Efficient removal of typical dye and Cr(VI) reduction using N-doped magnetic porous carbon

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Isotherm Model.

The Langmuir isotherm is often applicable to a homogeneous adsorption surface with all the adsorption sites having equal adsorbate affinity and is represented by the following equation:

$$q_e = \frac{q_m b C_e}{1 + b C_e}$$

The Freundlich isotherm model assumes heterogeneity of adsorption surfaces, expressed by the following equation:

$$q_e = K_F (C_e)^n$$

where q_e and C_e are the amount of organic pollutants adsorbed per unit weight of adsorbent (mg/g) and the equilibrium concentration (mg/L), respectively; b is the constant related to the free energy of adsorption (L/mg), and q_m is the maximum adsorption capacity; K_F is the Freundlich constant indicative of the relative adsorption capacity of the adsorbent (mg/g), and (n) is the adsorption intensity.

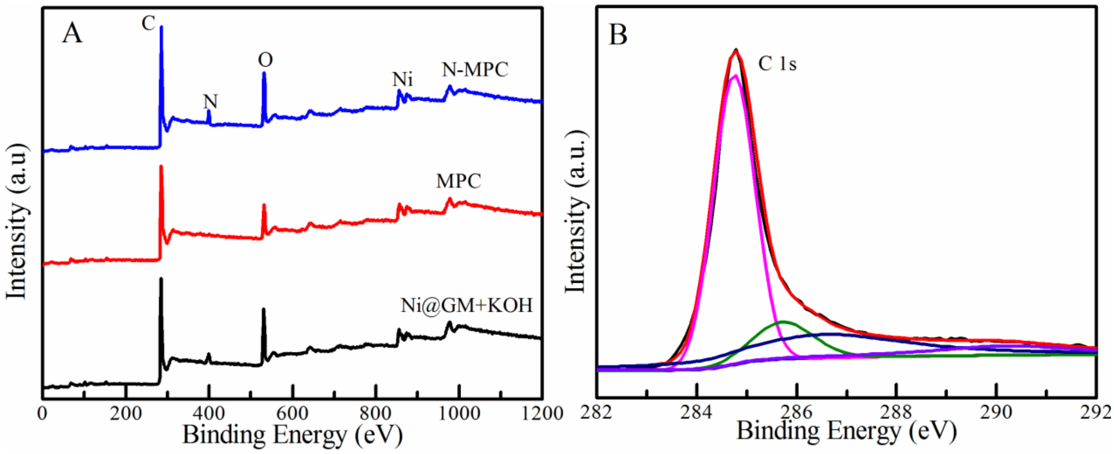


Figure S1. XPS survey spectra of as-prepared materials resulted from different experimental conditions (A) and the high resolution C 1s spectrum of N-MPC (B).

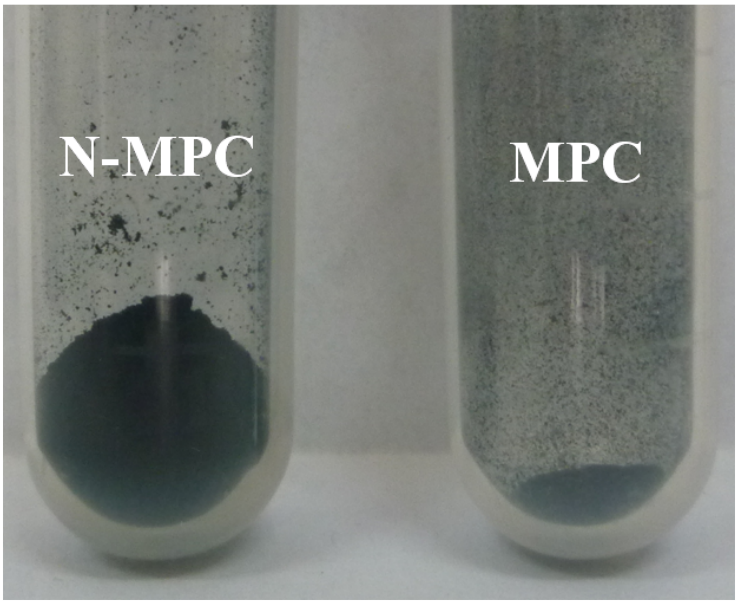


Figure S2. The digital image of 300 mg N-MPC and MPC in a plastic container.

