in evaluating the data. To find the appropriate model terms and fit the 2nd -order polynomial to the experimental data, a linear non-regression approach was employed. By considering all of the linear terms, square terms, and linear-by-linear interaction items, it is possible to explain the quadratic response model. Table 2 provides the actual experimental design matrix.

Table 1
Experimental design levels of three chosen variables

Variable	Unit	Factors	Level		
			Low (-1)	Middle (0)	High (1)
Adsorbent Dose	g. L^{-1}	A	0.15	0.225	0.3
Carbamazepine Concentration	mg. L^{-1}	B	100	200	300
Contact Time	min	C	20	100	180

Table 2
Experimental design obtained from Design Expert software (BBD)

Std	Run	Block	Adsorbent Dosage	Concentration	Time
11	1	Block 1	0.225	100	20
10	2	Block 1	0.225	200	100
3	3	Block 1	0.225	200	100
6	4	Block 1	0.225	100	180
5	5	Block 1	0.225	300	20
8	6	Block 1	0.15	300	100
2	7	Block 1	0.3	200	20
17	8	Block 1	0.3	200	180
7	9	Block 1	0.225	300	180
9	10	Block 1	0.225	200	100
12	11	Block 1	0.225	200	100
4	12	Block 1	0.15	100	100
13	13	Block 1	0.225	200	100
16	14	Block 1	0.15	200	20
14	15	Block 1	0.15	200	180
1	16	Block 1	0.3	100	100
15	17	Block 1	0.3	300	100

3 Results and Discussion

3.1 Comparison of removal % between Coconut husk-derived Activated carbon, MXene and AcC/MXene nanocomposite

To compare the removal efficiency of adsorbents, a study was conducted comparing MXene, coconut husk-derived activated carbon (AcC), and a composite of MXene and AcC called AcC/MXene. In this study, each adsorbent was tested in separate 100 mL Erlenmeyer flasks with a fixed dosage of 0.3 g.L^{-1} , initial carbamazepine concentration of 100 mg.L^{-1} , pH of 7, a temperature of 308 K, and agitation at 130 rpm on an incubator shaker. The experiment lasted 180 minutes, and the results showed that the highest removal rates for MXene, AcC, and AcC/MXene were 37.31%, 86.72%, and 98.11%, respectively. This indicates that the nano-composite had greater adsorption efficiency in removing carbamazepine from the solution. Consequently, further characterizations, batch adsorption studies, parameter optimization, and other analyses were performed only for the AcC/MXene nanocomposite. The comparison graph has been included in the supplementary material.

3.2 Physicochemical Characterization of the nano-composite

Surface morphology was determined by scanning electron microscopy (SEM). Figure 2a and 2b display the SEM image and EDX spectra of the AcC/MXene nanocomposite. The SEM image shows cracks, crevices, and grains of different sizes within the large holes on the surface of the AcC/MXene. The nanocomposite's surface appears rough and porous, likely due to efficient carbonization and activation. EDX analysis confirmed the presence of Ti, which was strongly evident on the porous surface with MXene nanosheets, indicating the successful synthesis of the nanocomposite. The microstructure of the composite was further analyzed by using transmission electron microscopy (TEM), as demonstrated in Fig. 2(c-e). The monolayer MXene nanosheets seem incredibly thin on the surface of the activated carbon. The AcC/MXene nanocomposite's selected area electron diffraction (SAED) pattern in Fig. 2f revealed the characteristic hexagonal diffraction crystal structure of the $Ti_3C_2T_x$ phase.

Thermal stability and the purity of the nanocomposite were determined by Thermo Gravimetric Analysis (TGA). The investigation was conducted at a steady $40\text{ K}\cdot\text{min}^{-1}$ heat rate with continuous flow of nitrogen gas. Figure 3a demonstrates the TGA graph and DTGA graph of the nanocomposite, from which the total mass loss of the AcC/MXene nanocomposite was calculated to be 19.26% up to a temperature of 1180 K. The mass loss steps with corresponding thermal events were highlighted in the DTGA graph. The decomposition of the nanocomposite took place in three stages. The first stage occurred at a temperature range of 310 K to 350 K, which involved the loss of moisture present in the sample, with approximately a weight loss of 1.33%. Weight loss of 15.23% was noted at the range of 400 K to 740 K due to the carbonization of the nanocomposite as well as the erosion of the AcC, and final weight loss of 2.77% was observed at the range of 740 K to 1180 K, revealing the breaking of the strong Ti and C bond and decomposition of carbon particles (Alzahrani et al., 2024; Arsyad et al., 2016; Kumar et al., 2021).

FTIR spectroscopy analysis of AcC/MXene is illustrated in Fig. 3b. Four wave numbers, 3857 cm^{-1} , 3681 cm^{-1} , 3347 cm^{-1} and 2671 cm^{-1} , featured the existence of O–H band stretching. These peaks denote both terminal OH groups with TiO_2 and bridging OH groups serve as sources of OH radicals on adsorption sites, respectively (Liu et al., 2019). The peak 2987 cm^{-1} represented the O–H or C–H band available in the composite (Chakarova et al., 2012; Kondratenko et al., 2020). C–H or H–C–H band stretching was identified by 2914 cm^{-1} (Potocki et al., 2019). The $O=C=O$ band stretching was focused on the wave number of 2332 cm^{-1} (Parker et al., 2024). Four consecutive peaks of 2117 cm^{-1} , 1559 cm^{-1} , 1236 cm^{-1} and 1012 cm^{-1} denoted as various groups of carbon monoxide, like $C\equiv O$, $C=O$ and C-O band stretching, respectively (Makita & Hastings, 2018; Murthy et al., 2021; Xia & Shi, 2016). Another peak of 1794 cm^{-1} reflected the presence of the CO_3^{2-} functional group on the surface of the adsorbent (Xu et al., 2007). One more small peak at the 617 cm^{-1} depicted either a C–C–C chain or a metal oxide band (Ti or Si) on the surface (Arjunan et al., 2012). All the results indicated that there were traces of functional bands that can identify the presence of both MXene and AcC.

The XRD pattern within the range $2\theta = 3^\circ$ to 60° of AcC/MXene nanocomposite is displayed in Fig. 3c. The effective conversion of the MAX phase to MXene was indicated by the (002) peak shifting from 9.5° to 8.8° . The produced MXene clearly exhibits distinctive peaks at $2\theta = 8.8^\circ$, 17.8° , 27.3° , 36.1° , 43.4° and 54.2° , which correspond to the crystal planes (002), (004), (006), (104), (105) and (121) respectively (JCPDS no. 72-2496) (Sarkar, Mukherjee, et al., 2025; Xue et al., 2023). The presence of these peak series is an additional indication of Al in Ti_3AlC_2 effectively etched to yield MXene. It is suggested that the irregularity of the crystal structure is the result of etching because the peaks of MXene are broad and low in intensity. The existence of amorphous carbon is indicated by a large peak seen for the activated carbon sample at 27.3° and 41.8° in the range of $2\theta = 20^\circ$ to 30° and $40^\circ - 50^\circ$. The steadily increasing nature of intensity in the figure suggests the existence of MXene nanosheets in their crystalline form on the surface of activated carbon. Moreover, AcC/MXene composites exhibit the broad (002) peak, confirming the production of MXene-bonded AcC (Aliyu et al., 2024).

