Electronic Supplementary Material (ESI) for Materials Advances.

Supporting information

Efficiently improving the adsorption capacity of Rhodamine B dye in a SO_3H-functionalized chromium-based metal-organic framework

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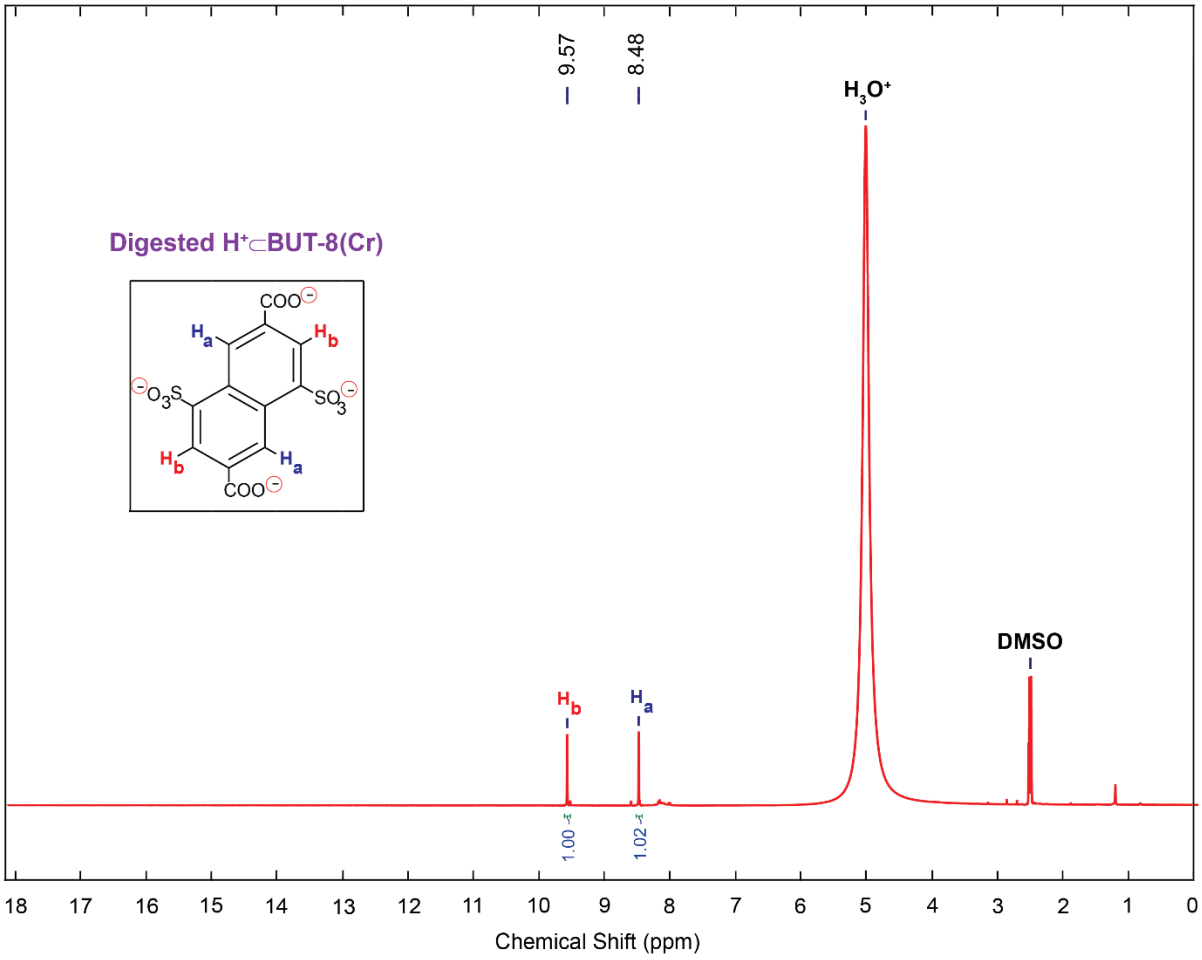


Figure S1. ^{1}H-NMR spectrum of digested $H^{+}\subset$BUT-8(Cr) in DMSO solvent