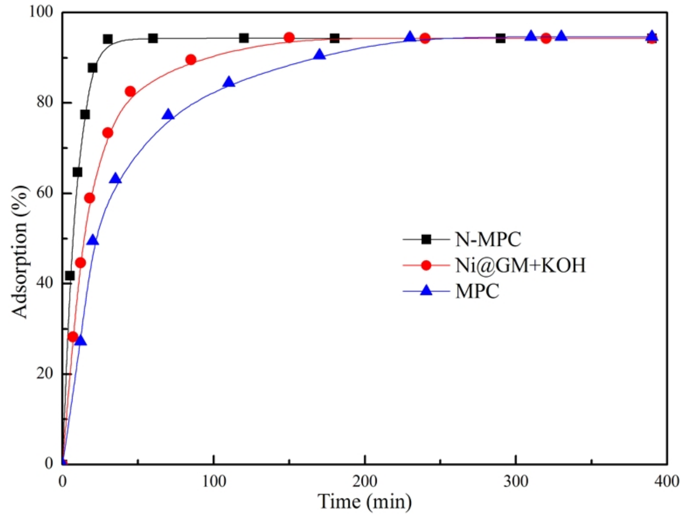


Figure S3. Effect of contact time of the remvoal of Cr(VI) from aqueous solutions to the three different adsorbents ($C_{adsorbent}$= 0.05 g/L, T= 25 ^{o}C, $C_{Cr(VI)initial}$= 6.0 mg/L, pH ~2.5).

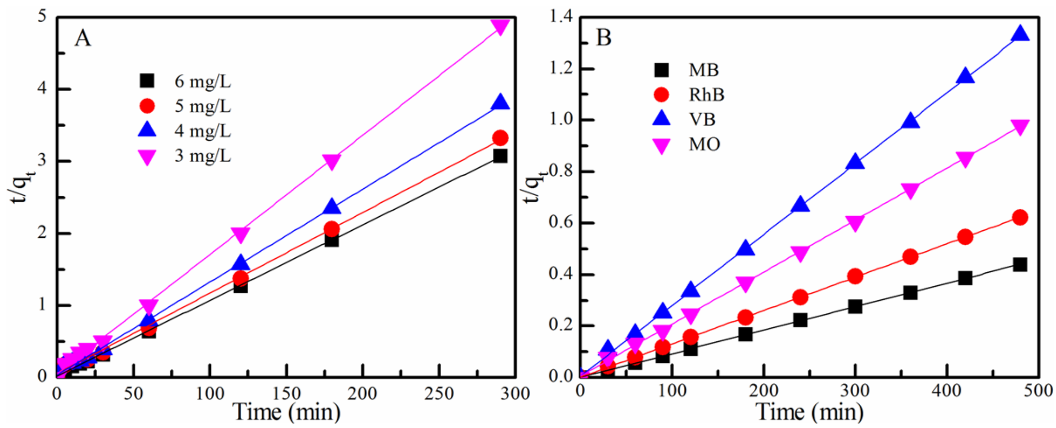


Figure S4. The pseudo-second order sorption kinetics of Cr(VI) (A) and dyes (B) onto N-MPC.