The nitrogen adsorption as well as desorption isotherms for BET analysis of AcC/MXene composites are depicted in Fig. 3d. The convex curve of adsorption justified the type IV isotherm according to the IUPAC classification and indicated the presence of micropores on their surface (Khurshid et al., 2025). According to the Density Functional Theory (DFT) method, the adsorption surface area, pore volume and pore radius details were mentioned in Table 3. Since the size of MXene is so small that it may block the void pores of larger-sized AcC particles. However, the positive effect of active sites was better than the negative effect of pore blocking after modifying AcC with MXene. The doping of MXene and AcC is therefore still advantageous for improving the performance of the composite material (Aliyu et al., 2024).

Table 3
BET details of AcC/MXene

Sample	BET Surface Area	Average Pore Diameter	Micropore Volume	Total Pore Volume
	$m^2\cdot g^{-1}$	nm	$cm^3\cdot g^{-1}$	$cm^3\cdot g^{-1}$
AcC/MXene	318.49	1.01	0.075	0.222

Dynamic Light Scattering (DLS) was used to measure the dispersive index and distinctive particle size distribution of AcC/MXene nanocomposite. The particle size distribution of AcC/MXene by intensity (percentage) indicated a characteristic sharp peak at 533.9 nm. The width of the particle size distribution of the nanocomposite was investigated by the polydispersity index (PDI), in which the value of 0.630 indicated that the composite was polydisperse in nature. This kind of polydispersity of the nano-composite might be the MXene nanosheets or particles that tend to agglomerate or cluster together, which are coated onto the surface of the activated carbon, increasing particle size and also in a wide range of particle size distribution (Park et al., 2022). The particle size analysis of AcC/MXene, as determined by the DLS method, is presented in the supplementary material.

3.3 Batch Study Result

3.3.1 Impact of solution’s pH on AcC/MXene of carbamazepine uptake

To examine the adsorbents' sensitivity to pH during carbamazepine adsorption, a batch adsorption experiment was carried out using the experimental solution at different pH conditions (2–10). Experiments were performed in a BOD Shaker with a constant amount of carbamazepine (100 mg.L^{-1}) and at 130 rpm, applying a nanocomposite dosage of 0.3 g.L^{-1} . From Fig. 4a, it was quite evident that after analyzing the Zeta potential of the composite, the pH_{PZC} value estimated was 7.2. The experimental result obtained by varying the pH of the solutions demonstrated in Fig. 4b indicated that the removal % as well as the adsorption capacity of the nanocomposite varied less within the range of experimental solutions pH. It was due to the carbamazepine primarily remains in non-ionized form in the experimental solution, as indicated by its reported values of $\text{pK}_{\text{a}1}=1$ and $\text{pK}_{\text{a}2}=13.9$. For carbamazepine adsorption, AcC/MXene had the maximum removal of 98.037% and the adsorption capacity of 326.79 mg.g^{-1} at pH 6. Consequently, further study on the adsorption of carbamazepine was conducted at pH 6.

3.3.2 Impact of AcC/MXene dosage on the removal of carbamazepine

The impact of adsorbent dosage was examined within the range of 0.1 to 0.3 g.L^{-1} , while the other variables that affected the adsorption performance, pH 6, rotational speed of 130 rpm, at 308 K and carbamazepine concentration of 100 mg.L^{-1} were fixed in the experiment examined for 180 minutes in the BOD incubator shaker. From Fig. 4c, it was quite evident that with increased dosage, the adsorption efficiency of the nanocomposite increased from 61.029% to 97.977% of carbamazepine removal. On the other hand, the highest adsorption capacity of the nano-composite was $406.862 \text{ mg.g}^{-1}$, which was calculated from the dosage of 0.1 g.L^{-1} . These phenomena could be explained as the dosage of the AcC/MXene nanocomposite rose, the total active sites, as well as the total surface area of the nanocomposite in a specific experimental solution also increased, which led to the enhanced removal % (Hasani Khaneghahi et al., 2023).

3.3.3 Impact of Carbamazepine concentration on AcC/MXene nanocomposite

Within a BOD incubator shaker, a range of carbamazepine concentrations from 100 to 300 mg.L^{-1} was examined for 180 minutes till the equilibrium point, while the other parameters remained constant. According to Fig. 4d, as the concentration of carbamazepine in the solution grew, the adsorption capacity increased, and the removal percentage dropped for the carbamazepine removal by the AcC/MXene nano-composite. From the experimental data, it indicated that the adsorption capacity rose from 326.666 to 427.47 mg.g^{-1} , and the removal % decreased from 98 to 50.363% as the experimental solution's concentration increased up to 250 mg.L^{-1} . Whereas, at an adsorbate concentration of 300 mg.L^{-1} a sudden drop in adsorption capacity of AcC/MXene occurred. At an adsorbate concentration of 300 mg.L^{-1} , a decrease in the adsorption capacity resulted because before that concentration, the active site for adsorption was preoccupied by the carbamazepine molecule, and increasing the concentration more might not adsorb on the surface of the AcC/MXene nano-composite, leading to a decrease in calculated adsorption capacity.

3.3.4 Impact of system temperature on the uptake of carbamazepine by AcC/MXene nanocomposite

The impact of system temperature on the uptake of carbamazepine was studied at four different temperatures from 293 to 308 K, while other factors remained unchanged in the above-mentioned study. Figure 4e indicates that with increased temperature, the removal % and the adsorption capacity also increased. The adsorption efficiency of AcC/MXene nano-composite on the removal of carbamazepine rose from 94.925 to 98.25%, and the adsorption capacity increased from 316.419 to 327.5 mg.g^{-1} as the temperature rose. Lower temperatures resulted in decreased adsorption capability because of the less active functional group. However, the pore spaces were enhanced as ascending temperature increasing the removal capacity to efficiently remove more adsorbate from the solution (Sarkar, Chakraborty, et al., 2025).

3.3.5 Impact of initial rotational speed on the uptake of carbamazepine by AcC/MXene nanocomposite

The effect of rotating speed was assessed over a range of 70–160 rpm while maintaining the same values for all the parameters. The result demonstrated in Fig. 4f indicated that a certain level of increase in the agitation speed led to the elevated removal % as well as the adsorption capacity. At 70 rpm, the adsorption efficiency and the adsorption capacity were 82.092% and $273.642 \text{ mg.g}^{-1}$, respectively, whereas at 130 rpm, the adsorption efficiency and the adsorption capacity were 98.657% and $327.654 \text{ mg.g}^{-1}$, respectively. Efficient adhesion of the adsorbate molecule on the adsorbent surface-active sites allowed for maximal removal at 130 rpm. Lower adsorption efficiency resulted from insufficient contact between the carbamazepine and the nanocomposite surface, caused by a decrease in speed (Sarkar, Mukherjee, et al., 2025). From the figure, it was also noted that at 160 rpm, both the efficiency and the capacity of adsorption dropped to 93.657% and $312.191 \text{ mg.g}^{-1}$, respectively. The adsorption efficiency dropped beyond 130 rpm, indicating that too much rotation has a negative impact on the removal of carbamazepine. In contrast, a speed increase higher than ideal resulted desorption of carbamazepine from the surface of the adsorbent, which decreased the removal effectiveness.

