SUPPORTING INFORMATION FOR:

Recyclable nanocomposite of flowerlike MoS_2@hybrid acid-doped PANI immobilized on porous PAN nanofibers for the efficient removal of Cr (VI)

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15 pages, 14 figures, 7 tables

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Figure S1. The physical appearance of the prepared MoS_2@PANI/PAN nanocomposite.

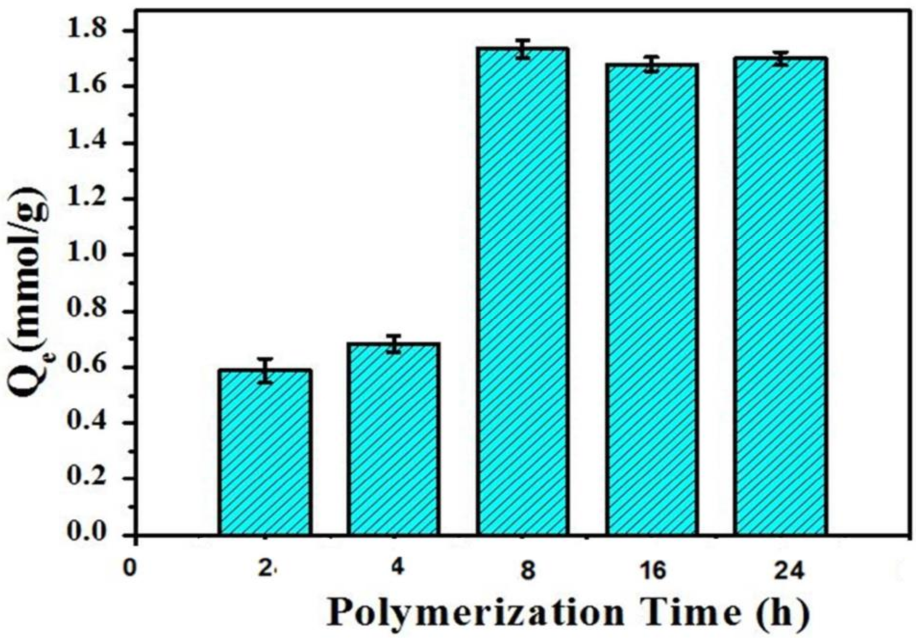


Figure S2. The effect of the polymerization time on the Cr(VI) removal capacity of the nanocomposite.

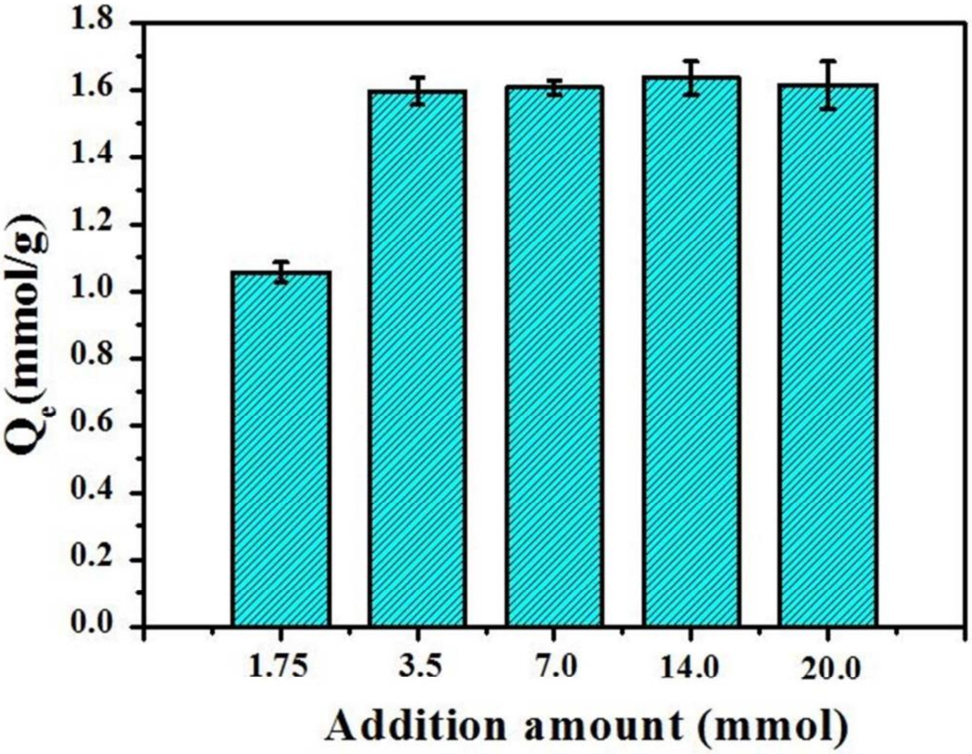


Figure S3. The effect of the added amount of APS on MoS_2@PANI/PAN polymerization and the Cr(VI) removal capacity.

