Supporting information

Efficiently improving the adsorption capacity of Rhodamine B dye in a SO$_3$H-functionalized chromium-based metal-organic framework

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Figure S1. $^1$H-NMR spectrum of digested $\text{H}^+\subset\text{BUT-8(Cr)}$ in DMSO solvent
Figure S2. The relationship between the absorbed intensity of RhB and different concentrations of 0 - 24 mg L\(^{-1}\) by linear fitting.
Figure S3. Elemental mapping by SEM-EDX of H⁺⊂BUT-8(Cr)
Figure S4. SEM images of H⁺⊂BUT-8(Cr) at different scale bars of 20.0 µm and 10.0 µm, respectively.
Figure S5. TEM images of H⁺⊂BUT-8(Cr) at at different scale bars of 500 nm and 200 nm, respectively
Figure S6. PXRD pattern of H⁺⊂BUT-8(Cr) before adsorption of RhB and immersed in water (black) as compared to the experimental pattern from the subjecting H⁺⊂BUT-8(Cr) after desorption of RhB.
Figure S7. FT-IR spectrum of H⁺⊂BUT-8(Cr) before adsorption of RhB (black) in comparison with FT-IR spectrum of H⁺⊂BUT-8(Cr) after desorption of RhB (red).
**N₂ adsorption measurement and surface area prediction**

The porosity analysis of activated H⁺⊂BUT-8(Cr) was measured by N₂ adsorption at 77 K.

![N₂ isotherm of H⁺⊂BUT-8(Cr) material at 77 K.](image)

**Figure S8.** N₂ isotherm of H⁺⊂BUT-8(Cr) material at 77 K.
$S = \frac{Q_m \times N_A \times A}{V}$

Where $S$ and $Q_m$ are the BET or Langmuir surface area and quantity adsorbed. $N_A$ is Avogadro’s number, $A$ is the molecular-sectional area and $V$ symbolizes the molar volume of adsorbed gas.

**Figure S9.** Plot of the linear region of the adsorption N$_2$ isotherm used for the BET equation (a), the Langmuir equation (b), and summary of parameters in the BET and Langmuir analysis (c).
Theoretical surface area prediction

The theoretical surface area of H⁺⊂BUT-8(Cr) was calculated through the Atom Volumes and Surfaces tool of Materials Studio 7.0 software with a grid interval of 0.25 Å and the solvent diameter, which is equal to a nitrogen probe diameter of 3.68 Å. The accessible solvent surface area of H⁺⊂BUT-8(Cr) was calculated to be 3482 Å². This data was converted into the surface area per gram, leading to a theoretical surface area of 2751 m² g⁻¹.

Table S1. Summary of surface area calculation for H⁺⊂BUT-8(Cr)

<table>
<thead>
<tr>
<th>H⁺⊂BUT-8(Cr)</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Crystal density (g cm⁻³)</td>
<td>0.707 [1]</td>
</tr>
<tr>
<td>Accessible solvent surface per cell (Å²)</td>
<td>3482</td>
</tr>
<tr>
<td>Calculated SA (m² g⁻¹)</td>
<td>2751</td>
</tr>
<tr>
<td>Unit cell volume (Å³)</td>
<td>17903 [1]</td>
</tr>
</tbody>
</table>

Figure S10. Accessible solvent surface and van der Waals surface of H⁺⊂BUT-8(Cr).

Figure S11. PXRD pattern of BUT-8(Cr) immersed in H₂O for 30 days in comparison with the simulated structure
Figure S12. Effect of the concentration of RhB on the adsorption capacity of H⁺⊂BUT-8(Cr) [m = 10 mg, V_{RhB} = 100 mL, C₀: 25-175 mg L⁻¹, t = 24 h] at pH = 5 (a); pH = 7 (b).
Adsorption isothermal models

The linear forms of the Langmuir, Freundlich, and Temkin are indicated by the equations (S1)-(S3):

\[
\frac{C_e}{q_e} = \frac{1}{K_L q_m} + \frac{C_e}{q_m} \quad (S1)
\]

\[
\log q_e = \log K_F + \frac{1}{n} \log C_e \quad (S2)
\]

\[
q_e = \frac{RT}{b} \ln(k_T C_e) \quad (S3)
\]

Where \(C_e\) (mg L\(^{-1}\)) and \(q_e\) (mg g\(^{-1}\)) are the RhB concentration and adsorption capacity at equilibrium, respectively, \(q_m\) (mg g\(^{-1}\)) is the theoretical maximum capacity of the RhB adsorption. \(K_L\) (L mg\(^{-1}\)) and \(K_F\) (mg g\(^{-1}\) (L g\(^{-1}\))\(^{1/n}\)) display the constants of Langmuir and Freundlich, respectively. 1/n value symbolizes the adsorption capacity index of Freundlich isotherm. Meanwhile, \(R\) is the gas constant, \(\beta\) and \(k_T\) are the constant of adsorption heat and the constant of Temkin, respectively, and \(T\) is the adsorption temperature.

The separation factor \((R_L)\) is used by equation (S4):

\[
R_L = \frac{1}{1 + K_L C_o} \quad (S4)
\]

Where \(C_o\) and \(K_L\) are the initial concentration of RhB and the constant of Langmuir, respectively.