3.4 Design of Experiments using Response Surface Methodology (RSM)

An equation for polynomial regression was generated using BBD to examine the relationship in the AcC/MX composite for its adsorption efficiency and adsorption of carbamazepine. To find the removal % for adsorption of carbamazepine, final empirical models of the coded factors excluding the undesirable terms are expressed in Eq. (14). The effect of the AcC/MX adsorbent derived from the studies and anticipated for carbamazepine removal is displayed in Fig. 5a.

$$\text{Removal \%} = +39.11 + 11.89 \times A - 24.91 \times B + 5.76 \times C - 5.66 \times A \times B + 1.53 \times A \times C - 3.26 \times B \times C - 0.74 \times A^2 + 11.46$$

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The predicted response and the experimental response are shown in Table 4 based on the adsorbents' removal % of carbamazepine. The ANOVA in Table 5 confirmed that the quadratic model was adequate. When the difference is smaller than 0.2, the corrected R^2 and the expected R^2 of the adsorbent are in reasonable agreement. The significance of the models was suggested by the greater F-values and P-values less than 0.05 for utilizing the adsorbent. With very low P-values and a high R^2 value, the second-order polynomial models were found to be highly significant and sufficient to represent the underlying relationship between the variables and the response, as indicated by the high F-values (Ravikumar et al., 2005).

Table 4
Predicted vs Actual values of Carbamazepine removal % by using AcC/MXene.

Standard Order	Actual Value (%)	Predicted Value (%)
1	92.96296	92.29167
2	40.92593	41.64352
3	40	39.11111
4	57.96296	57.18364
5	23.33333	21.83642
6	81.66667	83.16358
7	26.79012	26.83642
8	18.02469	18.69599
9	38.98148	39.11111
10	38.42593	39.11111
11	65.18519	65.13889
12	39.16667	39.11111
13	38.98148	39.11111
14	30.09259	29.375
15	30.37037	31.14969
16	20.09259	20.91821
17	57.03704	56.21142

Table 5
Results of ANOVA analysis for RSM model.

R^2	Predicted R^2	Adjusted R^2	F-Value	P-Value
0.9986	0.9795	0.9967	536.21	< 0.0001

3.4.1 Interaction effects on the carbamazepine removal

According to 3D graph in Fig. 5b, the percentage of carbamazepine removed by the composite varied with the initial carbamazepine concentration and the adsorbent dose. The 3D graph clearly shows that the carbamazepine removal % by AcC/MX increased as the initial concentration of the experimental solution was decreased, and on the other hand, the highest removal% can be estimated at the highest adsorbent dosage. This result may have been caused by the rise in the adsorbent's dosage, which also raised the adsorption's total surface area and the active sites, leading to a higher carbamazepine removal %. However, for a fixed number of adsorbent dosages, the increased initial concentration reduced the removal percentage because the adsorbate molecule occupied all of the adsorbent's active sites, which led to a reduction in the removal percentage from the experimental solution. The figure suggested that the highest removal percentage of carbamazepine can be seen at a low initial concentration of 100 mg.L^{-1} and at the dosage of 0.3 g.L^{-1} , which was in parallel to the experimental findings.

Figure 5c illustrates the combined effects of varying initial carbamazepine concentrations and contact periods in the removal of carbamazepine using AcC/MXene nanocomposite. According to the findings, the removal % by AcC/MXene progressively increased with increased contact duration and with increased initial carbamazepine concentration, the removal % by the nanocomposite was decreased. The higher percentage of carbamazepine was removed by the nanocomposite due to increased interaction between AcC/MXene and carbamazepine as their contact time increased. It was clear from the figure that the highest removal % of carbamazepine was estimated at the lowest starting concentration of around 100 mg.L^{-1} and the maximum contact time of about 175 min.

Figure 5d, the 3D plot demonstrates the simultaneous effects of adsorbent (AcC/MXene) dosage and contact time between the nanocomposite and carbamazepine. According to the figure, the parallel increase in dosage and the contact time increased the removal percentage of carbamazepine. As the

dosage increased, the active sites' total number and the total surface area of the adsorbent also increased, and the increased contact time increased the possibility of adsorption onto the surface of the nanocomposite, which led to the increased removal percentage. Based on the figure, a maximum removal of 99.25% could be achieved with an elevated adsorbent dosage of 0.27 to 0.30 mg.L⁻¹ and a contact time ranging from 160 to 180 minutes.

3.4.2 Process Optimization

Using the design program, the intended input for each parameter and response was selected from the list for numerical optimization. The study's input parameters included the total range of maximum and minimum values of the carbamazepine concentration, adsorbent as AcC/MXene dosage, experimental time, and maximizing the removal % of carbamazepine. The range of parameters that were assessed is covered in Table 1. Based on the responses an adsorbent dose of 0.29 g. L⁻¹ for 174.35 minutes with a carbamazepine concentration of 100.21 mg. L⁻¹ produced the best results out of 30 predicted optimized outcomes, with a desirability of 1 and with a 99.2515% removal for the removal of carbamazepine using AcC/MXene nanocomposite. A confirmatory test was conducted using the BBD to confirm that the desirability data was significant, and in optimized conditions, we found 98.56% of removal, which was closely related. The desirability optimization of the three selected inputs graph has been transferred to the supplementary material.

3.5 Isotherm analysis on the removal of carbamazepine by AcC/MXene

It was crucial to perform the isotherm analysis of the adsorption process to ascertain the adsorbent's adsorption capability as well as to assess its commercial application and financial prospects. The Langmuir, Freundlich, and Dubinin-Radushkevich isotherm models were fitted in this investigation, and Table 6 presents the results of the calculations for carbamazepine adsorption by AcC/MXene. With the maximum regression coefficient factor (R²) of 0.9974 and a theoretical q_{max} value of 416.667 mg. g⁻¹, which was closest to the experimental value, the results reflected that the AcC/MXene nanocomposite's carbamazepine adsorption was directed by the Langmuir isotherm model. This reveals that carbamazepine adsorption onto the surface of the nano-composite was distributed homogenously. Additionally, it stated that the adsorbent promoted the carbamazepine molecules in a monolayer covering the nano-composite's surface (Ghaedi et al., 2015). Furthermore, the adsorption process will be favourable for the Langmuir isotherm as the computed separation factor (R_L) values exist between 0 and 1. The Freundlich isotherm and the Dubinin-Radushkevich isotherm models are not comparable because of a low R² value of 0.8925 and 0.5094, respectively, and n_f value exceeding 10.

Table 6
Adsorption isotherm parameters for carbamazepine removal by AcC/MXene nanocomposite.

Langmuir Isotherm				Freundlich Isotherm			Dubinin-Radushkevich isotherm		
q _{max}	K _L	R _L	R ²	n _f	k _f	R ²	q _m	E	R ²
(mg.g ⁻¹)	(L.mg ⁻¹)				(L.mg ⁻¹)		(mg.g ⁻¹)	(kJ.mol ⁻¹)	
416.667	0.34783	0.01636	0.9974	18.315	311.1	0.8925	415.424	40.8	0.5094

3.6 Kinetic analysis on the removal of carbamazepine by AcC/MXene

A kinetics investigation was conducted between 293 and 308 K to determine the rate of carbamazepine absorption by the AcC/MXene, and two kinetic models — the pseudo-first-order and pseudo-second-order kinetic models—were used to fit the results. The results demonstrated that the pseudo-second order kinetic model could fit better to the carbamazepine uptake by using AcC/MXene nanocomposite because for various temperatures (293K–313K), the experimental equilibrium adsorption capacity (q_e) values were more in line with the theoretical values (q_t) for the pseudo-second-order model than for the pseudo-first-order model. Furthermore, the pseudo-second-order models exhibited the highest correlation coefficients (R²) for all temperatures (Table 7). There was a greater agreement with the pseudo-second-order model, suggesting that the rate-determining stage of the adsorption process involves surface activities.

