Article

N-cetyltrimethylammonium bromide-modified zeolite Na-A from waste fly ash for hexavalent chromium removal from in-dustrial effluent

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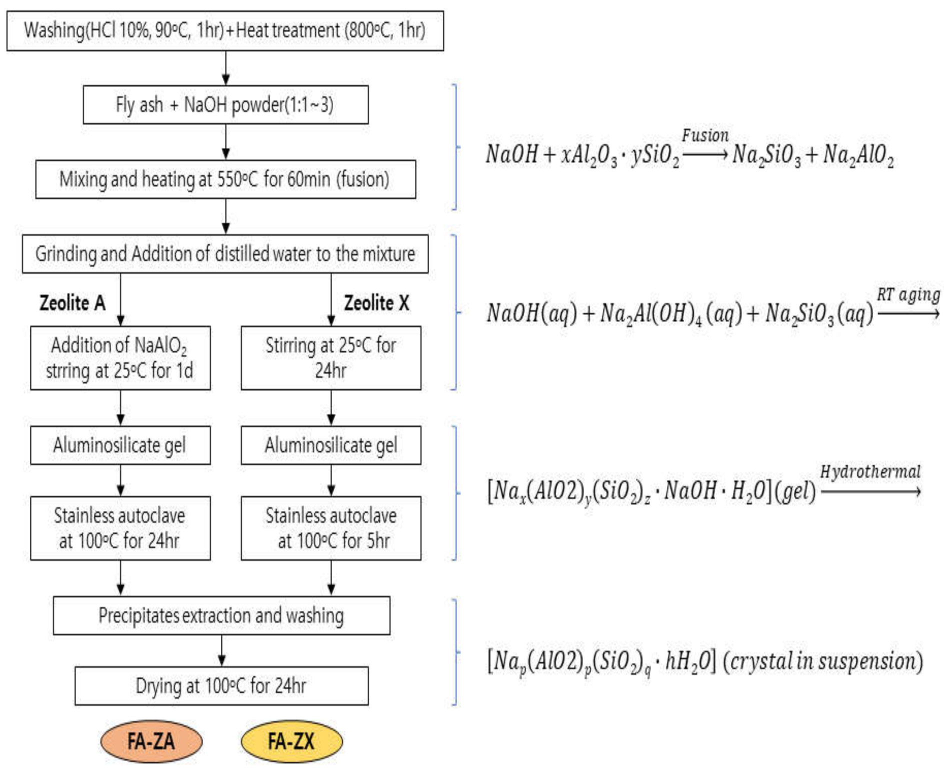

Figure S1. Synthesis of Zeolite (Na-A and Na-X) from Coal fly ash (Choi et al., 2019).

Assessment of sorption behavior

The influence of the reaction rate on the initial metal ion concentration was examined for the pseudo-first-order (PFO), pseudo-second-order (PSO), and Elvovich kinetic models using CTAB@FZA, as given in Eqs. (1),(2), and (3) respectively:

PFO kinetic equation: $$Log(Q_e - Q_t) = LogQ_e - \left(\frac{k_1}{2.03}\right)t \quad (1)$$

PSO kinetic equation: $$\frac{t}{Q_t} = \frac{1}{k_2 Q_e^2} + \left(\frac{1}{Q_e}\right)t \quad (2)$$

Elvovich kinetic equation: $$Qt = \beta \ln(t) + \beta \ln(\alpha) \quad (3)$$

where q_e and q_t are the numbers of metal ions removed at equilibrium (mg·g^{-1}); t is the adsorption duration (min); k_1 and k_2 are adsorption rate constants; α (mg/g·min) is the initial rate constant, and β (mg/g) is the desorption constant of the Elovich kinetics.

The adsorption isotherm behavior was analyzed using the isotherm models shown in Eqs. (4), (5), and (6):

Langmuir isotherm equation: $$\frac{C_e}{Q_e} = \left(\frac{1}{k_l + Q_m}\right) + \left(\frac{1}{Q_m}\right)C_e \quad (4)$$

Freundlich isotherm equation: $$\log Q_e = \log k_f + \left(\frac{1}{n}\right)\log K_c \quad (5)$$

Temkin isotherm equation: $$Q_e = \frac{RT}{bT}\ln AT + \frac{RT}{bT}\ln C_e \quad (6)$$

where the adsorbate equilibrium concentrations are represented by c_e (mg L^{-1}) for the liquid phase and q_e (mg g^{-1}) for the solid phases; q_m (mg g^{-1}) indicates the maximum removal efficiency; b denotes the Langmuir adsorption equilibrium constant; K_f is the Freundlich equilibrium constant, which symbolizes the adsorption efficiency; $1/n$ is the Freundlich adsorption constant, the reciprocate of the adsorption intensity; B is the Temkin isotherm constant; and K_T is the Temkin isotherm equilibrium binding constant.

The universal gas constant (R) was adjusted to 8.314 J^{-1}.mol^{-1}.K and the temperature was applied individually for each isotherm test. Thermodynamic characteristics, such as enthalpy, entropy, and Gibbs free energy [ΔH^0, ΔS, and ΔG^0] of the Cr(VI) removal by CTAB@FZA were subsequently determined using $ln\ Kc$ vs. $1/T$, as shown in Figure 5, and ΔG^0 was calculated as follows equation (7) and (8):

$$\Delta G = -RT\ln K_C \quad (7)$$

$$\Delta G = \Delta H - T\Delta S \quad (8)$$

where R is the ideal gas constant (8.314 kJ·mol^{-1}) and T is temperature (°C).

The adsorptive batch studies were conducted using a range of conditions, such as initial pH (2–7), contact time (1–30 min), initial metal concentration (10–300 mg/L at 298 K), temperature (298–338 K), coexisting anions (chlorine, phosphate, sulfate, and nitrate), and cations (sodium, potassium, calcium, and magnesium; 20 mg/L), to examine the adsorption process of CTAB@FZA towards Cr(VI). After removal, the supernatant was carefully decanted and used to determine the remaining concentrations of the pollutants in the solution.

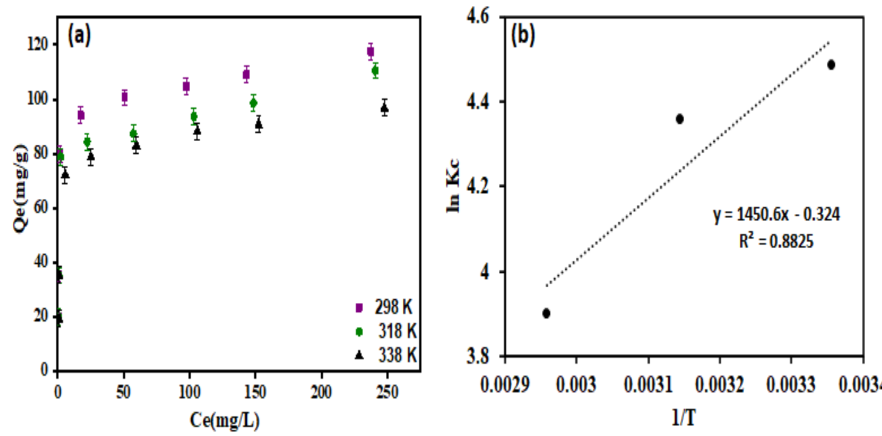

Figure S2. (a)Effect of temperature on Cr(VI) removal; (b) Adsorption thermodynamics.