Adsorption Behavior and Mechanisms of Cr(VI) on the

Functionalized Carboxymethyl Cellulose-based Sponge

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Equations involved in the paper

$$\varepsilon = \frac{C_0 - C_e}{C_0} \times 100\%$$

(1)

$$q_e = \frac{(C_0 - C_e)V}{m}$$

(2)

Where C_0 (mg L^{-1}) and C_e (mg L^{-1}) are the initial and equilibrium concentrations of Cr(VI), respectively; V (L) is the volume of solvent, and m (g) is the mass of PEI-PAM-CMC.

$$\ln(q_e - q_t) = \ln q_e - k_1 t$$

(3)

$$\frac{t}{q_t} = \frac{1}{k_2 q_e^2} + \frac{1}{q_e} t$$

(4)

$$q_t = k_d t^{0.5}$$

(5)

Where t (min) is the adsorption time; q_t and q_e (mg g^{-1}) represent the adsorption capacity at time t and equilibrium, respectively; k_1 (min^{-1}), k_2 (g mg^{-1} min^{-1}) and k_d (mg g^{-1} min$^{0.5}$) are the rate constants for the pseudo-first-order, pseudo-second-order kinetic models and intra-particle diffusion model, respectively.

$$\frac{c_e}{q_e} = \frac{1}{bq_{max}} + \frac{c_e}{q_{max}}$$

(6)

$$\ln q_e = \frac{1}{n} \ln c_e + \ln K_f$$

(7)

Where q_{max} (mg g^{-1}) is the theoretical maximum equilibrium adsorption capacity; b (L mg^{-1}) is adsorption constant of the Langmuir model, K_f (mg$^{1-1/n}$L$^{1/n}$g^{-1}) is the Freundlich equilibrium constant related to adsorption capacity; n is the Freundlich coefficient.

$$\Delta G = -RT \ln K_0 \qquad (8)$$

$$\ln K_0 = \frac{\Delta S}{R} - \frac{\Delta H}{RT} \qquad (9)$$

Where R is the ideal gas constant (8.314 J mol^{-1} K^{-1}), T is the temperature in Kelvin, and K_0 (L g^{-1}) is the adsorption equilibrium constant.
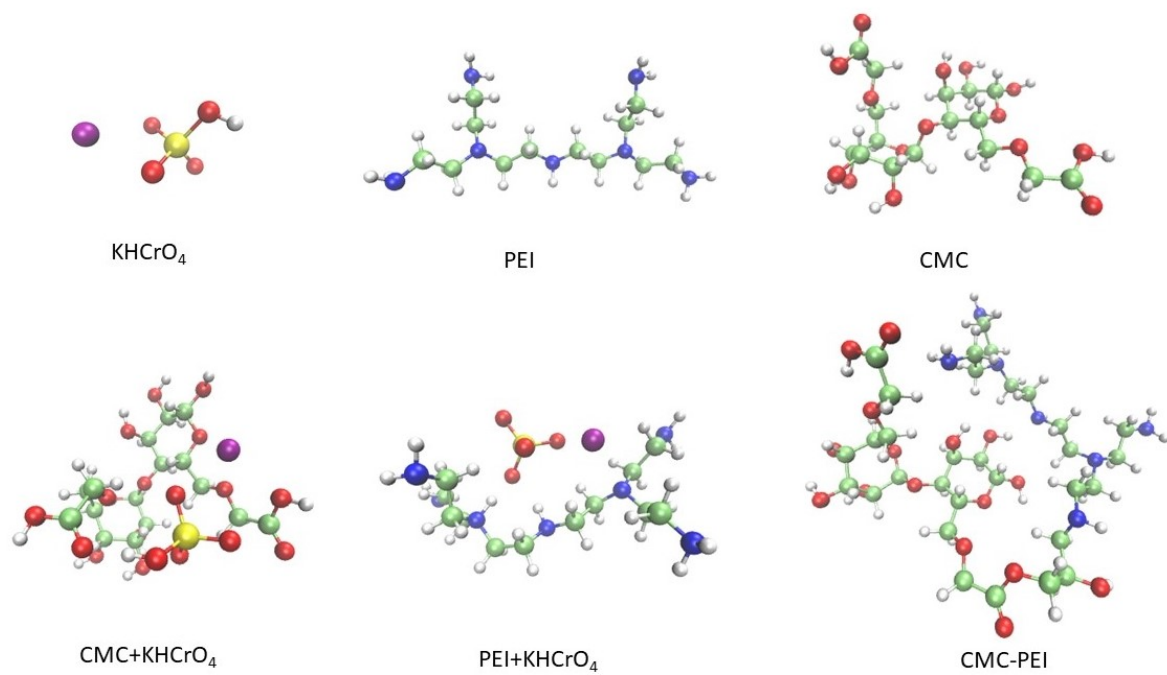
KHCrO₄