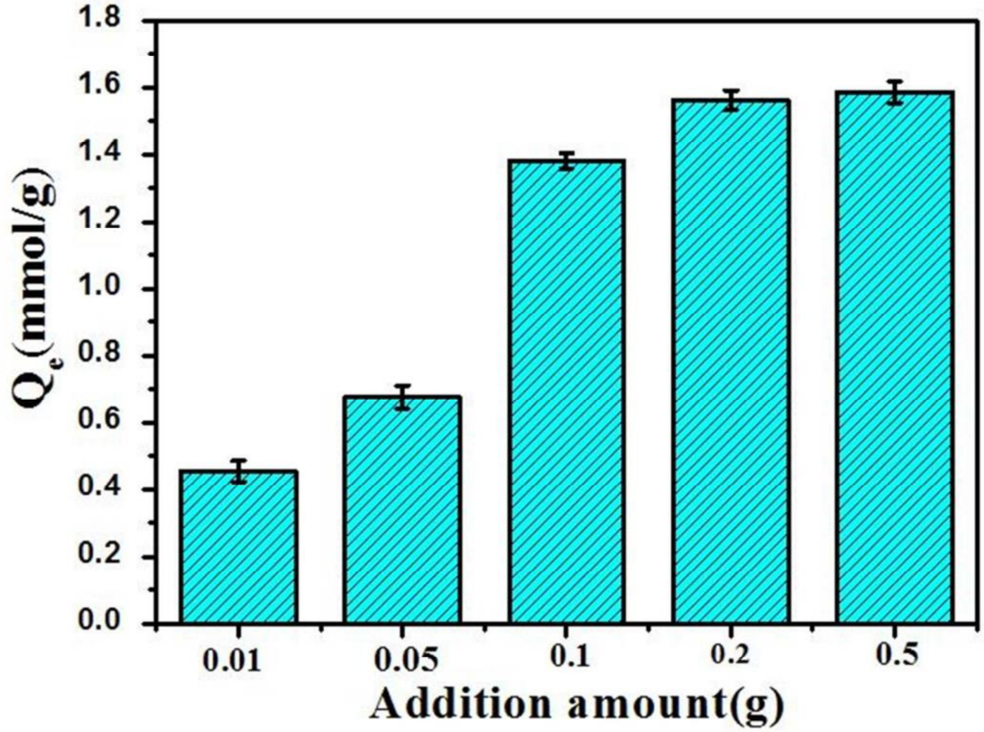


Figure S4. The effect of the added amount of MoS_2 on MoS_2@PANI/PAN polymerization and the Cr(VI) removal capacity.

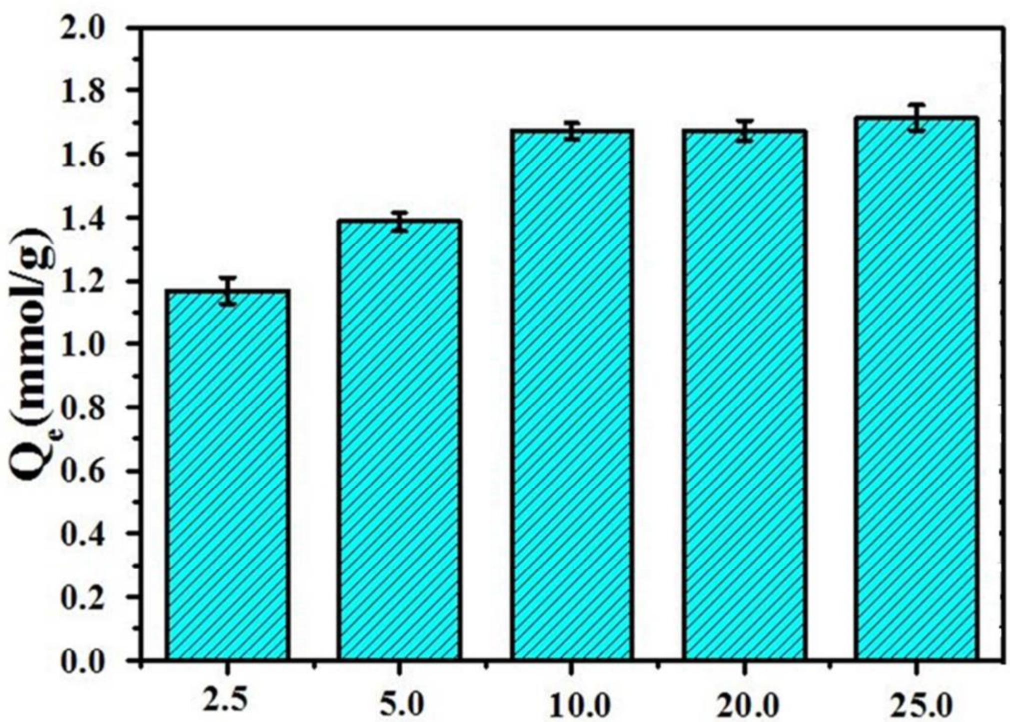


Figure S5. The effect of the added amount of aniline on MoS_2@PANI/PAN polymerization and the Cr(VI) removal capacity.

