Supporting Information

A Two-Dimensional Cationic Aluminoborate as a New Paradigm for Highly Selective and Efficient Cr(VI) Capture from Aqueous Solution

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References
Section 1. Synthesis of BAC(10).

Pure aluminoborate BAC(10) was synthesized via a hydrothermal route described previously with slight modification. A mixture with molar composition of 3.5B₂O₃:2.0AlCl₃:2.5NH₃·H₂O:200H₂O was prepared from boric acid (99%, Aladdin), anhydrous aluminum trichloride (99%, Sinopharm Chemical Reagent Co. LTD), ammonium hydroxide (25%-28%, Sinopharm Group Chemical Reagent Co. LTD), and deionized water (DI water). The mixture was stirred thoroughly at 70 °C for 1 h to ensure homogeneity. The resulting mixture was then transferred into a Teflon-lined stainless steel autoclave and heated at 150 °C for 18 h under autogenous pressure. The resulting product was filtered, washed with hot DI water, and dried in air at 100 °C.

Section 2. Thermal stability and unusual “structural memory effect” of BAC(10).

The as-synthesized BAC(10) was calcined in air for 2 h at 150 °C, 200 °C, 250 °C, and 300 °C with a heating rate of 10 °C/min, respectively. After cooling to ambient temperature, all samples were characterized by powder X-ray diffraction (PXRD).

The 300 °C calcined sample was immersed in DI water, 0.01 M NaCl or 0.01 M HCl aqueous solution. The mixture was stirred vigorously for 24 h at ambient temperature. The resulting solid samples were characterized by PXRD.

Section 3. Hydrolytic stability of BAC(10).

Hydrolytic stability of BAC(10) was studied by immersing 20 mg of BAC(10) in 10 mL aqueous solutions with pH values ranging from 2 to 12.5, adjusted with 0.1 M HCl or 0.1 M NaOH. The mixture was stirred vigorously for 12 h at ambient temperature and the resulting solid samples were characterized by PXRD.

Section 4. Commercials and other anion exchangers.

For comparison, hydrotalcite with formula of [Mg₆Al₂(OH)₁₆]CO₃·4H₂O (Mg-Al-LDH) was purchased from Shaoyang Tiantang Auxiliaries Chemical Co., Ltd., China, in powder form and then activated at 500 °C for 3 h (denoted as CLDH). Anion exchange resin Amberlite IRN78 was purchased from Sigma-Aldrich. The resin was washed several times with DI water before use. Granular activated carbon (denoted as GAC) was purchased from Tianjin Fuchen Chemical Reagents Company. The activated carbon was dried at 100 °C for 2 h before use.
Section 5. Batch experiments.

All experiments were conducted at 25 °C using the batch sorption method. The solid/liquid ratio performed in all batch experiments was 2 g/L. Typically, 40 mg of BAC(10) was added into 20 mL of aqueous solution containing certain amounts of K₂CrO₄ (98%, Aladdin). All pH values were adjusted with 0.01 to 0.1 M HCl or 0.01 to 0.1 M NaOH. The resulting mixture was stirred for a desired contact time and separated with a 0.22 μm membrane filter. All experiments were carried out in duplicate, and the average data were used for analysis.

Influence of initial pH. Initial concentration of Cr (VI) was 50 mg/L and the solid/liquid ratio is 2 g/L. Initial pH of the solution was within the range of 2.0 to 12.0. The contact time was 12 h under stirring.

Sorption kinetics. 100 mg of BAC(10) was added into 50 mL of solution with an initial pH of 3.0 and concentration of 20 mg/L for Cr(VI). The contact time was varied from 10 to 240 min with a pre-set interval. The sorption kinetics of CLDH and IRN78 were also investigated under the same conditions.

Sorption isotherms. 40 mg of BAC(10) was added into 20 mL of Cr(VI) solutions with an initial pH of 3.0 and different concentrations (50-800 mg/L) for Cr(VI). The contact time was 12 h under stirring. The sorption isotherms of CLDH and IRN78 were also investigated under the same conditions.

