Supplementary Material

## Insight into adsorption mechanisms of aqueous hexavalent chromium by EDTA intercalated layered double hydroxides: XRD, FTIR, XPS, and zeta potential studies

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## List of supplementary materials:

Formulas used in this work

Fig. S1. EDS element composition of LDH-EDTA (A) and Mag-LDH-EDTA (B).

Fig. S2. N<sub>2</sub> adsorption-desorption isotherms of LDH-EDTA and Mag-LDH-EDTA.

Fig. S3. XPS survey of LDH-EDTA (a, b) and Mag-LDH-EDTA (c, d) before adsorption (a, c) and after Cr(VI) adsorption (b, d).

Fig. S4. Images of Cr(VI) solution (A), adsorption of Cr(VI) by Mag-LDH-EDTA (B), and magnetic separation of Mag-LDH-EDTA after adsorption (C).

## Formulas used in this work

Adsorption kinetic equation

$$\lg(q_e - q_t) = \lg q_e - \frac{k_1 t}{2.303}$$
 Eq. S1

$$\frac{t}{q_t} = \frac{1}{k_2 q_e^2} + \frac{t}{q_e}$$
 Eq. S2

 $q_t$ : adsorbate amount of Cr(VI) at time t (min), mg/g;

 $q_e$ : adsorbate amount of Cr(VI) at equilibrium state, mg/g;

 $k_1$ : rate constant of the pseudo-first-order equation, 1/min;

 $k_2$ : rate constant of the pseudo-second-order equation, g/(mg·min).

## Adsorption isotherm model

$$\frac{c_e}{q_e} = \frac{c_e}{q_m} + \frac{1}{bq_m}$$
Eq. S3

$$\ln q_e = \ln k_f + \frac{1}{n} \ln c_e$$
 Eq. S4

 $c_{\rm e}$ : equilibrium concentration of Cr(VI) in aqueous solution, mg/L;

 $q_e$ : equilibrium adsorption capacity of adsorbents, mg/g;

 $q_{\rm m}$ : theoretical saturated adsorption capacity of adsorbents, mg/g;

- *b*: Langmuir isotherm model constant, L/mg;
- *k*<sub>f</sub>: constant of the Freundlich isotherm model, no dimension;

*n*: constant of the Freundlich isotherm model, no dimension.

$$R_L = \frac{1}{1 + bc_0}$$
 Eq. S5

*b*: Langmuir isotherm model constant, L/mg;

 $c_0$ : initial Cr(VI) concentration, mg/L.



Fig. S1. EDS element composition of LDH-EDTA (A) and Mag-LDH-EDTA (B).



Fig. S2. N<sub>2</sub> adsorption-desorption isotherms of LDH-EDTA and Mag-LDH-EDTA.



Fig. S3. XPS survey of LDH-EDTA (a, b) and Mag-LDH-EDTA (c, d) before adsorption (a, c) and after Cr(VI) adsorption (b, d).



Fig. S4. Images of Cr(VI) solution (A), adsorption of Cr(VI) by Mag-LDH-EDTA (B), and magnetic separation of Mag-LDH-EDTA after adsorption (C).