Table 7
Adsorption kinetic parameters for carbamazepine removal by AcC/MXene.

Temp (K)	Pseudo-First-Order				Pseudo-Second-Order			
	K ₁	q _t	q _e	R ²	K ₂	q _t	q _e	R ²
(min ⁻¹)	(mg.g ⁻¹)	(mg.g ⁻¹)		(g.mg ⁻¹ .min ⁻¹)	(mg.g ⁻¹)	(mg.g ⁻¹)		
293	0.06103	316.42	403.924	0.7698	0.00072	316.42	322.581	0.9997
298	0.0525	320.31	311.96	0.7585	0.0008	320.31	322.58	0.9992
303	0.0504	326.36	388.78	0.7223	0.0005	326.36	333.33	0.9971
308	0.0442	327.5	317.61	0.7616	0.0005	327.5	333.33	0.9978

3.7 Thermodynamic analysis on the removal of carbamazepine by AcC/MXene

Thermodynamic characteristics, including spontaneity (ΔG), entropy (ΔS) and enthalpy (ΔH), were evaluated for the novel adsorbent AcC/MXene from batch adsorption experiments at four different temperatures. Table 8 demonstrated that the ΔG value was negative at working temperatures, suggesting that the adsorption occurred spontaneously. The decreasing trend of the ΔG value at increasing process temperature indicates more feasibility of the adsorption for the removal of carbamazepine at higher temperatures. The positive magnitude of the ΔH value of 59.47836 KJ mol⁻¹ for the AcC/MXene nanocomposite

corroborated the endothermic character of the adsorption process, while the positive ΔS value of $237.1901 \text{ J mol}^{-1} \text{ K}^{-1}$ suggests that the carbamazepine on the adsorbent's surface is more randomly distributed (Sarkar et al., 2024). It has been proposed that ΔH values range from 2.1 to 20.9 KJ mol^{-1} during physisorption and from 80 to 200 KJ mol^{-1} during chemisorption. Taking into account the range of ΔH values for this work, the physico-chemical adsorption process was responsible (Saha & Chowdhury, 2011).

Table 8
Parameters derived from thermodynamics for the adsorption of carbamazepine onto AcC/MXene.

Temperature	ΔG	ΔH	ΔS
(K)	(kJ.mol^{-1})	(kJ.mol^{-1})	($\text{J.mol}^{-1} \text{ K}^{-1}$)
293	-10.077	59.478	237.1901
298	-10.927		
303	-12.737		
308	-13.423		

3.8 Adsorption Mechanism

Activated carbon (AC) provides a highly porous structure and large surface area, facilitating the entrapment of hydrophobic carbamazepine molecules through pore-filling and hydrophobic partitioning. Incorporating MXene nanosheets enhances functionality through abundant terminal groups (-OH), excellent hydrophilicity and high surface reactivity. The MXene coating prevents AC pore fouling and increases adsorption selectivity.

The adsorption mechanism involves multiple interactions: (i) π - π electron donor-acceptor interactions between carbamazepine's aromatic rings and the delocalized p-electrons of AcC/MXene surfaces, (ii) hydrogen bonding between carbamazepine's amide group (-NH₂, C = O) and MXene surface functionalities, (iii) electrostatic interactions depending on solution pH and surface charge and (iv) hydrophobic interactions and pore filling with AC's porous network. These combined effects enable strong and stable binding of carbamazepine molecules. Overall, the AcC/MXene composite integrates the structural advantages of AC with the chemical versatility of MXene, resulting in superior adsorption capacity, faster kinetics and better reusability compared to individual materials.

Activated carbon (AC), with its graphitic and aromatic domains, provides delocalized π electron clouds that strongly attract the aromatic rings of carbamazepine. Adsorption affinity is increased by π - π stacking between the carbon structure of AC and the aromatic rings of carbamazepine (Bizi & El Bachra, 2021). Despite the lack of direct carbamazepine–MXene π - π evidence, MXene composites have demonstrated comparable behaviour for aromatic medicines. According to Dehghani and team (2025), MXene (Ti₃C₂T_x) eliminates medications like carbamazepine through interactions of the electron donor-acceptor (EDA) type (Dehghani et al., 2025). To promote cooperative adsorption, carbamazepine most likely participates in π - π stacking with both AC and MXene sheets in AcC/MXene. Amide groups (-NH₂, C = O) in carbamazepine can create hydrogen bonds with oxygen-containing surface groups on AC. The numerous -OH terminations on MXene surfaces can potentially function as acceptors or donors of hydrogen bonds. The adsorption of pollutant hydroxylated MXene is frequently ascribed to interactions between hydrogen bonds (Ahmaruzzaman, 2022; Igwegbe et al., 2019). Because of its high pK_a value (~ 13.9), carbamazepine is mostly neutral in normal water (pH ~ 7), which reduces the prominence of direct electrostatic attractions for AC alone. However, charged functional groups on AC can still facilitate interactions through dispersion forces and hydrogen bonding. From the Zeta potential analysis, the pH_{PZC} of the composite was 7.2. This indicates that below that pH, the composite surface charge will be positive below that pH and negative above that pH. Despite the neutrality of carbamazepine, the charge profile of MXene may have an indirect impact on adsorption through changes to carbamazepine orientation or proximity to active sites, as well as through interactions with co-pollutants that modify carbamazepine behaviour. The impact of pH on the adsorption study indicated that the change of pH within the range 2 to 10 did not show any significant changes in the removal % of carbamazepine. Therefore, it can be concluded that the electrostatic interactions contributed to the removal of carbamazepine by AcC/MXene composite, but did not play a pivotal role. Activated carbon's high surface area and extensive micropores and mesopores enable effective hydrophobic partitioning of carbamazepine, driven by its moderate hydrophobicity. From the BET analysis of the adsorbent high surface area of $318.49 \text{ m}^2 \text{ g}^{-1}$ with a total pore volume of $0.222 \text{ cm}^3 \text{ g}^{-1}$ might be a probable reason for the enhanced carbamazepine uptake. Without completely obstructing pore surfaces or coating pore entrances, MXene sheets in AcC/MXene composites offer more chemical functionality without sacrificing pore accessibility (Ahmaruzzaman, 2022). As the Langmuir isotherm fits best for the removal of carbamazepine by the AcC/MXene composite, it can be stated that carbamazepine molecules form a monolayer that covers the surface of the nano-composite. The thermodynamic calculations yielding a positive ΔH value ($5.9478 \text{ kJ.mol}^{-1}$) indicate that the adsorption of carbamazepine onto the AcC/MXene nanocomposite was an endothermic process. This value falls between typical ranges for physisorption (2.1 – 20.9 kJ.mol^{-1}) and chemisorption (80 – 200 kJ.mol^{-1}), suggesting a physico-chemical adsorption mechanism.

