

Supplementary Information

Facile synthesis of MgAl layered double hydroxides by co-precipitation method for efficient nitrate removal from water: Kinetics and mechanisms

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Fifteen Expressions and One Figure Included
(Expression 1-14 and Figure S1)

The calculation expressions related to adsorption is as follows:

$$RE=(C_0-C_t)/C_0 \quad (1)$$

$$Q_t = (C_0-C_t)V/m \quad (2)$$

$$Q_e = (C_0-C_e)V/m \quad (3)$$

Where RE is removal rate, C_0 is the NO_3^- initial concentration ($\text{mg}\cdot\text{L}^{-1}$), C_t and C_e are the NO_3^- concentration at time t and equilibrium ($\text{mg}\cdot\text{L}^{-1}$), m is the mass of adsorbent (g), V is the volume of the aqueous solution (L), Q_t and Q_e are the adsorption capacity at time t and equilibrium ($\text{mg}\cdot\text{g}^{-1}$).

Pseudo-first-order model:

$$Q_t = Q_e(1-e^{-k_1t}) \quad (4)$$

Pseudo-second-order model:

$$Q_t = k_2Q_e^2t/(1+k_2Q_et) \quad (5)$$

Intraparticle diffusion model:

$$Q_t = k_it^{0.5}+C \quad (6)$$

Where k_1 (min^{-1}), k_2 ($\text{g mg}^{-1} \text{min}^{-1}$), k_i ($\text{mg g}^{-1} \text{min}^{-1/2}$) are the rate constant individually for the corresponding model in the Exp 4-6, C (mg g^{-1}) is the intercept.

Langmuir model:

$$Q_e = Q_mK_LC_e/(1+K_LC_e) \quad (7)$$

Freundlich model:

$$Q_e = K_F C_e^n \quad (8)$$

Temkin model:

$$Q_e = b_T \ln(K_T C_e) \quad (9)$$

D-R model:

$$Q_e = Q_m e^{(-K_{D-R}\varepsilon^2)} \quad (10)$$

$$E = RT \ln(1+1/C_e) \quad (11)$$

$$E = 1/(2K_{D-R}^{1/2}) \quad (12)$$

Where C_e is the equilibrium concentration ($\text{mg}\cdot\text{L}^{-1}$), Q_m is the maximum adsorption capacity ($\text{mg}\cdot\text{g}^{-1}$), K_L is the adsorption equilibrium constant of Langmuir adsorption isotherm mode ($\text{L}\cdot\text{mg}^{-1}$), K_F is the empirical constant of Freundlich model ($\text{mg}\cdot\text{g}^{-1}$), K_T is the equilibrium binding constant ($\text{L}\cdot\text{mg}^{-1}$), b_T is the Temkin constant ($\text{J}\cdot\text{mol}^{-1}$), K_{D-R} is the constant of D-R model ($\text{mol}^2\cdot\text{J}^{-2}$), ε is the Polanyi adsorption potential energy ($\text{J}\cdot\text{mol}^{-1}$), E is the adsorption free energy ($\text{kJ}\cdot\text{mol}^{-1}$).

Van't Hoff equation:

$$\Delta G^\circ = -RT\ln(Q_e/C_e) \quad (13)$$

Gibbs-Helmholtz equation:

$$\Delta G^\circ = \Delta H^\circ - T\Delta S^\circ \quad (14)$$

Where ΔG° is the free energy change (kJ mol^{-1}), R is the universal gas constant ($8.314 \text{ kJ mol}^{-1} \text{ K}^{-1}$), T is the absolute temperature (K), ΔH° is the enthalpy change (kJ mol^{-1}), ΔS° is the entropy change ($\text{kJ mol}^{-1} \text{ K}^{-1}$).

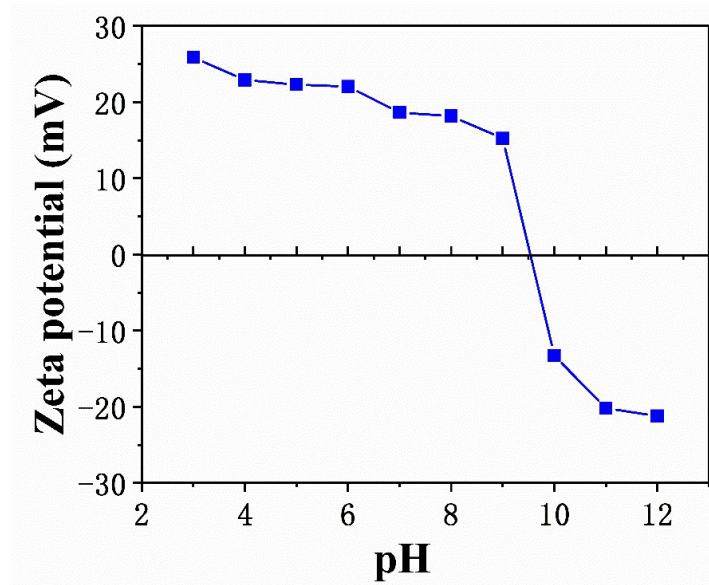


Fig. S1. Zeta potential of Mg_5Al -LDH.