Selectivity. The influence of coexisting anions (NO₃⁻, Br⁻, Cl⁻, HCO₃⁻, F⁻, and CO₃²⁻) with concentrations ranging from 0.4 to 8 mM was investigated in 20.8 mg/L (0.4 mM) Cr(VI) solution. The pH of the mixed solution was adjusted to 7 and the contact time was 12 h under stirring.

Removal efficiency at low concentration. The solution with the initial concentration of 2.5 to 20 mg/L for Cr(VI) was prepared with DI water and tap water, respectively. The pH was adjusted to 7 and the contact time was 12 h under stirring.

Reusability. 100 mg of BAC(10) was immersed in 50 mg/L Cr(VI) solution (50 mL, pH=3) under stirring for 12 h. After Cr(VI) sorption, the sample was regenerated using 1 M NaCl solution (50 mL) under stirring for 12 h. The solid was recovered by centrifugation and washed with DI water for three times. The sorption-regeneration procedure was repeated for
up to five cycles. The regenerated BAC(10) samples were denoted as BAC(10)-R-cycle number.

**Removal of other toxic oxyanions.** The solution of Re, Mo, Se, P, and V oxyanions used in this experiment was prepared from NH\(_4\)ReO\(_4\) (99.999\%, Innochem), Na\(_2\)MoO\(_4\)·2H\(_2\)O (99\%, Innochem), Na\(_2\)SeO\(_4\)·10H\(_2\)O (99.9\%, Alfa), Na\(_2\)HPO\(_4\) (99\%, Innochem), and Na\(_3\)VO\(_4\) (99\%, Innochem), respectively. The initial concentration for Re, Mo, Se, P, and V oxyanions was 20 mg/L. The pH was adjusted to 6 and the contact time was 12 h under stirring. All the concentrations in aqueous solution were determined by ICP-OES.

**Calculation of removal efficiency and sorption capacity.** The adsorption of Cr(VI) on adsorbents could be calculated from the difference between the initial concentration (C\(_o\), mg/L) and the equilibrium one (C\(_e\), mg/L). The removal efficiency of Cr(VI) (R, %) was calculated by the following equation:

\[
R = \left( \frac{C_o - C_e}{C_o} \right) \times 100\%
\]  

(1)

The adsorption capacity of Cr(VI) (q, mg/g) was calculated by the following equation:

\[
q = \frac{C_o - C_e}{m} \times V
\]

(2)

where V (L) and m (g) represent the volume of the suspension and the mass of adsorbents, respectively. The concentration and the adsorption capacity in this work are expressed by the elements, not the whole oxo-anions.

**Adsorption Kinetics.** To understand the characteristics of the adsorption process, the kinetics of Cr(VI) adsorption on BAC(10), CLDH and IRN78 are analyzed by pseudo-first-order (eq. S1) and pseudo-second-order (eq. S2) kinetic models, which are presented as follows:

\[
\text{lg}(q_e - q_t) = \text{lg} q_e - \frac{k_1}{2.303}t \\
\frac{t}{q_t} = \frac{1}{k_2q_e^2} + \frac{t}{q_e}
\]

(eq.S1)

(eq.S2)

where k\(_1\) (min\(^{-1}\)) and k\(_2\) (g·mg\(^{-1}\)·min\(^{-1}\)) are the rate constants of pseudo-first-order and pseudo-second-order kinetic model, respectively; The kinetics plot feature is achieved and presented in Figure 4, and the relevant parameters are listed in Table 1. All the correlation coefficient values (R\(^2\)) of the pseudo-second-order model are higher than that of the pseudo-first-order.
model, which indicates that the kinetics adsorption can be described by the pseudo-second-order rate equation well; \( q_t \) and \( q_e \) (mg·g\(^{-1}\)) are the adsorption capacity at contact time \( t \) (min) and equilibrium state, respectively.