3.9 Regeneration study

One important factor in determining the adsorbent's financial viability for industrial application is its reusability (Misran et al., 2022). The adsorbent was separated and successively treated with 0.2 M HCl solution and 0.2 M NaOH solution after the adsorption tests carried out by AcC/MXene to adsorb carbamazepine from the experimental solution. The regenerated adsorbent was dried at 323 K and reused to remove carbamazepine again. This cycle was conducted up to seven consecutive times, and the results are displayed in Fig. 6c. From the figure, it was evident that after every cycle, the adsorption efficiency decreased gradually and dropped to 51.018% for the carbamazepine removal by AcC/MXene nanocomposite. Although the chemical treatment led to the removal of carbamazepine from the active site of the nanocomposite, the loss of some components and the lack of active binding sites, the removal

decreased by the nanocomposite in each cycle. After reusing the adsorbent seven times, surface morphology was analyzed by SEM. Figure 6a and 6b display the SEM image and EDX spectra of the AcC/MXene nanocomposite after being reused. The EDAX spectra confirm the presence of Ti on the composite surface, which indicates the presence of MXene nanosheets on the composite surface even after several chemical treatments in each regeneration cycle. The weight% analysis from the EDX spectra shows the reduction of Ti, which may have resulted from the continuous chemical treatment of HCl and NaOH for the regeneration study, which may break some of the composite structure. Table 9 demonstrates the removal capacity of AcC/MXene for carbamazepine from the aqueous solution by previously reported research articles, and also the removal of other pollutants by MXene nanosheets.

Table 9
Comparative analysis of different types of adsorbents for carbamazepine and other pollutants.

Adsorbent Type	Targeted Pollutant	Adsorption Capacity (mg.g ⁻¹)	References
Granular CNT/Al ₂ O ₃	Carbamazepine	154.5	(Wei et al., 2013)
Hydroxyl-modified zirconia/porous carbon nanocomposite	Carbamazepine	186.21	(Cheng et al., 2022)
Multi-walled CNTs	Carbamazepine	105.0	(Oleszczuk et al., 2009)
Ti ₃ C ₂ T _x nanosheets	Cr (VI)	250	(Ying et al., 2015)
MXene: Fe3O4 = 2:1	Phosphate	9.42	(Zhang et al., 2016)
H ₃ PO ₄ /K ₂ CO ₃ activated modified hydrocar	Carbamazepine	376.11	(Zhong et al., 2025)
Ti ₃ C ₂ T _x nanosheets	Methyl Orange	94.8	(Karthikeyan et al., 2021)
Magnetic nanoparticle	Carbamazepine	77.30	(Yoon et al., 2016)
Fe ₃ O ₄ -activated carbon from Coconut shell (Ac/Fe3O4)	Carbamazepine	135.1	(Shan et al., 2016)
AcC/Mxene nanocomposite	Carbamazepine	427.47	This study

4 Conclusion

The current study revealed that the development of a novel composite of coconut husk-derived activated carbon and MXene exhibits remarkable efficiency in adsorbing carbamazepine from aqueous solution. Because of the synergistic combination of increased surface area, higher porosity, and rich functional groups, the composite material outperformed individual components and achieved a higher removal rate under optimum conditions. In this batch adsorption study, the nanocomposite displayed the highest adsorption capacity of 427.47 mg.g⁻¹ for the uptake of carbamazepine under controlled conditions. Based on the RSM optimization, the adsorbent dose of 0.29 g. L⁻¹ for 174.35 minutes with a carbamazepine concentration of 100.21 mg. L⁻¹ removed 99.2515% of carbamazepine from the experimental solutions. The regeneration study demonstrated the removal of 51.018% of carbamazepine at the 7th cycle by the AcC/MXene nanocomposite, which indicated that the adsorbent is efficient enough to remove carbamazepine multiple times and is suitable for economic application in wastewater treatment. This demonstrates the potential of agricultural waste valorization, coupled with advanced materials, for sustainable wastewater treatment. Although the study highlights promising findings, the complex structure of real wastewater matrices was not taken into consideration because the adsorption studies were conducted in a controlled laboratory conditions. Therefore, future investigation should be focused on evaluating the composite's increase in adsorption capacity and performance in real wastewater treatment by targeting multiple pollutants like dyes, pharmaceuticals, heavy metals and many more.

Declarations

Ethical Approval:

Not applicable.

Competing Interest:

The authors declared that there is no conflict of interest.

Consent to participate:

All authors agree to publish the work.

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Author Contribution

Sampad Sarkar- Conceptualization, Manuscript writing. Suryanshu Mukherjee- Manuscript writing. Papita Das- Supervised the work, Visualization, and Validation. Avijit Bhowal- Conceptualization.

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Data Availability

Data will be made available upon reasonable request.

