Electronic supplementary information

Cr(III) adsorption by fluorinated activated boron nitride: a combined experimental and theoretical investigation

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Fax: +86-22-60202660; Tel: +86-22-60202660;
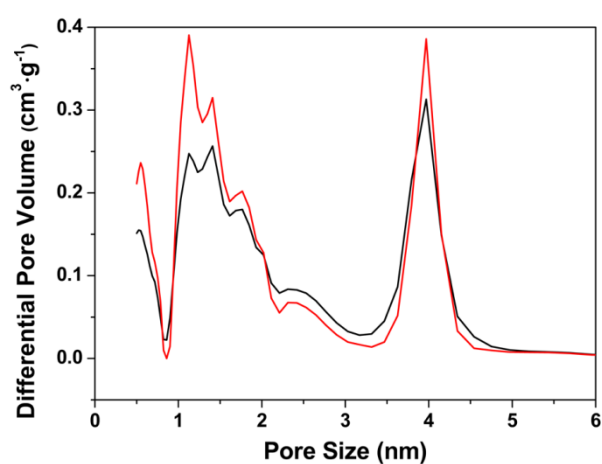*E-mail: china.peng.jin@gmail.com.(P. J.) ; tangcc@hebut.edu.cn (C. T.)*

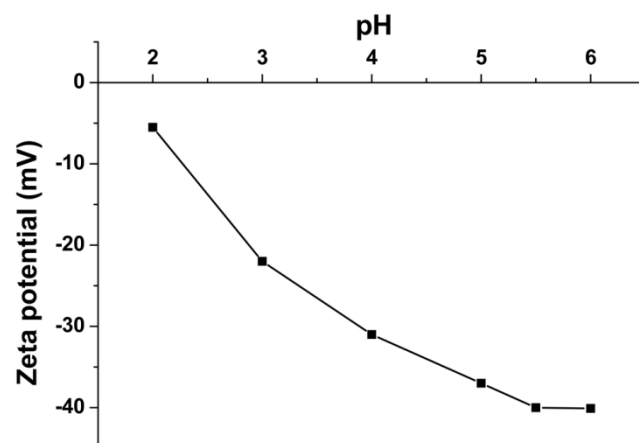**Fig. S1** Pore size distributions of ABN (black) and F-ABN (red).

Fig. S2 Zeta potential vs. pH value of F-ABN.

Kinetic model

The pseudo-first-order and pseudo-second-order models are displayed in Eqs. S1 and S2, respectively:

$$\ln(q_e\text{-}q_t) = \ln q_e - k_1 t \tag{S1}$$

$$t/q_t = 1/k_2 q_e^2 + t/q_e \tag{S2}$$

where q_e and q_t (mg/g) are the amounts of Cr(III) adsorbed at equilibrium and time t, respectively; k_1 (min^{-1}) and k_2 (g mg^{-1} min^{-1}) are the rate constants of the pseudo-first-order and pseudo-second-order adsorptions, respectively.

Table S1 Comparison between the adsorption kinetic data of the pseudo-first-order and pseudo-second-order models.

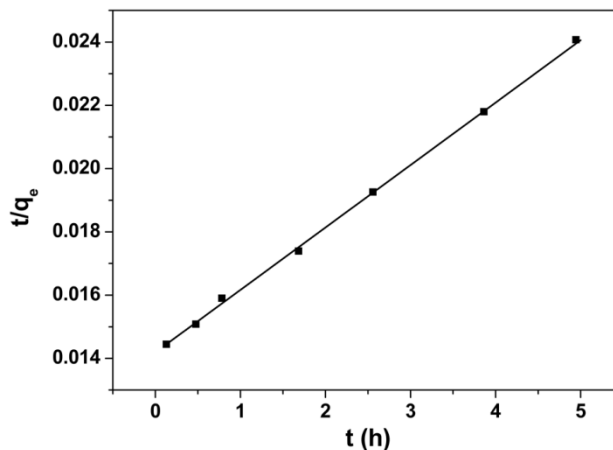| adsorbent	pseudo-first-order			pseudo-second-order		
	k_1(min^{-1})	q_e (mg g^{-1})	R^2	k_2(g mg min^{-1})	q_e (mg g^{-1})	R^2
F-ABN	1.125×10^{-5}	153	0.721	1.61×10^{-5}	207.79	0.992

Fig. S3 The fitting of Cr(III) adsorption by F-ABN using the pseudo-second-order kinetic model (initial concentration of Cr(III): 52 mg/L; pH: 5.5; adsorbent: 50 mg; T: 30 °C).

Thermodynamic model

Using the values of Langmuir constant b (3.45) and Eqs. S3 - S5, one can calculate the variations of apparent enthalpy (ΔH), apparent free energy (ΔG), and apparent entropy (ΔS) of chromium sorption on F-ABN:

$$\ln b = - (\Delta H/RT) + \text{constant} \qquad (S3)$$

$$\Delta G = - RT \ln b \qquad (S4)$$

$$\Delta S = (\Delta H - \Delta G)/T \qquad (S5)$$

where R is the gas law constant and T is the absolute temperature.

Table S2 The apparent thermodynamic parameters of Cr(III) adsorption on F-ABN.

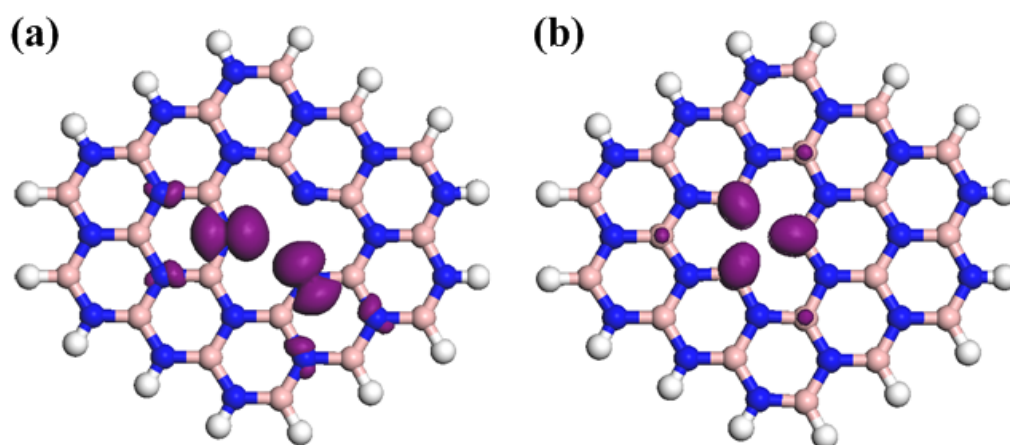| T (K)	ΔG (kJ/mol)	ΔH (kJ/mol)	ΔS (J/mol K)
283	-0.71	-0.68	0.106
293	-2.51	-2.49	0.068
303	-3.16	-3.15	0.033

Fig. S4 Spin density distributions of the (a) BNF_{Bv} and (b) BNF_{Nv}.