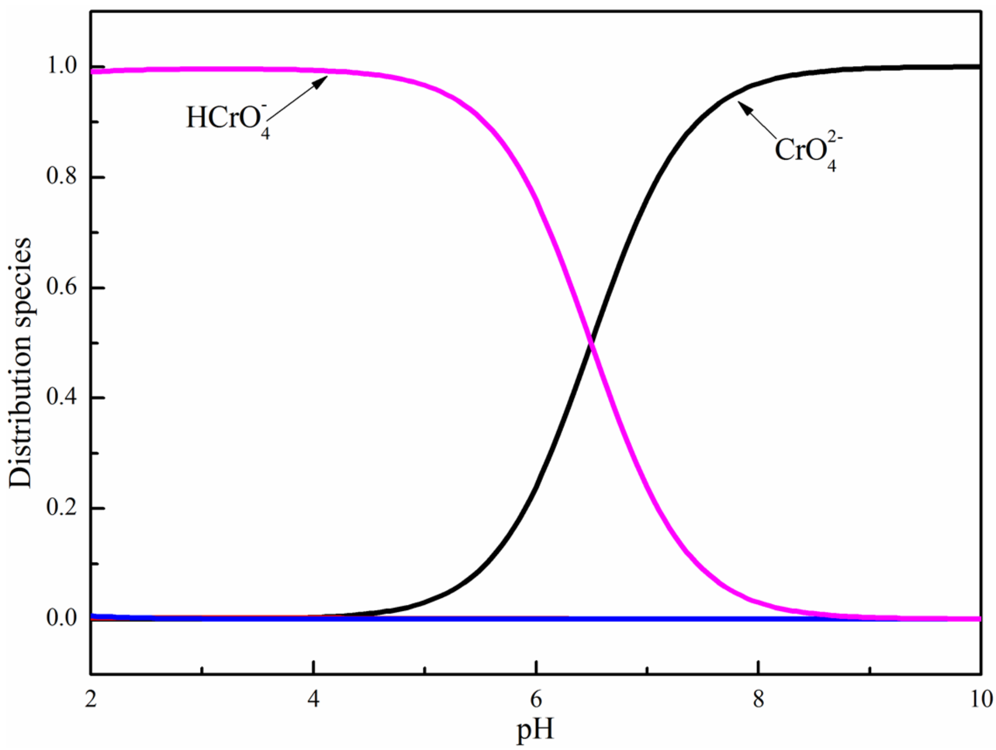


Figure S5. Relative proportion of Cr species as a function of pH values.

Brunauer-Emmett-Teller (BET) isotherm is a theoretical equation, most widely applied in the gas-solid equilibrium systems. This model assumes multilayer adsorption and was developed to describe adsorption phenomena when successive molecular layers of adsorbate form after the completion of a monolayer.

The extinction of this model to liquid-solid interface is described by Eq. (1), which is linearized in Eq. (2).

$$q_e = \frac{C_{BET} C_e q_s}{(C_s - C_e)[1 + (C_{BET} - 1)(C_e/C_s)]} \quad (1)$$

$$\frac{C_e}{(C_s - C_e)q_e} = \frac{1}{C_{BET} q_s} + (\frac{C_{BET} - 1}{C_{BET} q_s})(\frac{C_e}{C_s}) \quad (2)$$

q_e amount of adsorbate in the adsorbent at equilibrium (mg/g)
C_e equilibrium concentration (mg/L)
C_s adsorbate monolayer saturation concentration (mg/L)
C_{BET} BET adsorption isotherm relating to the energy of surface interaction (L/mg)
q_s theoretical isotherm saturation capacity (mg/g)

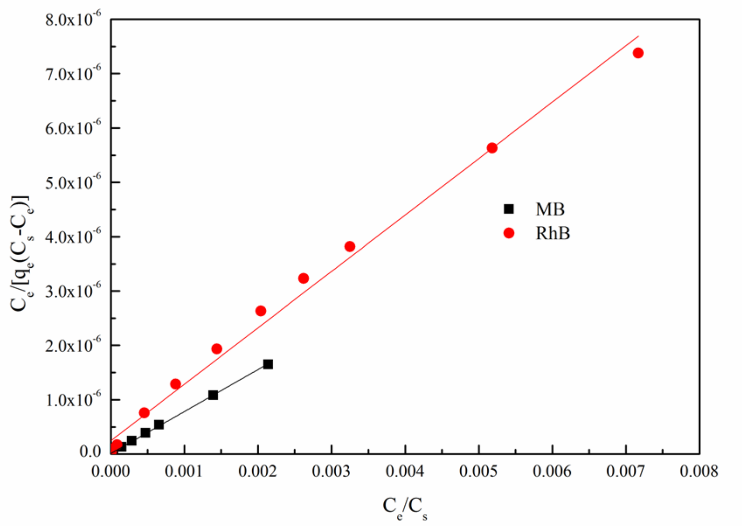


Figure S6. Linearized forms of BET model for adsorption of MB and RhB by N-MPC.