**Adsorption isotherms.** The linear equation of the Langmuir isotherm model (eq.S3) of BAC(10), CLDH and IRN78 are expressed as followed:

\[
\frac{C_e}{q_e} = \frac{1}{bq_m} + \frac{C_e}{q_m}
\]

(eq.S3)

where \( q_m \) is the maximum adsorption capacity corresponding to complete monolayer adsorption (mg/g) and \( b \) is a Langmuir constant related to the affinity of binding sites (L/mg), which characterizes the affinity of Cr(VI) with the adsorbent.

The Freundlich equation is an empirical equation based on Cr(VI) sorption on a heterogeneous surface. The isotherm assumes that adsorbent surface sites have a spectrum of different binding energies. The linear equation of the Freundlich isotherm model (eq.S4) can be expressed by:

\[
\lg q_e = \lg k_f + \frac{1}{n} \lg C_e
\]

(eq.S4)

where \( k_f \) (mg/g) represents the adsorption capacity, and \( n \) represents the sorption intensity, respectively.

The linear plot was obtained by plotting \( \lg q_e \) against \( \lg C_e \), and the values of \( k_f \) and \( n \) were calculated from the slope and intercept of the straight line. All the sorption isotherm can be well fitted by the Langmuir model, suggesting that monolayer sorption mode are more appropriate to explain the adsorption mechanism.

**Section 6. Preparation of Cr(VI)@ BAC(10).**

To reach saturation adsorption, 100 mg of BAC(10) was added into 50 mL of solution with initial pH of 3.0 and concentration of 800 mg/L Cr(VI). The resulting mixture was stirred for 12 h at 25 °C and then centrifuged at 10000 rpm for 5 min. The solid was washed with DI water for three times and dried in air at ambient temperature. The saturated Cr(VI) loaded material was denoted as Cr(VI)@BAC(10).

**Section 7. Crystal structure determination of Cr(VI)@BAC(10).**

**Morphology.** The boroaluminate crystal has a plate-like morphology (Figure S1a).
**Continuous Rotation Electron Diffraction (cRED).** Cr(VI)@BAC(10) crystals were crushed, dispersed in absolute ethanol, and sonicated for 1 min before mounting onto a holey carbon film covered copper grid. cRED was collected on JEOL JEM-2100 transmission electron microscope (TEM) operated at an acceleration voltage of 200 kV by continuously tilting goniometer. Electron diffraction patterns (Figure S1b) were collected continuously on a high-speed hybrid detection Timepix Quad camera (ASI) using software *Instamatic.*\(^1\) The cRED data was processed with X-ray Detector Software (XDS).\(^2\) All framework atoms were resolved *ab initio* using SHELXT,\(^3\)\(^-\)\(^4\) and refinement was performed using SHELXL-2018\(^5\) via Olex2 software,\(^6\) with atomic scattering factors for electrons derived by Peng.\(^7\)

Attributed to the preferred orientation of the nanosheets, about the \(b^*\)-axis containing 0\(k0\) reflections is missing. Based on the reflection conditions observed in the cRED data, three possible space groups were deduced: *Pn* (No. 7), *P2/n* (No. 13), and *P2_1/n* (No. 14). Structure solutions could be obtained from SHELXT for each of the three space groups, and therefore the space group with the highest symmetry *P2_1/n* was used. Two chromium ions that were yet to be fully tetrahedral were directly located between the layers. After the initial refinement, all but one oxygen of the tetrahedra could be located from the difference Fourier map. The last oxygen was placed based on the geometry. The occupancies of the two chromate ions CrA and CrB were refined to 77% and 32%, respectively. Finally, additional chromium ion (CrC) was located in the difference Fourier map and the occupancy was refined to 24%. CrC is coordinated to two AlO\(_6\) in the layer. Due to the low occupancy, no oxygen atoms are added to complete the tetrahedral coordination of CrC.