PEI

CMC

CMC+KHCrO₄

PEI+KHCrO₄

CMC-PEI

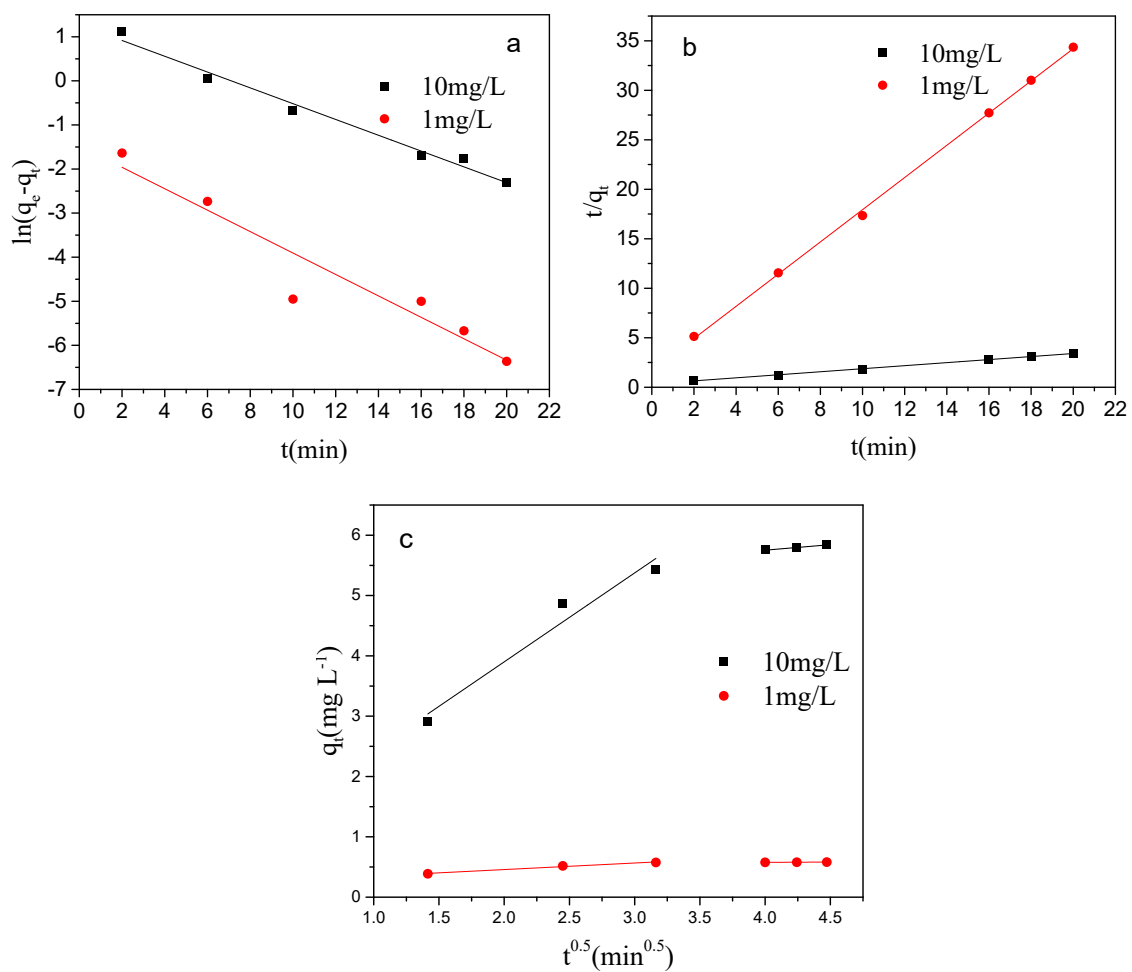Fig. S1 Models of the theoretical calculation.

Fig. S2 Linearly fitting results obtained by pseudo-first-order kinetic model (a), pseudo-second-order kinetic model (b) and intra-particle diffusion model (c).
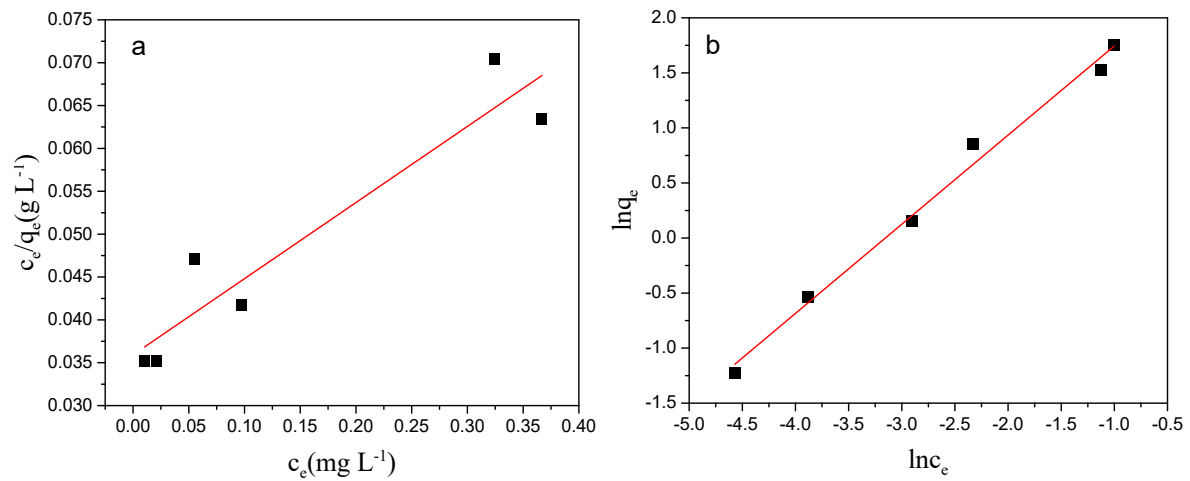
Fig. S3 Linearly fitting results obtained by Langmuir isotherm model (a) and Freundlich isotherm model (b).