Electronic Supplementary Material

Immobilization of nano-zero-valent irons by carboxylated cellulose nanocrystals for wastewater remediation

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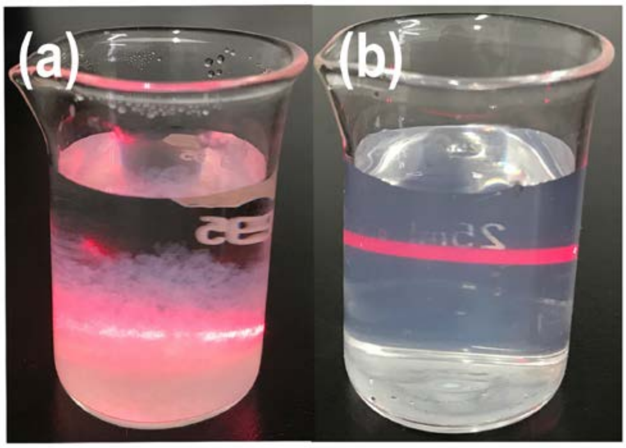

Fig. S1. Physical appearances of CNC (a) and CCNC (b) in aqueous solution (photos taken immediately after solution preparation).

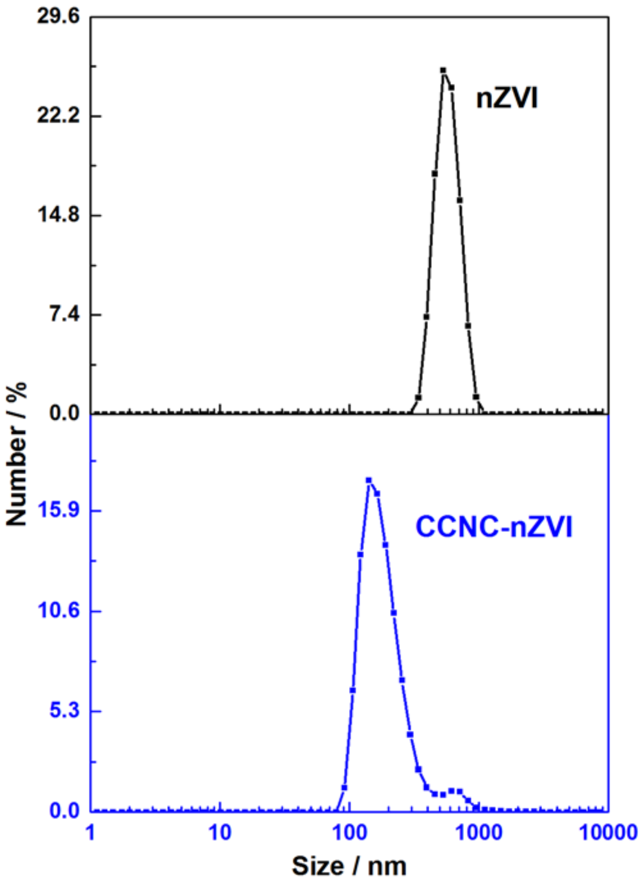

Fig. S2. The hydraulic diameter of nZVI and CCNC-nZVI.

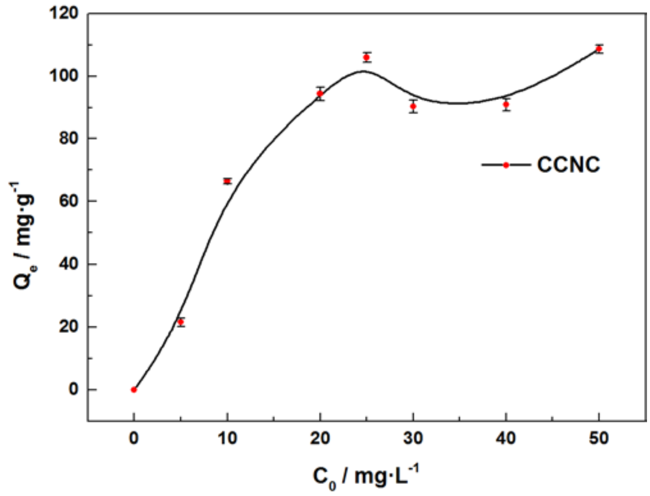

Fig. S3. Saturated adsorption of Fe(III) ions on CCNC (m = 0.1 g·L^{-1}, C_0 = 25 mg·L^{-1}, pH = 4.0, temperature at 298.15 K).