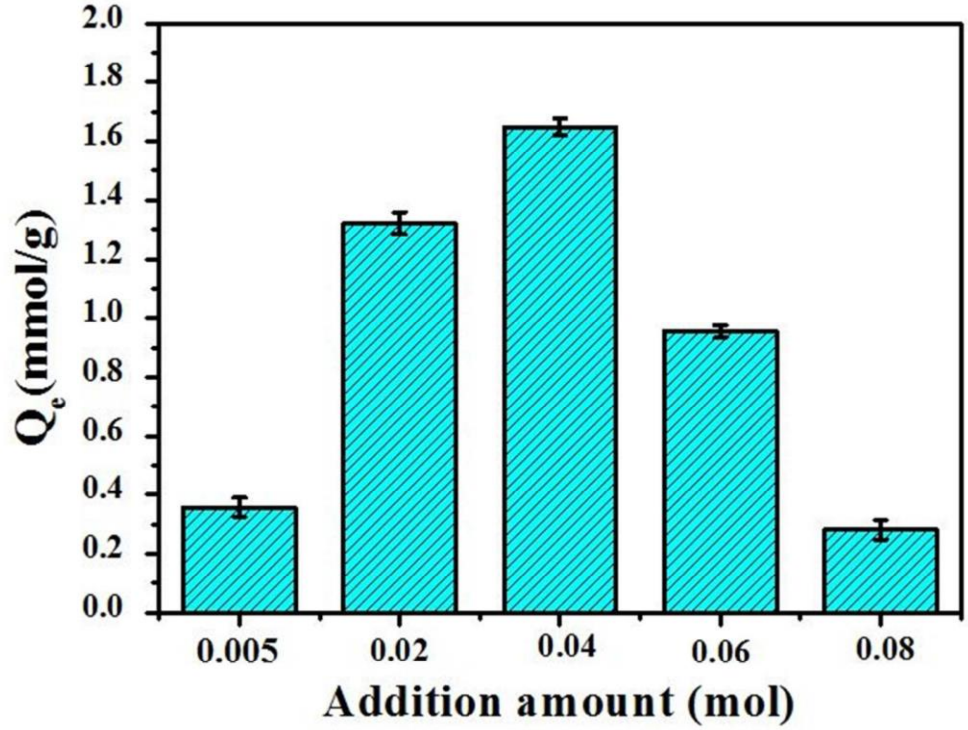
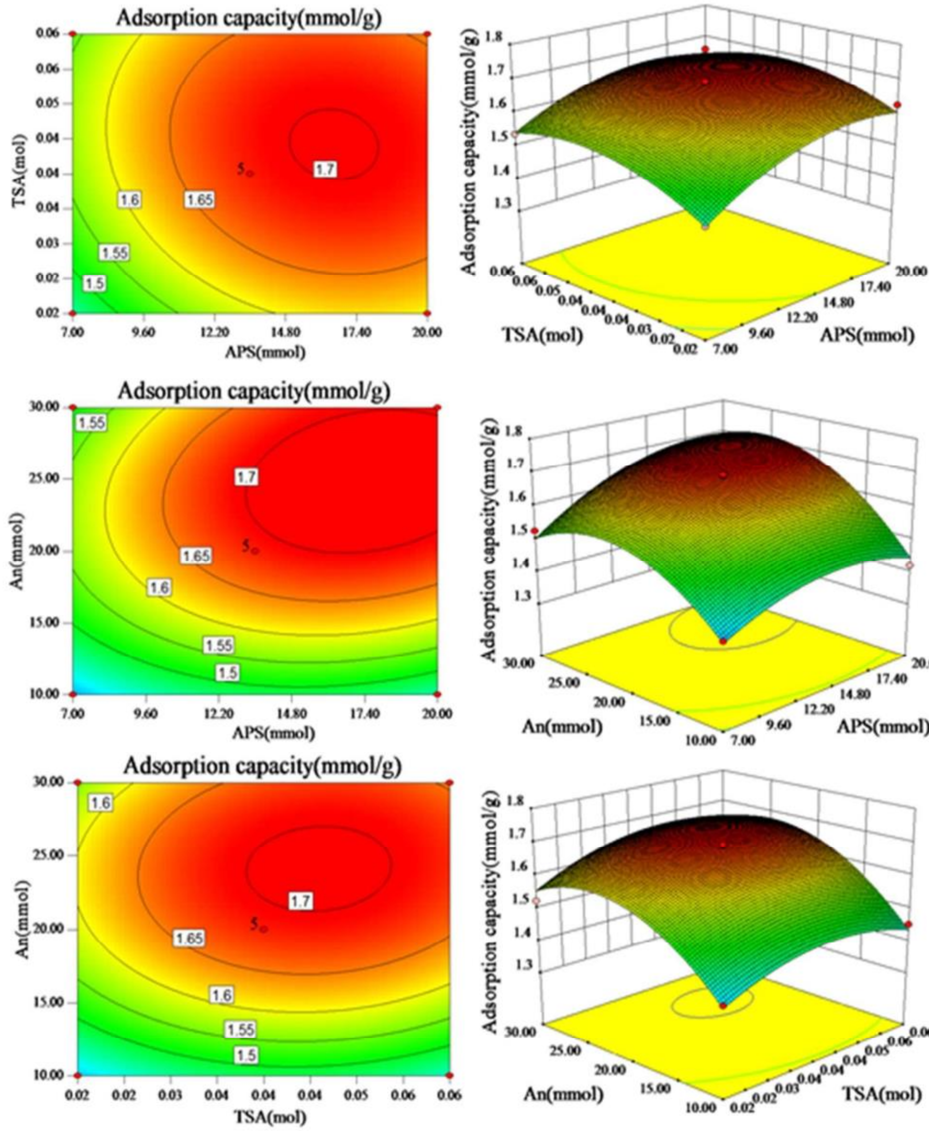