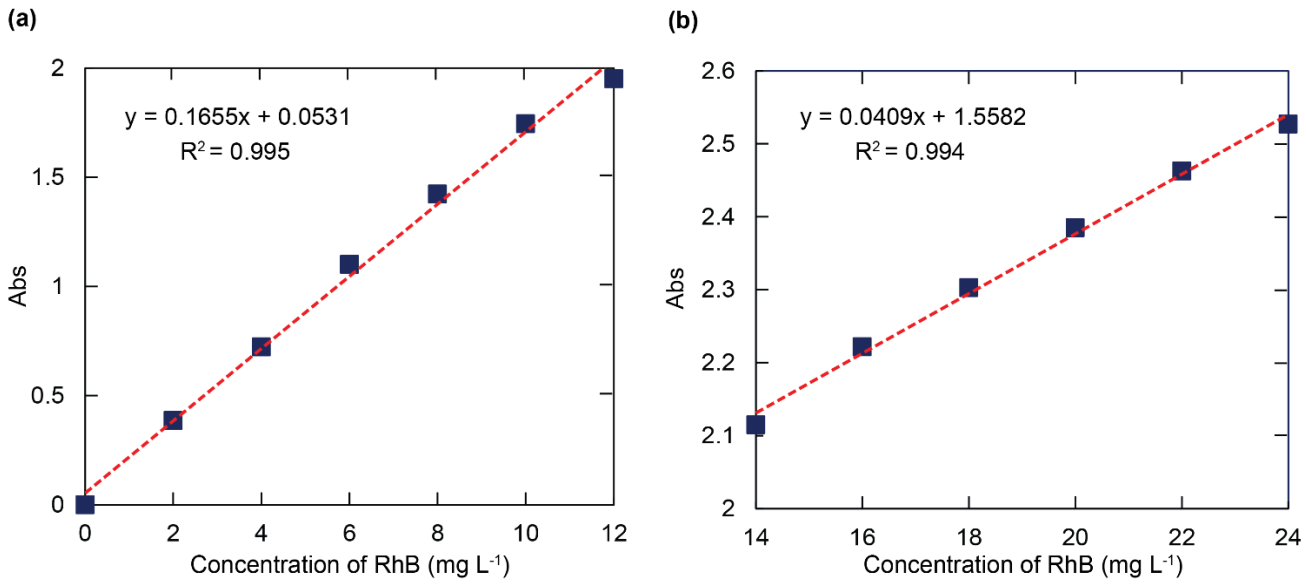


Figure S2. The relationship between the absorbed intensity of RhB and different concentrations of 0 - 24 mg L^{-1} by linear fitting.