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Figures

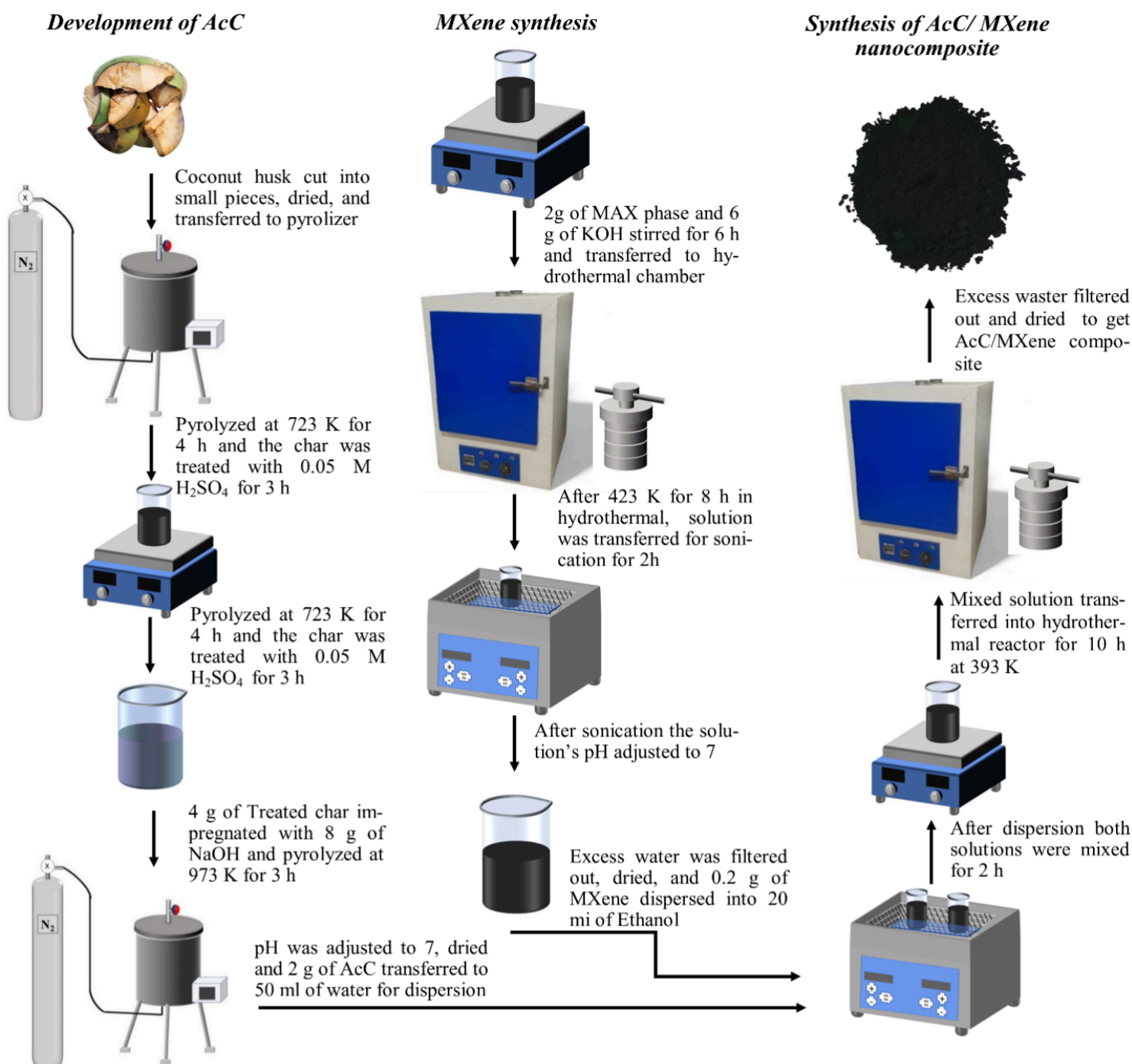


Figure 1

Schematic illustration of the synthesis process of AcC, MXene and AcC/MXene nanocomposite.

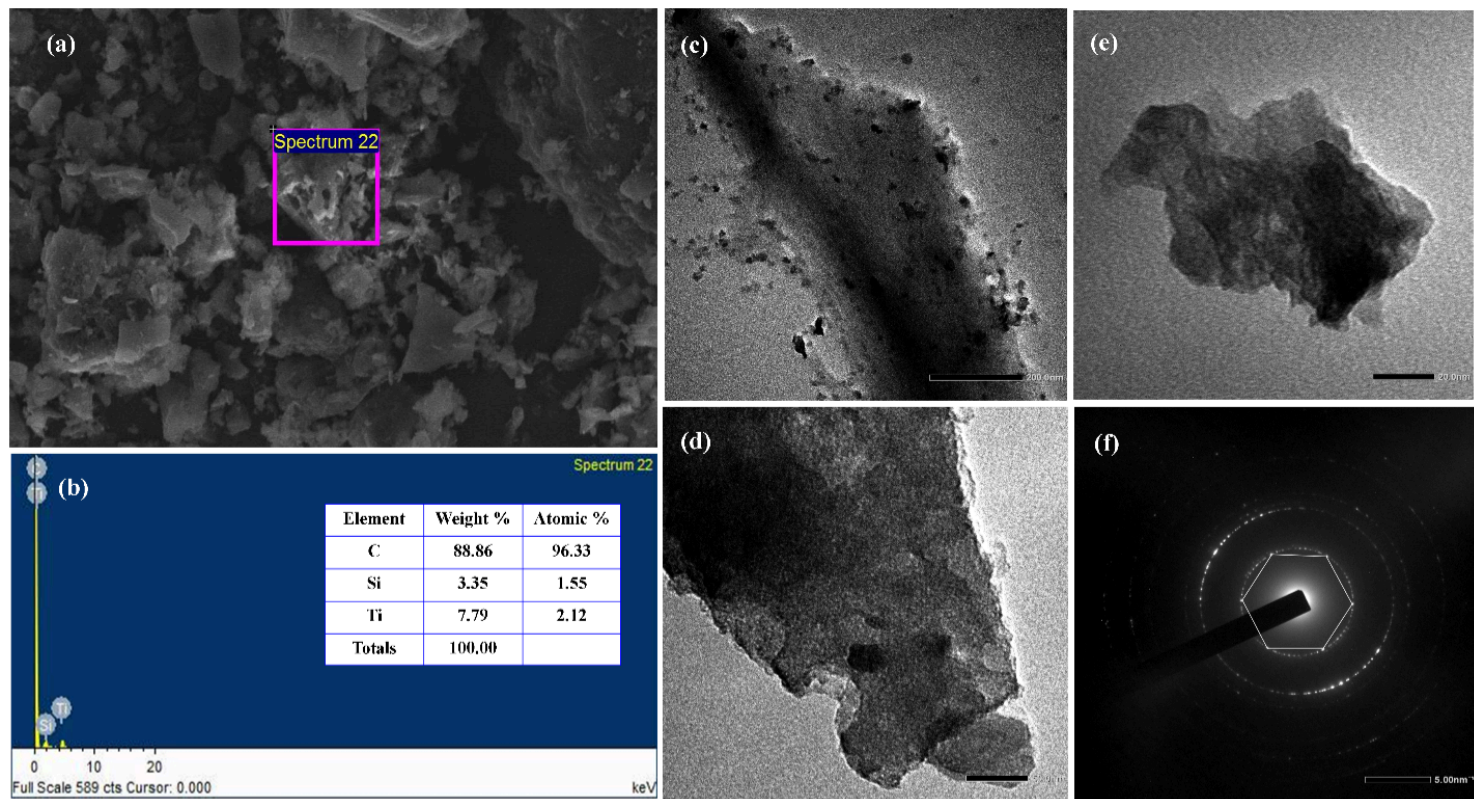


Figure 2
(a-b) Scanning electron microscopic image and EDX spectra of AcC/MXene nanocomposite, respectively. (c-e) TEM image, and (f) SAED pattern of AcC/MXene nanocomposite.