Figure S6. The effect of the added amount of TSA on MoS_2@PANI/PAN polymerization and the Cr(VI) removal capacity.


Adsorption capacity(mmol/g)
TSA(mol)
APS(mmol)
1.5
1.55
1.6
1.65
1.7
5
Adsorption capacity(mmol/g)
TSA(mol)
APS(mmol)
Adsorption capacity(mmol/g)
An(mmol)
APS(mmol)
1.55
1.7
1.65
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Adsorption capacity(mmol/g)
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Adsorption capacity(mmol/g)
An(mmol)
TSA(mol)

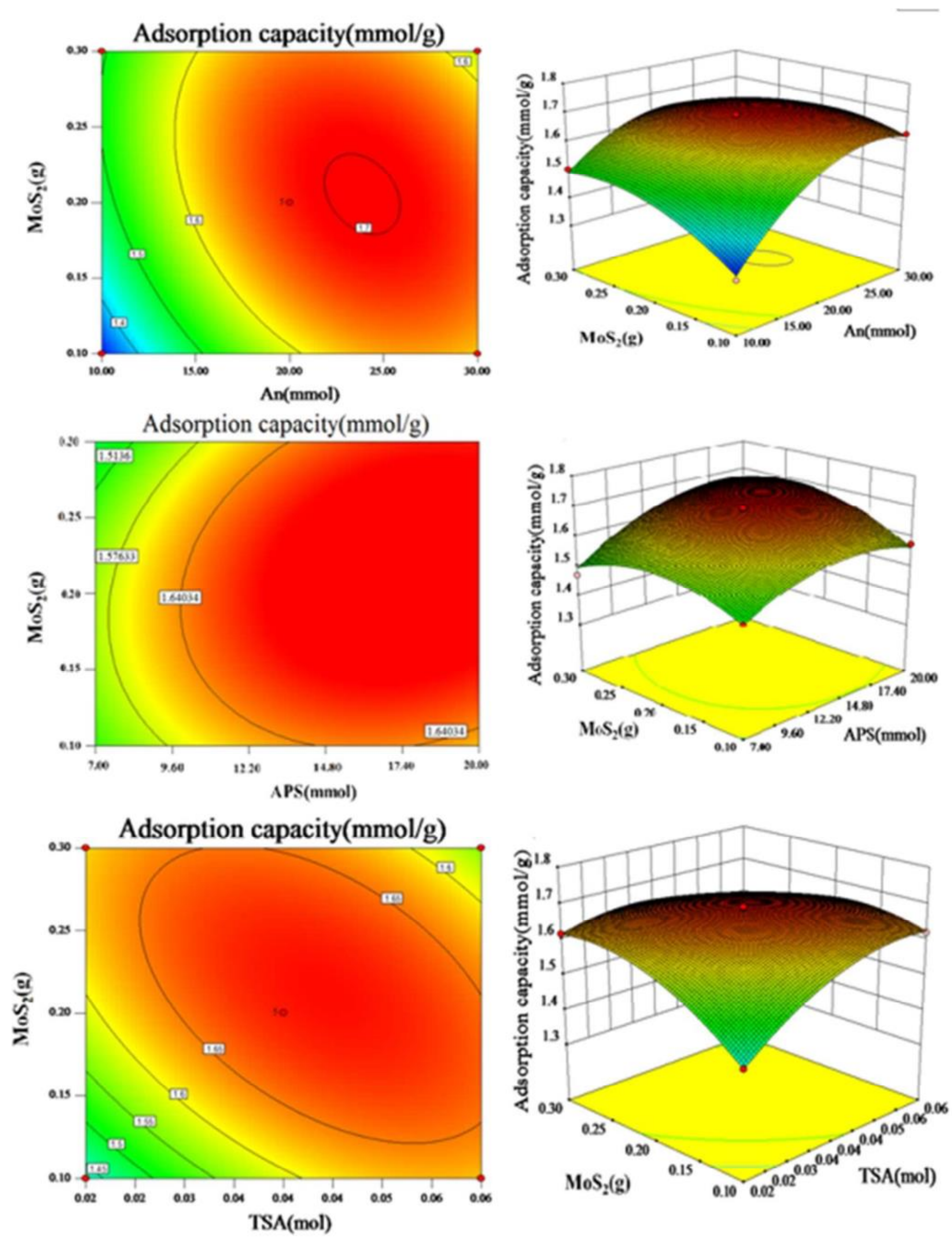

Figure S7. Contour maps and response surfaces for Cr(VI) removal.

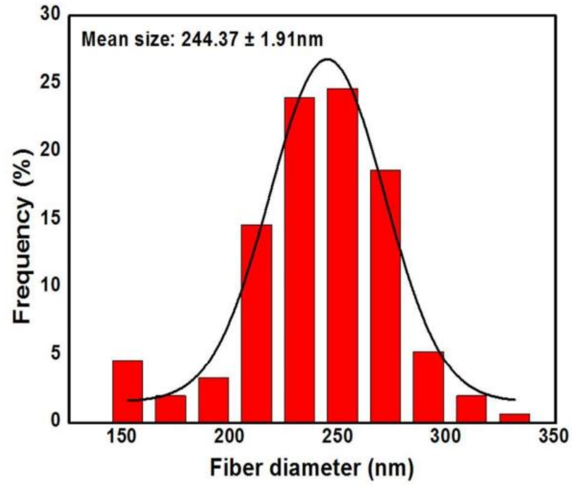

Figure S8. The diameter distribution of pure PAN nanofibers.

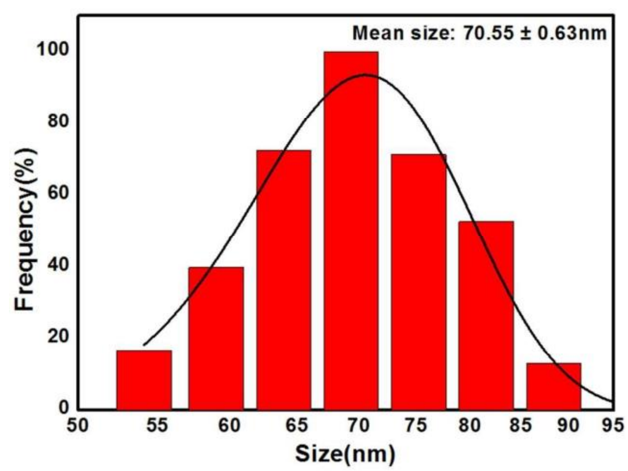

Figure S9. The diameter distribution of pure MoS_2 nanoparticles.

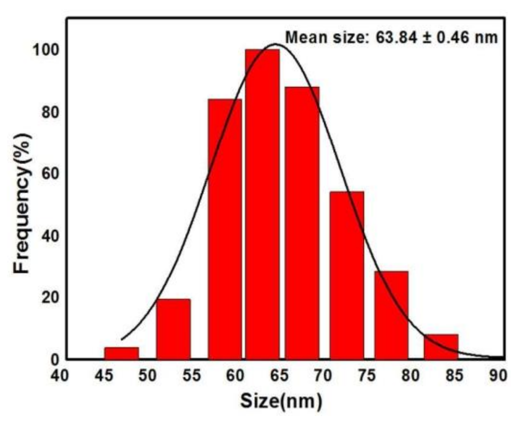

Figure S10. The diameter distribution of pure PANI nanoparticles.

Table S1. The specific surface area of the obtained materials and information on their porous texture

Properties	Bare PAN nanofibers without pores	Bare porous PAN nanofibers	MoS_2@PANI/PAN nanocomposite	Pure MoS_2 nanoparticles
BET surface area (m^2/g)	21.52	13.99	27.06	10.89
Average pore Diameter (nm)	4.36	7.39	10.14	13.08
Pore volume(cm^3/g)	0.023	0.026	0.069	0.036

Table S2. The mechanical properties of PAN fibers before and after modification

Program	Breaking strength(N/mm^2)	Elongation at break (%)	Elasticity modulus (Mpa)
Before modification	39.8	26	150.5
After modification	25.6	16	164.2

The kinetic equations are expressed as follows:

$$\ln\left(q_e - q_t\right) = \ln q_e - k_1 t \qquad (Eq.1)$$

$$\frac{t}{q_t} = \frac{1}{k_2 q_e^2} + \frac{t}{q_e} \qquad (Eq.2)$$

where q_t and q_e (mmol/g) are the amounts of adsorbates adsorbed at time t (min) and at equilibrium, respectively. k_1 (min^{-1}) and k_2 (g $mmol^{-1}$`min^{-1}) are the rate constants of the two models, respectively.