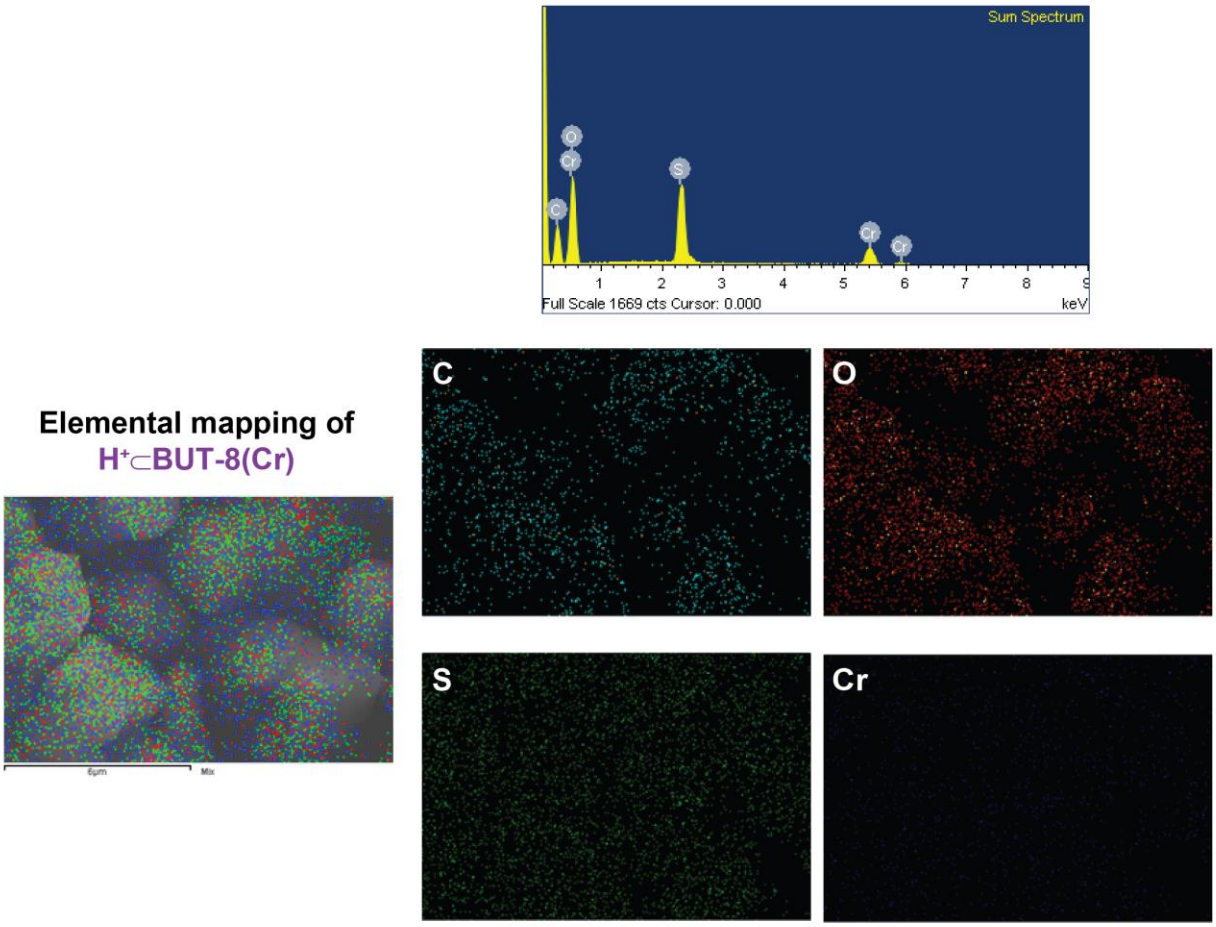


Figure S3. Elemental mapping by SEM-EDX of $H^{+}\subset$BUT-8(Cr)

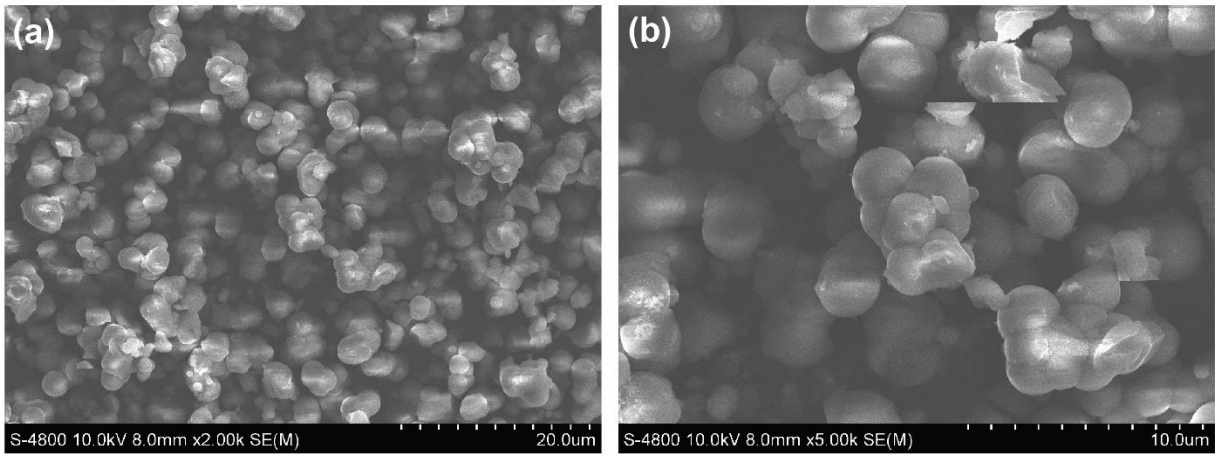


Figure S4. SEM images of H^+⊂BUT-8(Cr) at different scale bars of 20.0 μm and 10.0 μm, respectively

