Supporting information

Engineering of efficient functionalization in a zirconium-hydroxyl-based metal-organic framework for ultra-high adsorption of Pb\textsuperscript{2+} ion from an aqueous medium: an elucidated uptake mechanism

Hang M. N. Pham,\textsuperscript{a} Anh V. N. Phan,\textsuperscript{a} Anh N. T. Phan,\textsuperscript{a} Vi P. Nguyen,\textsuperscript{a} Khang M. V. Nguyen,\textsuperscript{a} Hung N. Nguyen,\textsuperscript{a} Thai M. Nguyen\textsuperscript{a} and My V. Nguyen\textsuperscript{*a}

\textsuperscript{a}Faculty of Chemistry, Ho Chi Minh City University of Education, Ho Chi Minh City, 700000, Vietnam.

*To whom correspondence should be addressed: mynv@hcmue.edu.vn

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Figure S1. $^1$H-NMR spectrum of H$_2$NDC(OH) linker in DMSO solvent
Figure S2. $^{13}$C-NMR spectrum of $\text{H}_2\text{NDC(OH)}$ linker in DMSO solvent
Figure S3. Mass spectroscopy of H$_2$NDC(OH) linker
Figure S4. The relationship between the absorbed intensity of Pb$^{2+}$ and various concentrations of 0 - 20 mg L$^{-1}$ by linear fitting
Figure S5. The structure of the Zr-bcu-NDC backbones is constructed from the \( \text{Zr}_6\text{O}_8(\text{H}_2\text{O})_8(\text{CO}_2)_8 \) SBU\text{s with the H\text{2}NDC linker. Atom colors: Zr polyhedra, green; C, black; O, red. All H atoms are omitted for clarity.
Figure S6. Raman spectrum of activated HCMUE-2 (red) in comparison with H$_2$NDC(OH) linker (black)
Figure S7. The FT-IR spectrum of HCMUE-2 (red) in comparison with H$_2$NDC(OH) (black)
Figure S8. The effect of the initial pH on the final pH for determining $pH_{\text{pzc}}$ of HCMUE-2. In detail, HCMUE-2 (150 mg) was introduced to 100 mL of glass bottles containing 50 mL of 0.01 M NaCl solutions with different initial pH ranges ($pH_i$) from 2 to 11. The mixtures were stirred for 48 h. The final pH value ($pH_f$) of the solutions was recorded using a pH meter. The intersection points between $pH_i$ and $pH_f$ values exhibited the $pH_{\text{pzc}}$ value.
Figure S9. Effect of low initial concentrations on the adsorption uptake of Pb$^{2+}$ over HCMUE-2 \([m = 15 \text{ mg}, V = 100 \text{ mL}, C_0: 10 - 50 \text{ mg L}^{-1}, \text{pH} = 5.5, t = 24 \text{ h}] \) (a); The kinetic curve for the adsorption of Pb$^{2+}$ at low concentrations onto HCMUE-2 \([m = 5 \text{ mg}, V = 50 \text{ mL}, C_0 = 10 \text{ mg L}^{-1}, t = 1 - 60 \text{ min}, \text{pH} = 5] \) (b)
Adsorption kinetics

The pseudo-first-order, pseudo-second-order, and intra-particle diffusion models are determined the equations (S1), (S2), and (S3):

\[ q_t = q_e \cdot (1 - e^{-k_1 t}) \]  \hspace{1cm} (S1)

\[ \frac{t}{q_t} = \frac{1}{k_2 q_e^2} + \frac{t}{q_e} \]  \hspace{1cm} (S2)

\[ q_t = k_i t^{1/2} + c \]  \hspace{1cm} (S3)

Where $q_t$ (mg g\(^{-1}\)) and $q_e$ (mg g\(^{-1}\)) symbolize the Pb\(^{2+}\) adsorption capacity at $t$ and equilibrium time, respectively. $k_1$ (min\(^{-1}\)), $k_2$ (g mg\(^{-1}\) min\(^{-1}\)), and $k_i$ (g mg\(^{-1}\) min\(^{-1}\)) represent the rate constants of pseudo-first-order, pseudo-second-order, and intra-particle diffusion models, and $c$ is the constant, exhibiting the boundary layer thickness.