Table S3. The kinetics parameters of Cr(VI) removal by the MoS_2@PANI/PAN nanocomposite

		Pseudo-First-Order			Pseudo-Second-Order			
C_0 (mmol/L)	*Q_{exp}* (mmol/g)	*Q_{eq}* (mmol/g)	*k_1* (min^{-1})	R^2	*Q_{eq}* (mmol/g)	*k_2* (g/mmol min)	*h* (mmol/g min)	R^2
2.0	1.73	1.77	0.08	0.99	1.96	0.06	0.23	0.97

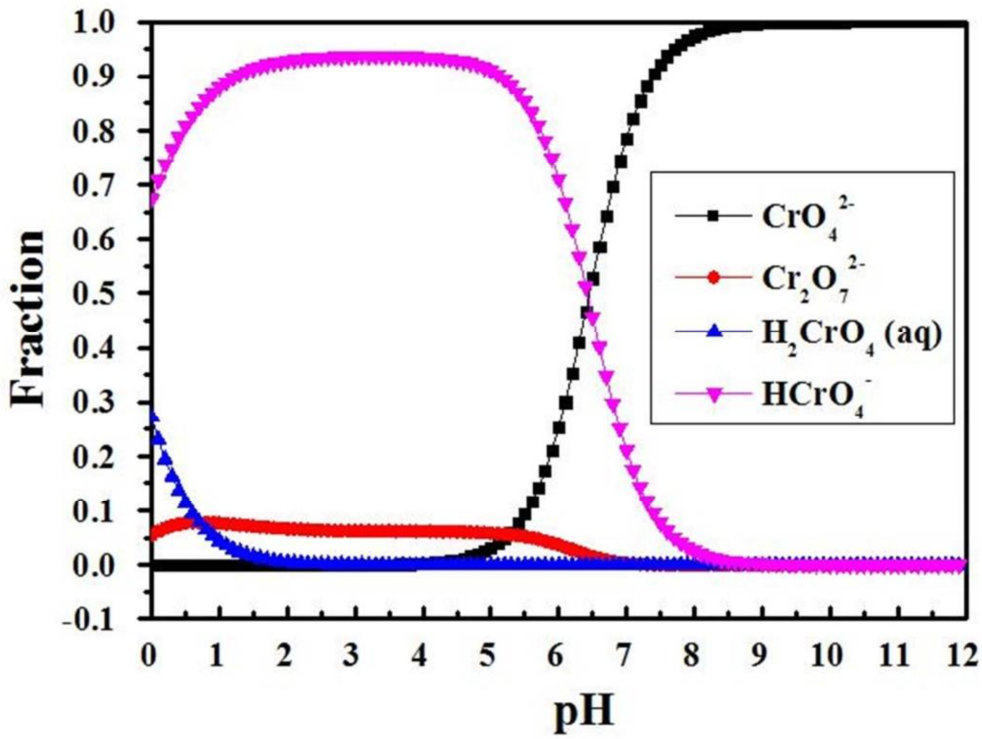

Figure S11. Cr species distribution at different pH values.

Adsorption isotherm models were applied to describe the adsorption behaviors between the liquid and solid phases. The primary theory of Langmuir isotherm model was based on the hypothesis of molecular layer adsorption, and there was no interaction among the adsorbed molecules, indicating the active sites on the adsorbents were equal for the adsorbed molecules. Whereas, the Freundlich isotherm model demonstrated the heterogeneous binding sites on the surface of adsorbents.

The form of the Langmuir isotherm is as *Eq*.3:

$$\frac{C_e}{q_e} = \frac{C_e}{q_m} + \frac{1}{q_m K_L} \qquad (Eq.3)$$

where q_e (mmol/g) is the amount of adsorbates adsorbed at the equilibria, q_m (mmol/g) is the maximum adsorption capacity, C_e (mmol/L) is the equilibrium concentration of adsorbates in the solution and K_L (L/mmol) is the Langmuir adsorption constant.

The Freundlich adsorption equation is given as *Eq*.4:

$$q_e = K_f C_e^{1/n} \qquad (Eq.4)$$

where K_f is the Freundlich adsorption coefficient, which is an index of the adsorption capacity and *1/n* refers to a constant depicting the adsorption intensity.

Table S4. The isothermal parameters of Cr(VI) removal by MoS_2@PANI/PAN nanocomposite

	Langmuir model			Freundlich model		
T (K)	Q_{max} *(mmol/g)*	K_L *(L/mmol)*	R^2	k_f	*n*	R^2
298	5.90	94.7	0.999	28.5	1.92	0.976
308	6.45	102.2	0.999	30.9	1.95	0.972
318	6.57	113.3	0.999	30.6	2.01	0.966

The thermodynamic equations are expressed as follows:

$$\ln K_d = \frac{\Delta S^\circ}{R} - \frac{\Delta H^\circ}{RT} \qquad (Eq.5)$$

$$\Delta G^\circ = -RT \ln K_d \qquad (Eq.6)$$

where K_d (L/mmol) is the adsorption equilibrium constant obtained from Langmuir model, T (K) is the temperature, and R is the universal gas constant (kJ mol^{-1} k^{-1}), respectively.