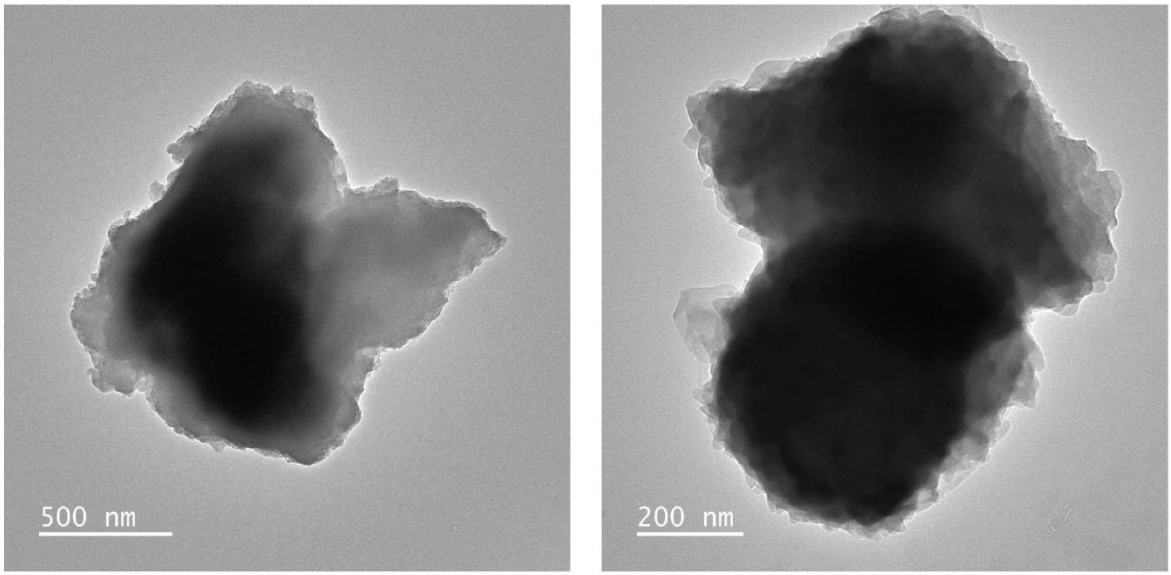


Figure S5. TEM images of H^+⊂BUT-8(Cr) at at different scale bars of 500 nm and 200 nm, respectively