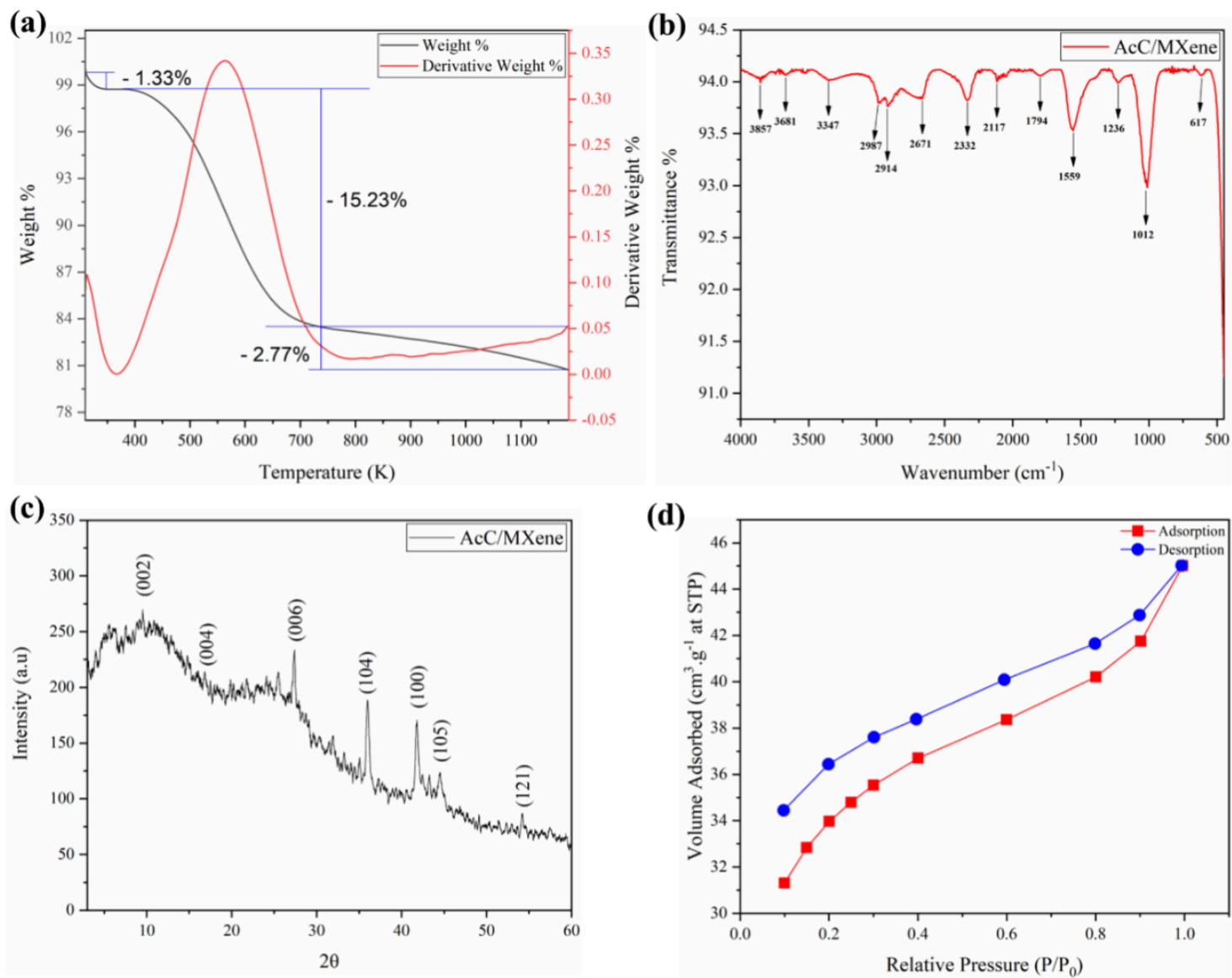


Figure 3

Characterization of AcC/MXene. Plots **(a-d)** TGA-DTGA graph, the ATR-FTIR spectrum, the XRD spectrum, and the nitrogen adsorption isotherm of AcC/MXene used in this study, respectively.

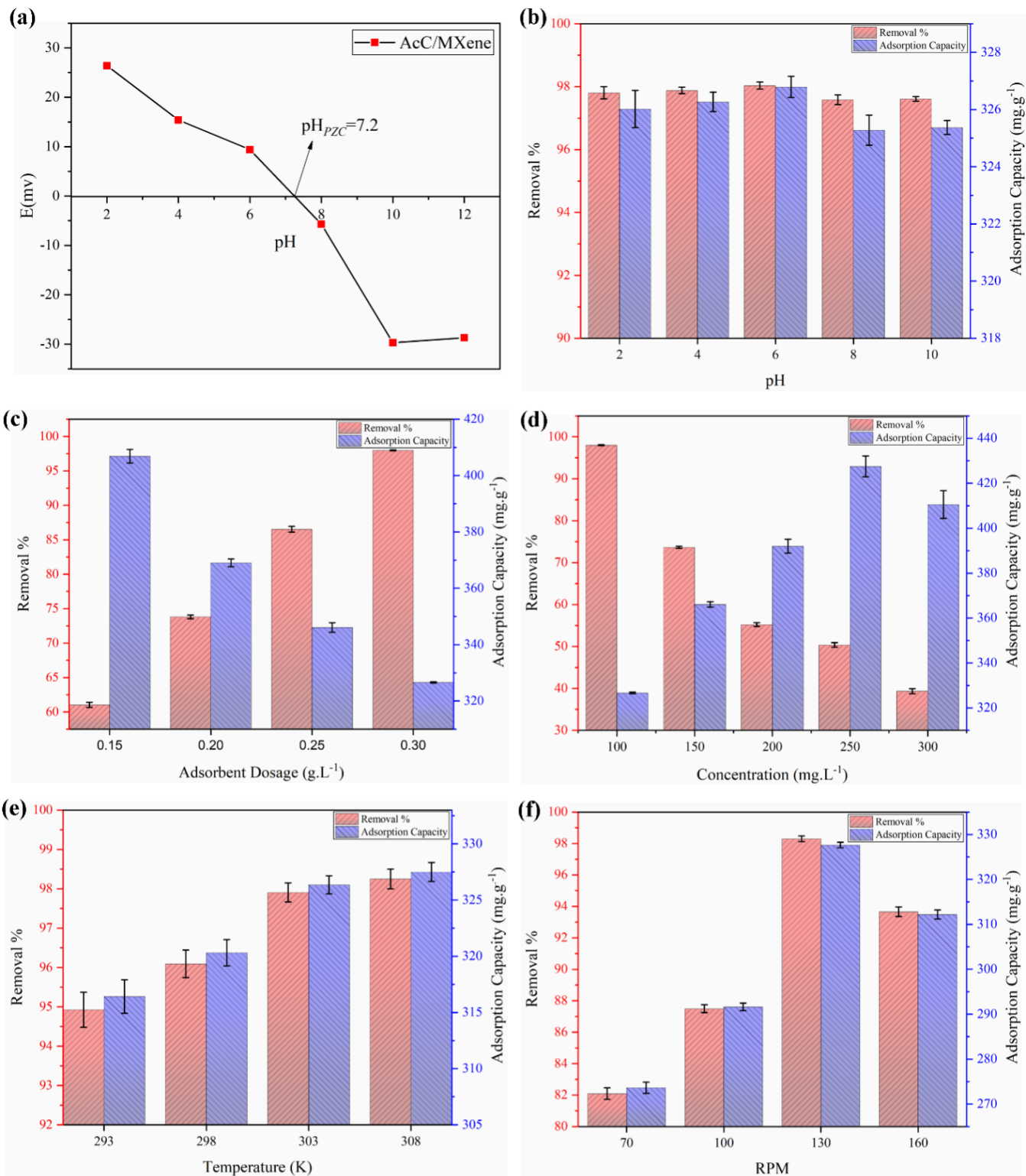


Figure 4

(a) ZetaPotential of AcC/MXene nanocomposite. Effects of different parameters (b) pH of the experimental solutions, (c) adsorbent dosage, (d) concentration of carbamazepine in experimental solutions, (e) system temperature, and (f) agitation speed of the incubator on the removal efficiency and adsorption capacity of AcC/MXene.