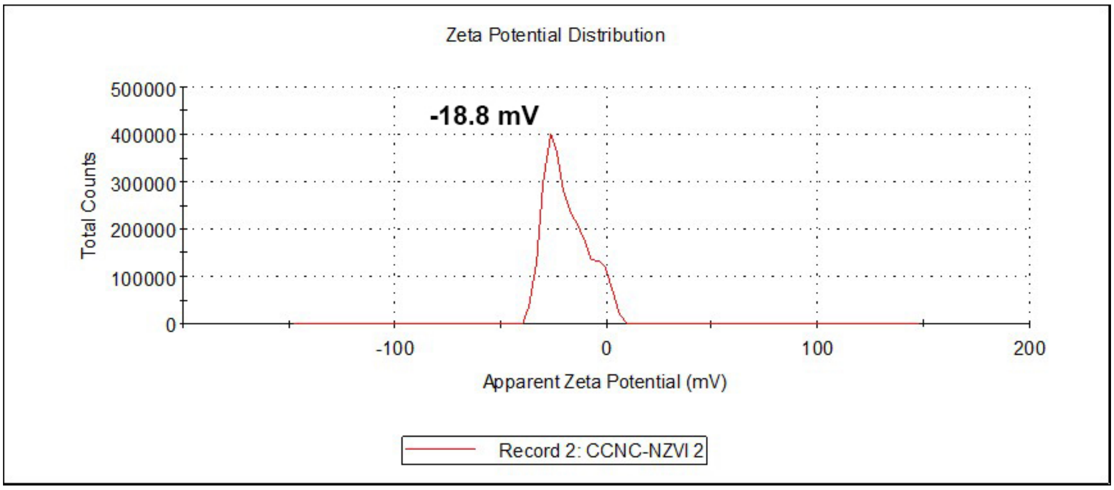

Fig. S4. The Zeta potential of CCNC-nZVI.

Adsorption kinetics, isotherms and thermodynamic studies

Pseudo-first-order and pseudo-second-order kinetic models were usually used to describe the relationship between adsorption rate and substrate concentration. The kinetics equations were shown as follows:

$$\ln\left(1-\frac{q_t}{q_e}\right)=-k_1\times t \tag{1}$$

$$\frac{t}{q_t}=\frac{1}{k_2q_e^2}+\frac{t}{q_e} \tag{2}$$

where q_e denotes the equilibrium adsorption capacity (mg·g^{-1}), q_t is the adsorption capacity (mg·g^{-1}) at a certain time; k_1 (min^{-1}) and k_2 (g·(mg·min)$^{-1}$) are the rate constants.

The Langmuir model considers that the monolayer adsorption occurs on the uniform surface of the adsorbent. The equation is expressed as follows:

$$\frac{C_e}{q_e}=\frac{1}{c_Lq_{\max}}+\frac{C_e}{q_m} \tag{3}$$

where C_e (mg·L^{-1}) and q_e (mg·g^{-1}) represents the equilibrium adsorption concentration and equilibrium adsorption capacity, respectively; q_{max} (mg·g^{-1}) represents the maximum adsorption capacity and c_L (L·mg^{-1}) is the Langmuir constant.

The Freundlich adsorption model considers adsorption to occur on the nonuniform surface and is calculated by the following Eqs. :

$$\log q_e = \log c_F + \frac{\log C_e}{\mathrm{n}} \quad (4)$$

where C_e ($mg\cdot L^{-1}$) and q_e ($mg\cdot g^{-1}$) denotes the equilibrium concentration and the equilibrium adsorption capacity at a certain solution concentration, respectively; Freundlich constant c_F ($L\cdot mg^{-1}$) and 1/n can be obtained from the linear plot of $\log q_e$ versus $\log C_e$.

The change thermodynamic values of enthalpy (ΔH, $kJ\cdot mol^{-1}$), Gibbs free energy (ΔG, $kJ\cdot mol^{-1}$) and entropy (ΔS, $J\cdot mol^{-1}\cdot K^{-1}$) were represented as follows：

$$K_C = \frac{q_e}{C_e} \quad (5)$$

$$\Delta G = -RT \ln K_C \quad (6)$$

$$\Delta G = \Delta H - T\Delta S \quad (7)$$

where T (K) is the temperature, K_c is the equilibrium constant and R (8.314 $J\cdot mol^{-1}\cdot K^{-1}$) is the ideal gas constant. q_e ($mg\cdot g^{-1}$) and C_e ($mg\cdot L^{-1}$) are the equilibrium adsorption capacity of adsorbents and equilibrium concentrations of metal ions at certain solution concentration, respectively.

Table S1. Thermodynamic parameters for Pb(II) adsorption on CCNC-nZVI.

Ion concentration /mg·L^{-1}	Δ*H* /kJ·mol^{-1}	Δ*S* /kJ·K^{-1}·mol^{-1}	Δ*G* /kJ·mol^{-1}		
			298.15 K	308.15 K	318.15 K
50	-220.93	-0.66	-21.11	-21.82	-7.87
100	-58.75	-0.16	-10.39	-8.95	-7.15
150	-32.44	-0.09	-6.45	-6.63	-4.73
200	-32.38	-0.09	-5.40	-5.38	-3.61
250	-52.71	-0.16	-5.69	-4.30	-2.54
300	-42.14	-0.13	-4.16	-2.79	-1.61