**High-resolution transmission electron microscopy (HRTEM) image.** HRTEM image was taken from Cr-exchanged Cr(VI)@BAC(10) crystals on a JEOL JEM-2100F TEM operated at an acceleration voltage of 200 kV with a Gatan Ultrascan 1000 CCD camera under low-dose conditions to obtain more information regarding the structure (Figure S4). We used the through-focus method\(^8\) for structure projection reconstruction from a series of 25 HRTEM images acquired with a constant defocus step of 53.2 Å. A through-focus series of HRTEM images along the \(b\)-axis of a Cr(VI)@BAC(10) nanosheet was acquired using a DigitalMicrograph script\(^8\) that is modified to allow the brightness of the image to be adjusted without changing the electron dose on the TEM. Then the projections were reconstructed using the program *QFocus.*\(^9\) Projected potential maps were obtained by crystallographic image processing using the software CRISP.\(^10\) The symmetry \(p2\) was imposed in the map (Figure S4b).
Section 8. Characterizations.

PXRD analyses were performed by Rigaku D/Max 2550 X-ray diffractometer in the scanning range of 2θ between 4° and 40° using copper Kα as the source of radiation (λ=1.5418Å). The morphology and microstructure were obtained with field emission scanning electron microscopy (SEM, JSM-7800F) and transmission electron microscopy (TEM, Tecnai F20), respectively. Energy-dispersive spectroscopy (EDS) mapping was recorded on JSM-7800F. Atomic force microscopy (AFM) data were acquired with a Bruker Dimension FastScan AFM system. In AFM analyses, the samples were prepared by depositing one droplet of the corresponding suspension on single crystal silicon substrate and dried at ambient temperature. The concentrations of Cr(VI) in aqueous solution were determined by inductively coupled plasma optical emission spectrometry (ICP-OES, Thermo Fisher Scientific iCAP7600 DUO). N₂ adsorption/desorption measurements were carried out on a Micromeritics 2020 analyzer at 77 K. Prior to measurement, the samples were degassed at 250 °C for at least 6 h. Fourier transform infrared (FTIR) spectroscopy was performed on a Nicolet Impact 410 spectrometer following the standard KBr disk method. TGA-MS was carried out from ambient temperature to 800 °C with a heating rate of 10 °C/min on a thermal analyzer (Netzsch STA449C) equipped with a quadrupole mass spectrometer (Balzers MID). The X-ray photoelectron spectroscopy (XPS) was recorded on a Thermo Scientific ESCALAB 250Xi spectrometer.
**Table S1.** Crystallographic data and experimental and refinement details for the cRED data of Cr(VI)@BAC(10). The formula is based on the refinement result, with hydrogen atoms added for charge balance.

### Crystal Data

|                |                             |
|----------------|-----------------------------|
| **Formula**    | Al$_{48}$ B$_{24}$ Cr$_{5.25}$ O$_{187.65}$ |
| **Formula Weight (g/mol)** | 4835.92 |
| **Crystal System** | Monoclinic |
| **Space group** | $P2_1/n$ |
| **$a$, $b$, $c$ (Å)** | 16.020(3), 16.910(3), 16.390(3) |
| **$α$, $β$, $γ$ (°)** | 90, 112.69(3), 90 |
| **Volume, Å$^3$** | 4096.4(16) |

### Data Collection

|                         |                             |
|-------------------------|-----------------------------|
| **Temperature (K)**    | 293                         |
| **Radiation (Å)**      | Electrons, 0.02508          |
| **$d_{\text{min}}$, $d_{\text{max}}$ (Å)** | 0.90, 11.13 |
| **Dataset $(h, k, l)$** | -17→17, -16→15, -17→17 |
| **Tot., Uniq. Data, $R_{\text{int}}$** | 10601, 3541, 9.70 |
| **Completeness, %**    | 60.42                       |
| **<I/σ(I)>**           | 5.9                         |
| **$R_{\text{meas}}$** | 0.118                       |
| **CC$_{1/2}$**         | 0.989                       |
| **Tilt range (°)**     | 129.49                      |
| **No. ED frames**      | 412                         |
| **Tilt step per frame (°)** | 0.23                  |
| **Exposure time per frame (s)** | 0.6                   |