It was found that the experimental data fit the BET model isotherm well, and the correlation coefficients R^2 was 0.9997 (MB) and 0.9983 (RhB), respectively. Hence, the BET model is more suitable for describe the adsorption behavior of MB and RhB over N-MPC.

Table S1. Kinetics parameters of Cr(VI) adsorption on N-MPC.

		The second-order kinetics		
	q_{exp} (mg/g)	k_2(g/(mg·min))	q_{cal}(mg/g)	R^2
6.0 mg/L	96.27	0.0023	95.42	0.999
5.0 mg/L	90.27	0.0032	89.45	0.997
4.0 mg/L	78.33	0.0044	77.52	0.999
3.0 mg/L	59.33	0.0049	60.42	0.999

Table S2. The adsorption capacities for different dyes on different adsorbents.

adsorbents	MB (mg/g)	RhB (mg/g)	VB (mg/g)	MO (mg/g)
AC	330.25	194.32	157.52	202.76
N-MPC	1284.09	819.39	376.29	565.41
MPC	937.34	599.73	210.65	270.12
Ni@GM+KOH	1054.78	635.24	270.59	342.81

Table S3. Molecular ball and spring model, molecular size for the four dyes.

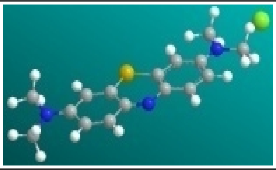
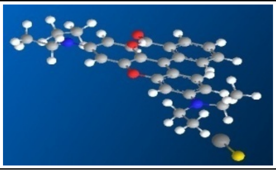
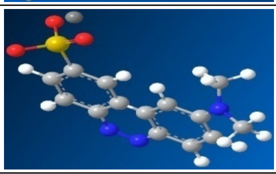
Dye	Molecular model	Molecular size (nm)	Molecular weight (g/mol)	Nature	UV absorption (nm)
MB		1.26×0.77×0.65	320	basic	665
RhB		1.59×1.18×0.56	478	basic	554
VB		1.47×1.41×0.44	506	basic	603
MO		1.31×0.55×0.18	327	acidic	465

Table S4. Kinetics parameters for the different dyes on N-MPC.

		The second-order kinetics		
	q_{exp} (mg/g)	k_2(g/(mg·min))	q_{cal} (mg/g)	R^2
MB	1091.31	0.00048	1094.09	0.999
RhB	770.50	0.00111	769.23	0.999
VB	360.91	0.00125	363.64	0.999
MO	489.47	0.00063	495.05	0.999

Table S5. Comparison of the adsorption capacities of MB, MO, RhB and CV onto various adsorbents.

Dyes	Adsorbents	Adsorption capacity (mg/g)	Ref.
MB	anaerobic granular sludge	212	1
	graphene/magnetite composite	43.08	2
	CNTs-A	400	3
	copper silicate hollow spheres	162	4
	Metal silicate nanotubes	400	5
	N-MPC	1284.09	This work
MO	hyper-cross-linked polymeric	70	6
	silkworm exuviae	87	7
	chitosan/Fe_2O_3/CNTs	66	8
	CNTs-A	149	3
	N-MPC	565.41	This work
RhB	activated carbons	400.0	9
	Zeolite	37.8	10
	Porous carbon	479.0	11
	Carbonaceous adsorbent	82.8	12
	N-MPC	819.39	This work
VB	Perlite	21.7	13
	BSD	39.3	14
	G-SO_3H/Fe_3O_4	200.6	15
	N-MPC	819.39	This work

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