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Table S5. The thermodynamic parameters of Cr(VI) removal by MoS_2@PANI/PAN nanocomposite

K_d (L/mmol)			ΔH^o (kJ/mol)	ΔS^o (J/ mol·K)	ΔG^o (kJ/mol)		
298K	308K	318K			298K	308K	318K
94.7	102.2	113.3	7.1	61.5	-18.3	-18.9	-19.6

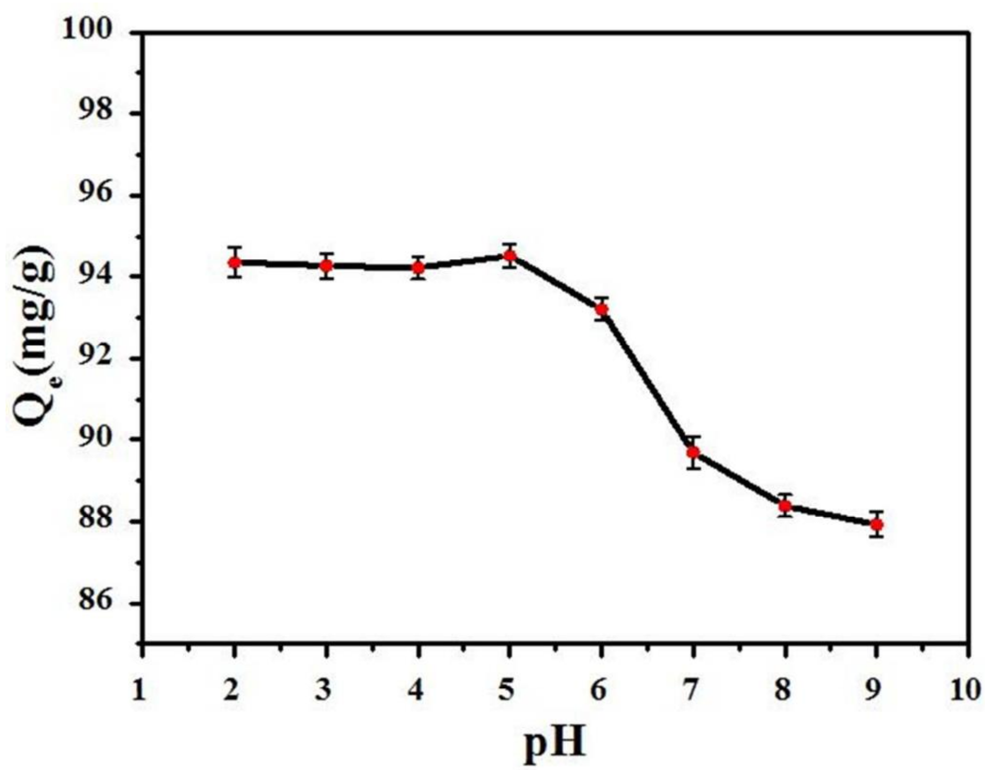

Figure S12. The effect of pH on the removal of humic acid (HA).