### Refinement

|                         |                             |
|-------------------------|-----------------------------|
| **$N_{\text{reflections}}$, $N_{\text{parameters}}$, $N_{\text{restraints}}$** | 3541, 279, 2 |
| **$N_{\text{parameters}}$, $N_{\text{restraints}}$** | 284, 1 |
| **$R_1$, $I>I(2σ)$, all data** | 0.2769, 0.2983 |
| **GooF**                | 1.067                       |
Table S2. Kinetic parameters for Cr(VI) sorption on BAC(10), IRN78, and CLDH.

| Samples   | First-order-model |                | Second-order-model |                |
|-----------|------------------|----------------|-------------------|----------------|
|           | k₁ (min⁻¹)       | q₁ (mg/g)     | R²        | k₂ (g mg⁻¹ min⁻¹) | q₂ (mg/g) | R²    |
| BAC(10)  | 22.6             | 1.43          | 0.978     | 0.0344         | 10.1      | 0.999 |
| IRN78    | 23.5             | 3.42          | 0.942     | 0.0220         | 10.2      | 0.999 |
| CLDH     | 42.5             | 12.2          | 0.926     | 0.0027         | 11.4      | 0.997 |

Table S3. Langmuir and Freundlich isotherm parameters for Cr(VI) sorption on BAC(10), CLDH, and IRN78.

| Sample   | Langmuir | Freundlich |
|----------|----------|------------|
|          | qₘ (mg/g) | B (L mg⁻¹) | R² | kᵢ (mg/g) | 1/n | R²  |
| BAC(10)  | 139.1    | 0.027      | 0.997 | 19.1      | 0.325 | 0.980 |
| CLDH     | 81.43    | 0.024      | 0.996 | 14.1      | 0.272 | 0.989 |
| IRN78    | 62.77    | 0.188      | 0.999 | 29.8      | 0.125 | 0.905 |
Table S4. Comparison of adsorption capacity of Cr(VI) with the reported anion exchangers

| Types          | Samples          | $q_m$ (mg/g) | References |
|----------------|-----------------|--------------|------------|
| MOFs           | SLUG-21         | 26.9         | 12         |
|                | ABT-2ClO$_4$    | 102.6        | 13         |
|                | 1-SO$_4$        | 79.9         | 14         |
|                | MOR-1-HA        | 116.5        | 15         |
|                | MOR-2           | 194          | 16         |
|                | UiO-66-NH$_2$@silica | 133.4     | 17         |
|                | JLU-MOF50       | 44.3         | 18         |
| LDHs           | Mg-Al-Cl        | 112          | 19         |
|                | NiMgAl-LDOs     | 103.4        | 20         |
|                | Ca-Al-Cl        | 55           | 21         |
|                | CH-Mg/Al        | 85.9         | 22         |
|                | CLDH            | 81.43        | This work  |
| Anion exchange resins | RQA           | 48           | 23         |
|                | Lewatit MP 500  | 21.3         | 24         |
|                | Dowex 1×8       | 28.1         | 25         |
|                | IRN78           | 62.77        | This work  |
| Cationic aluminum oxyhydroxide | JU-111       | 105.4        | 26         |
| Aluminoborate  | BAC(10)         | 139.1        | This work  |

Note: The Cr adsorption capacity is presented in its elemental form.
Figure S1. TEM images of Cr(VI)@BAC(10).

Figure S2. EDS mapping profiles of Cl and Cr in BAC(10) (a) and Cr(VI)@BAC(10) (b).

Figure S3. N₂ adsorption-desorption isotherms of BAC(10) and Cr(VI)@BAC(10).
Figure S4. (a) TEM image showing the morphology of Cr(VI)@BAC(10) and (b) selected area electron diffraction (SAED) pattern perpendicular to the nanosheet, which corresponds to the [010] zone axis. The weak extra spots in the SAED pattern are from the elongated first order (h1l) reflections due to the few repeating unit cells along the b-axis.

Figure S5. 3D reciprocal space reconstructed from the cRED data depicting diffuse streaks along the \( b^* \)-axis.
**Figure S6.** 3D structure of Cr(VI)@BAC(10) viewed along (a) the [010] and (b) the [101] direction.