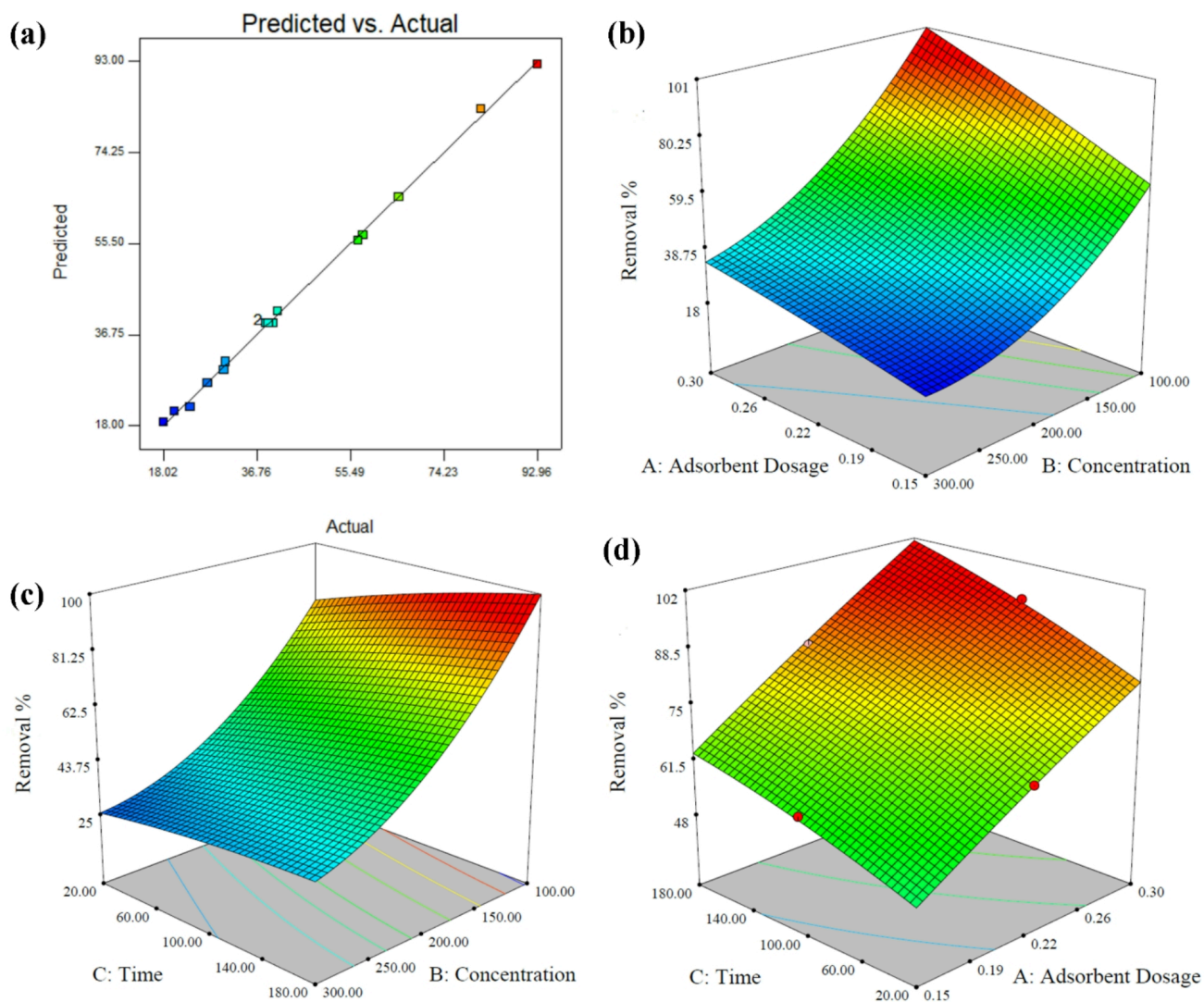


Figure 5

(a) Predicted vs. Actual values for carbamazepine removal by using AcC/MXene. 3D surface plots of (b) the combined effect of adsorbent dosage and carbamazepine concentration, (c) the combined effect of carbamazepine concentration and contact time, and (d) the combined effect of adsorbent dosage and contact time on carbamazepine removed by the AcC/MXene nanocomposite.

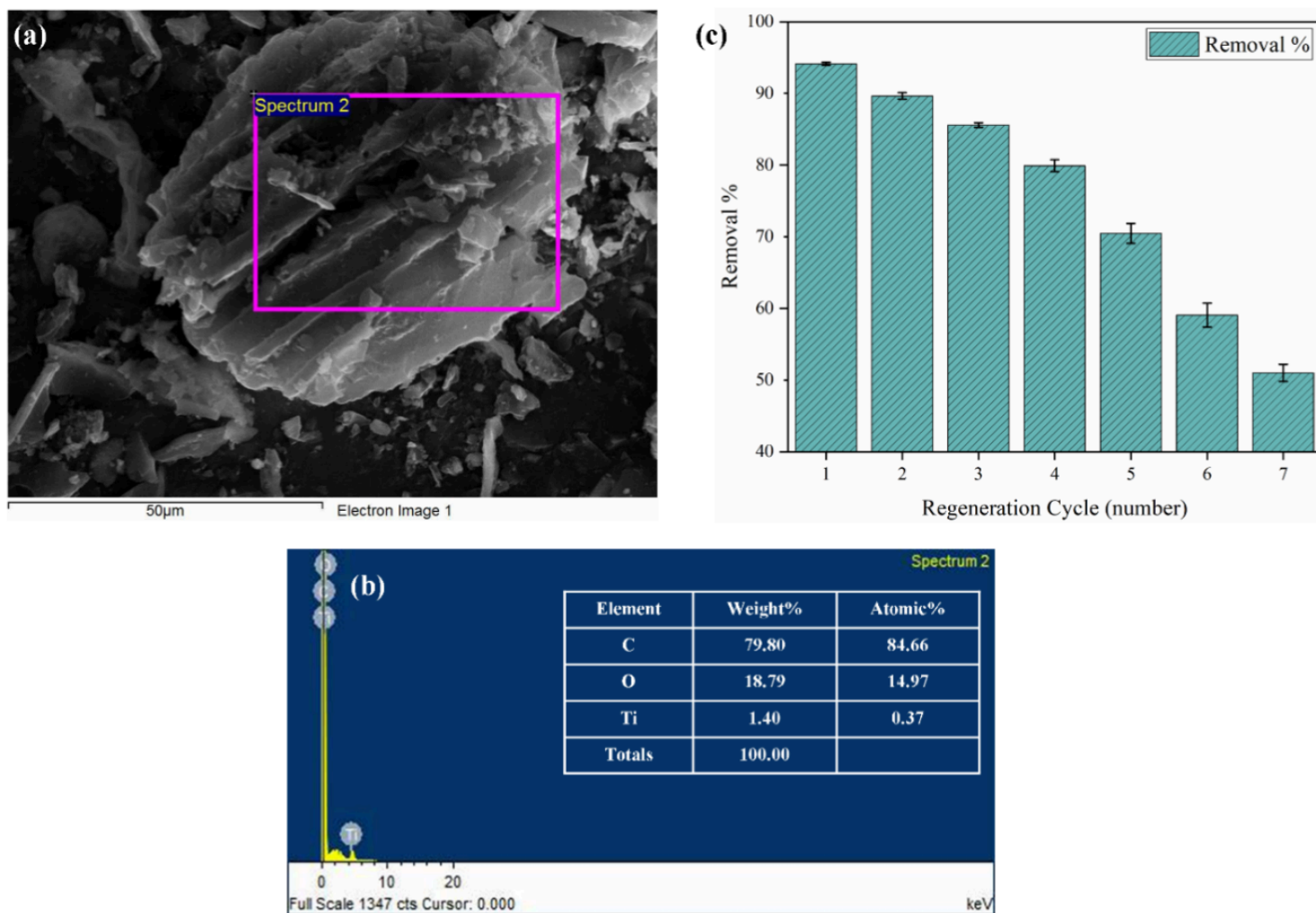


Figure 6

(a-b) SEM image and EDX spectra of AcC/MXene nanocomposite after reuse, respectively; **(c)** regeneration of AcC/MXene for the removal of carbamazepine. Each cycle used a constant dosage of 0.3 g.L^{-1} , an initial carbamazepine concentration of 100 mg.L^{-1} , a solution pH of 6, a temperature of 308 K, and an agitation speed of 130 rpm of the incubator shaker.

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