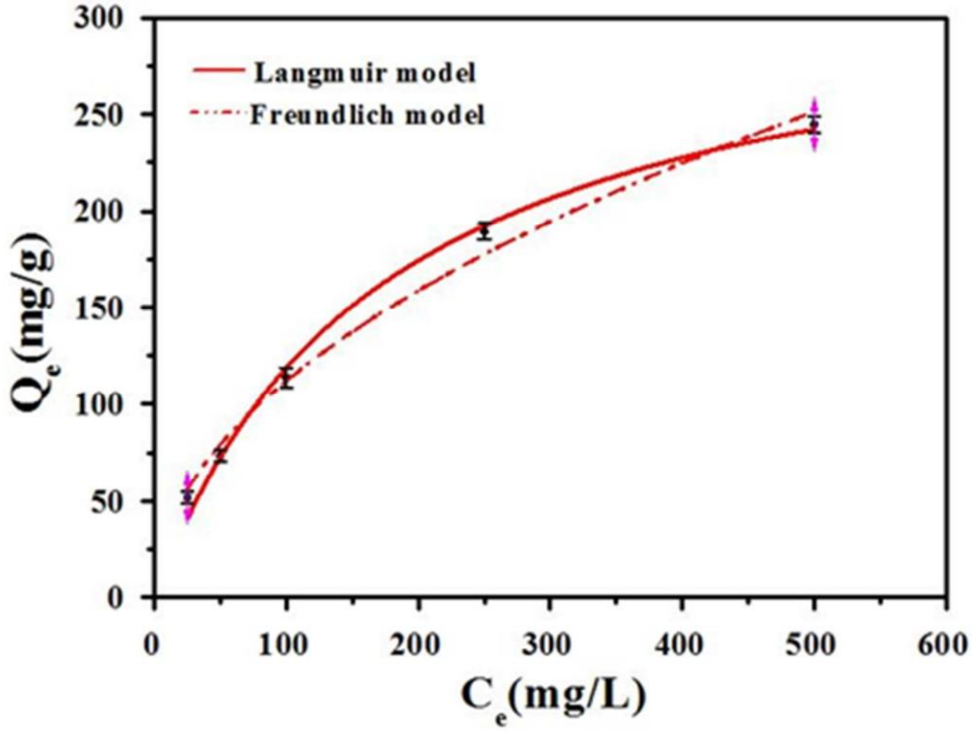

Figure S13. The isotherm of HA removal by MoS_2@PANI/PAN nanocomposite.

Table S6. The geometrical parameters of complex

Program	E (a.u.)	ΔE (kJ/mol)	Bond length (Å)	Bond angle (°)
Single Cr atom	-84.13	---	---	---
PANI^0 PANI^0-Cr	-1375.12	---	---	---
	-1460.41	-794.43	1.94	39.01

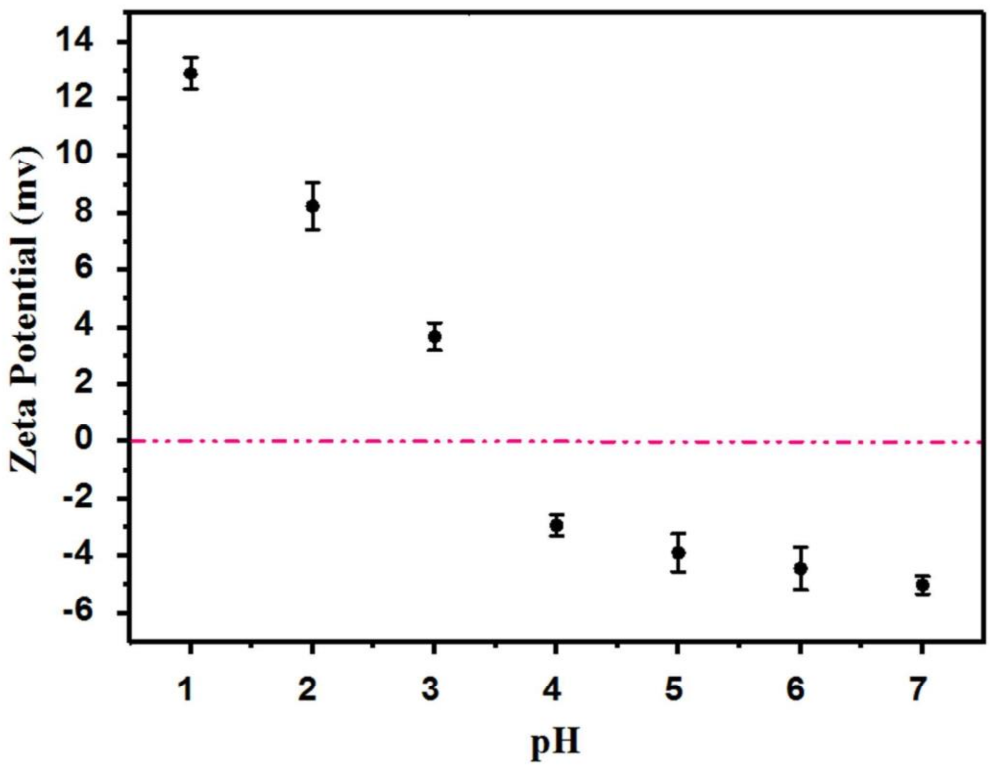

Figure S14. The zeta potential of MoS_2 nanoparticles at different pH values.

Table S7. Comparison of the Cr(VI) removal efficiency of the MoS_2@PANI/PAN nanocomposite and other, previously reported materials

Materials		Removal capacity (mmol/g)	Reference
Equilibrium time (h)			
PANI/H-TNBs	5.0	3.0	28
PANI@ Mg/Al LDH	5.0	7.6	38
HA@PAN Hybrid Nanotubes	0.17	1.2	39
AC modified PEI	3.3	7.7	40
Pyridine copolymer resin	2.0	1.4	41
Fe_3O_4/PANI microspheres	1.2	3.8	42
Rare earth doped titanium dioxide coated carbon sphere	6.0	1.6	43
Nitrogen-doped chitosan-Fe(III) composites	3.3	1.1	44
Al-substituted ferrihydrites	0.66	0.77	45
MoS_2@PANI/PAN nanocomposite	0.50	6.6	This work