**Figure S7.** (a) Structure projection along the [010] direction from a through-focus series of 25 HRTEM images of Cr@BAC(10). Inset: Fourier transformation of the image. (b) Projected potential map with the symmetry \( p2 \) imposed. The processed area is from the entire region in (a); The structure model of Cr@BAC(10) is superimposed in the image (b).
Figure S8. Influence of the initial pH on the structure of BAC(10).

Figure S9. The distribution of Cr(VI) species at various pHs.
Figure S10. Linear fitting with pseudo-first-order kinetic model for IRN78 and CLDH.

Figure S11. Linear fitting with pseudo-second-order kinetic model for IRN78 and CLDH.
Figure S12. PXRD patterns of regenerated BAC(10) samples after 1-5 cycles.
Figure S13. The EDS spectra of regenerated BAC(10) samples after 1-5 cycles.
Figure S14. Photographs of BAC(10), Cr(VI)@BAC(10), and the BAC(10) after the first regeneration (BAC(10)-1st).
References

1. Smeets, S.; Wang, B.; Cichocka, M. O.; Ångström, J.; Wan W. (2017, December 5) https://zenodo.org/record/1090389#.WmdJUHIG1hE.
2. Kabsch, W., XDS. Acta Cryst. 2010, D66, 125-132.
3. Sheldrick, G. M., A Short History of SHELX. Acta Cryst. 2008, A64, 112-122.
4. Sheldrick, G. M., SHELXT – Integrated Space-Group and Crystal-Structure Determination. Acta Cryst. 2015, A71, 3-8.
5. Sheldrick, G. M., Crystal Structure Refinement with SHELXL. Acta Cryst. 2015, C71, 3-8.
6. Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A. K.; Puschmann, H., OLEX2: a Complete Structure Solution, Refinement and Analysis Program. J. Appl. Cryst. 2009, 42(2), 339-341.
7. Peng, L.-M, Electron Atomic Scattering Factors and Scattering Potentials of Crystals. Micron 1999, 30(6), 625-648.
8. Kirkland, E. J.; Siegel, B. M.; Uyeda, N.; Fujiyoshi, Y., Digital Reconstruction of Bright Field Phase Contrast Images from High Resolution Electron Micrographs. Ultramicroscopy 1980, 5(4), 479-503.
9. DigitalMicrograph database, www.felmi-zfe.tugraz.at/dm_scripts/.
10. Wan, W.; Hovmöller, S.; Zou, X., Structure Projection Reconstruction from Through-Focus Series of High-Resolution Transmission Electron Microscopy images. Ultramicroscopy 2012, 115, 50-60.
11. Hovmöller, S., CRISP: Crystallographic Image Processing on a Personal Computer. Ultramicroscopy 1992, 41, 121-135.
12. Fei, H.; Bresler, M. R.; Oliver, S. R. J., A New Paradigm for Anion Trapping in High Capacity and Selectivity: Crystal-to-Crystal Transformation of Cationic Materials. J. Am. Chem. Soc. 2011, 133 (29), 11110-11113.
13. Li, X.; Xu, H.; Kong, F.; Wang, R., A Cationic Metal–Organic Framework Consisting of Nanoscale Cages: Capture, Separation, and Luminescent Probing of Cr$_2$O$_7^{2-}$ through a Single-Crystal to Single-Crystal Process. Angew. Chem. Int. Ed. 2013, 52 (51), 13769-13773.
14. Desai, A. V.; Manna, B.; Karmakar, A.; Sahu, A.; Ghosh, S. K., A Water-Stable Cationic Metal–Organic Framework as a Dual Adsorbent of Oxoanion Pollutants. Angew. Chem. Int. Ed. 2016, 55 (27), 7811-7815.
15. Rapti, S.; Pournara, A.; Sarma, D.; Papadas, I. T.; Armatas, G. S.; Tsipis, A. C.; Lazarides, T.; Kanatzidis, M. G.; Manos, M. J., Selective Capture of Hexavalent Chromium from an Anion-Exchange Column of Metal Organic Resin-Alginic Acid Composite. Chem. Sci. 2016, 7 (3), 2427-2436.
16. Rapti, S.; Sarma, D.; Diamantis, S. A.; Skliri, E.; Armatas, G. S.; Tsipis, A. C.; Hassan, Y. S.; Alkordi, M.; Miliakas, C. D.; Kanatzidis, M. G.; Lazarides, T.; Plakatouras, J. C.; Manos, M. J., All in One Porous Material: Exceptional Sorption and Selective Sensing of Hexavalent Chromium by Using a Zr$^{4+}$ MOF. J. Mater. Chem. A 2017, 5 (28), 14707-14719.
17. El-Mehalmy, W. A.; Ibrahim, A. H.; Abugable, A. A.; Hassan, M. H.; Haikal, R. R.; Karakalos, S. G.; Zaki, O.; Alkordi, M. H., Metal-Organic Framework@Silica as a Stationary Phase Sorbent for Rapid and Cost-Effective Removal of Hexavalent Chromium. J. Mater. Chem. A 2018, 6 (6), 2742-2751.
18. Sun, X.; Yao, S.; Yu, C.; Li, G.; Liu, C.; Huo, Q.; Liu, Y., An Ultrastable Zr-MOF for Fast Capture and Highly Luminescence Detection of Cr$_2$O$_7^{2-}$ Simultaneously in an Aqueous Phase. J. Mater. Chem. A 2018, 6 (15), 6363-6369.
19. Li, Y.; Gao, B.; Wu, T.; Sun, D.; Li, X.; Wang, B.; Lu, F., Hexavalent Chromium Removal from Aqueous Solution by Adsorption on Aluminum Magnesium Mixed Hydroxide. Water Res. 2009, 43 (12), 3067-3075.
20. Lei, C.; Zhu, X.; Zhu, B.; Jiang, C.; Le, Y.; Yu, J., Superb Adsorption Capacity of Hierarchical Calcined Ni/Mg/Al Layered Double Hydroxides for Congo Red and Cr(VI) Ions. *J. Hazard. Mater.* 2017, **321**, 801-811.

