Supporting Information

Sol–Gel Derived Benzo-Crown Ether-Functionalized Silica gel for Selective Adsorption of Ca^{2+} Ions

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Adsorption isotherms

The linearized equations of Langmuir and Freundlich isotherm can be expressed as Eqs. (S1) and (S2), respectively.

$$C_e/q_e = 1/(q_{max}\, b) + C_e/q_{max} \quad \text{(S1)}$$

$$\log q_e = \log k_F + (1/n) \log C_e \quad \text{(S2)}$$

$$q_e = B_T \ln A_T + B_T \ln C_e \quad \text{(S3)}$$

$$B_T = RT/b_T \quad \text{(S4)}$$

where q_e (mg g^{-1}) is the amount of Ca^{2+} ions adsorbed per unit mass of BCES at equilibrium; C_e (mg L^{-1}) is the concentration at equilibrium; q_{max} (mg g^{-1}) is the maximum adsorption at monolayer coverage; b (L mg^{-1}) is the adsorption equilibrium constant; K_F (L g^{-1}) is a Freundlich constant; n is a constant; B_T and b_T are the Temkin constant (KJ mol^{-1}) which related to heat of adsorption, A_T is the equilibrium binding constant (mg L^{-1}), R is the universal gas constant (8.314 J mol^{-1} K^{-1}) and T (K) is the solution temperature.

Kinetic analysis

The pseudo-first-order and pseudo-second-order rate expressions are linearly expressed as:

$$\log(q_e - q_t) = \log q_e - k_1 t/2.303 \quad \text{(S5)}$$

$$t/q_t = 1/k_2 q_e^{\,2} + t/q_e \quad \text{(S6)}$$

where k_1 (min^{-1}) is the rate constant of the pseudo-first-order adsorption. q_e and q_t (mg g^{-1}) are the adsorption capacity at equilibrium and the adsorption amount at time t (min), respectively. k_2 (g mg^{-1} min^{-1}) is the rate constant of the pseudo-second-order equation.

The intraparticle diffusion model is linearly expressed as

$$q_t = k_{pi} t^{0.5} + C_{pi} \quad \text{(S7)}$$

Where k_{pi} is the intraparticle diffusion rate constant of stage i (mg g^{-1} $min^{-0.5}$), C_{pi}, the intercept of stage i, gives an idea about the thickness of boundary layer, i.e., the larger of the intercept, the greater of the boundary layer effect.