21. Qian, G.; Feng, L.; Zhou, J. Z.; Xu, Y.; Liu, J.; Zhang, J.; Xu, Z. P., Solubility Product (Ksp)-Controlled Removal of Chromate and Phosphate by Hydrocalumite. *Chem. Eng. J.* 2012, **181-182**, 251-258.

22. Xiao, L.; Ma, W.; Han, M.; Cheng, Z., The Influence of Ferric Iron in Calcined Nano-Mg/Al Hydrotalcite on Adsorption of Cr (VI) from Aqueous Solution. *J. Hazard. Mater.* 2011, **186**(1), 690-698.

23. Atia, A. A., Synthesis of a Quaternary Amine Anion Exchange Resin and Study its Adsorption Behaviour for Chromate Oxyanions. *J. Hazard. Mater.* 2006, **137**(2), 1049-1055.

24. Pehlivan, E.; Cetin, S., Sorption of Cr(VI) Ions on Two Lewatit-Anion Exchange Resins and their Quantitative Determination Using UV–Visible Spectrophotometer. *J. Hazard. Mater.* 2009, **163**(1), 448-453.

25. Edebali, S.; Pehlivan, E., Evaluation of Amberlite IRA96 and Dowex 1×8 Ion-Exchange Resins for the Removal of Cr(VI) from Aqueous Solution. *Chem. Eng. J.* 2010, **161**(1-2), 161-166.

26. Bai, P.; Dong, Z.; Wang, S.; Wang, X.; Li, Y.; Wang, Y.; Ma, Y.; Yan, W.; Zou, X.; Yu, J., A Layered Cationic Aluminum Oxyhydroxide as a Highly Efficient and Selective Trap for Heavy Metal Oxyanions. *Angew. Chem. Int. Ed.* 2020, **59**(44), 19539-19544.