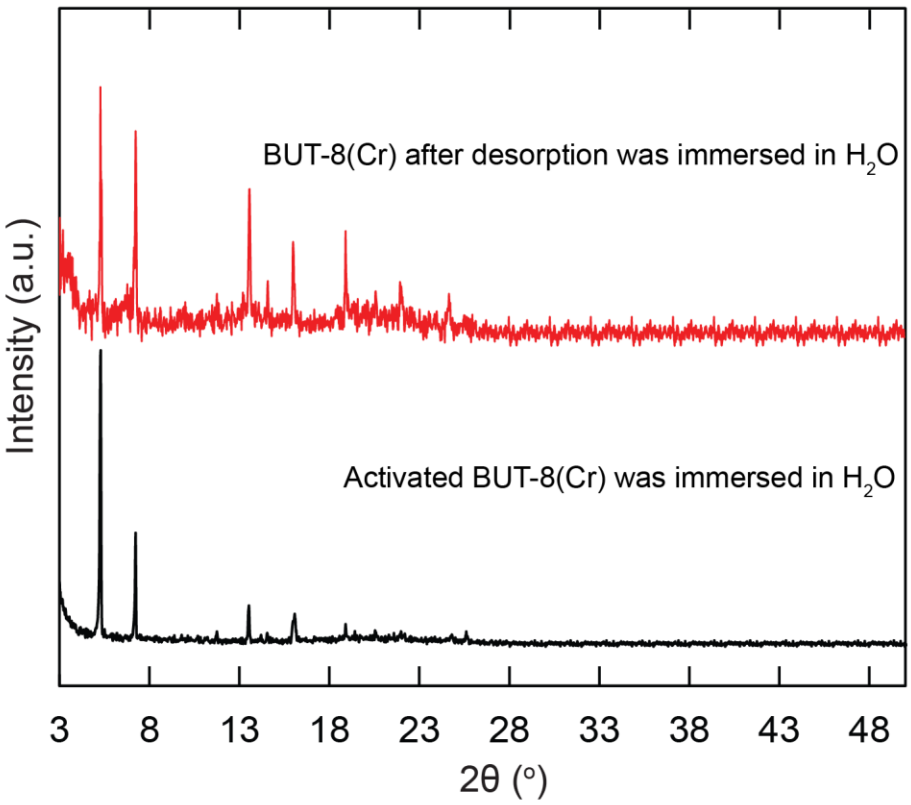


Figure S6. PXRD pattern of H^+⊂BUT-8(Cr) before adsorption of RhB and immersed in water (black) as compared to the experimental pattern from the subjecting H^+⊂BUT-8(Cr) after desorption of RhB.

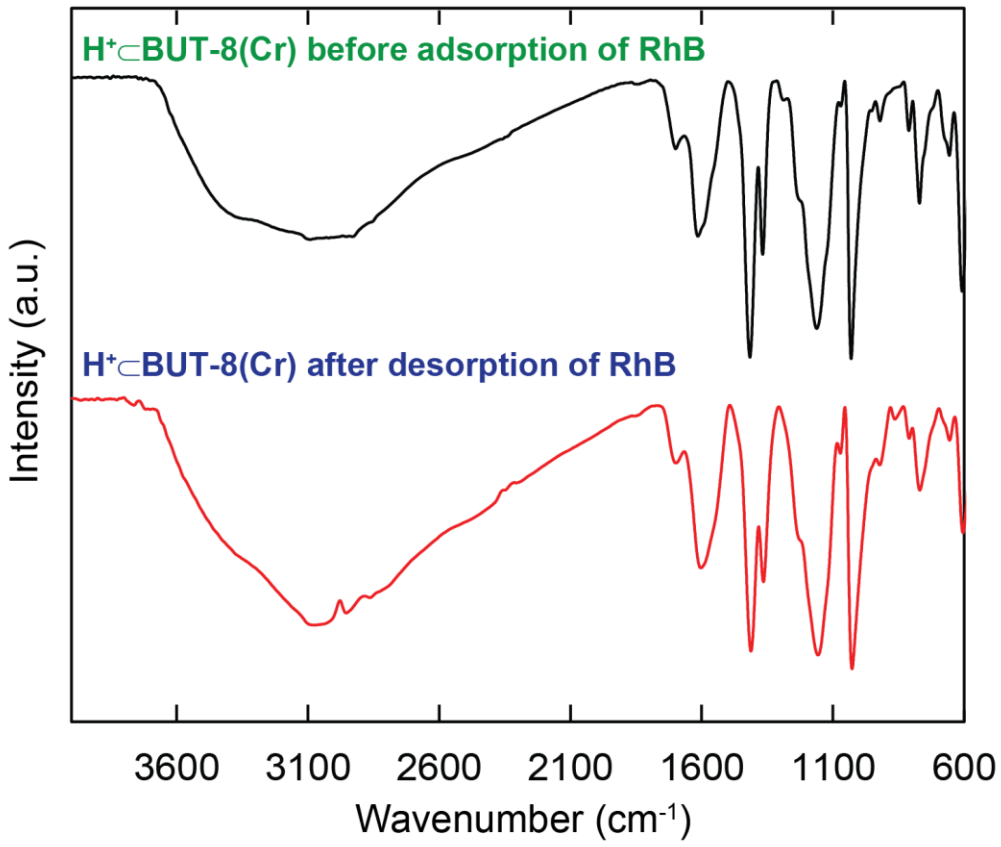


Figure S7. FT-IR spectrum of H^+⊂BUT-8(Cr) before adsorption of RhB (black) in comparison with FT-IR spectrum of H^+⊂BUT-8(Cr) after desorption of RhB (red).

N_2 adsorption measurement and surface area prediction

The porosity analysis of activated H^+⊂BUT-8(Cr) was measured by N_2 adsorption at 77 K.

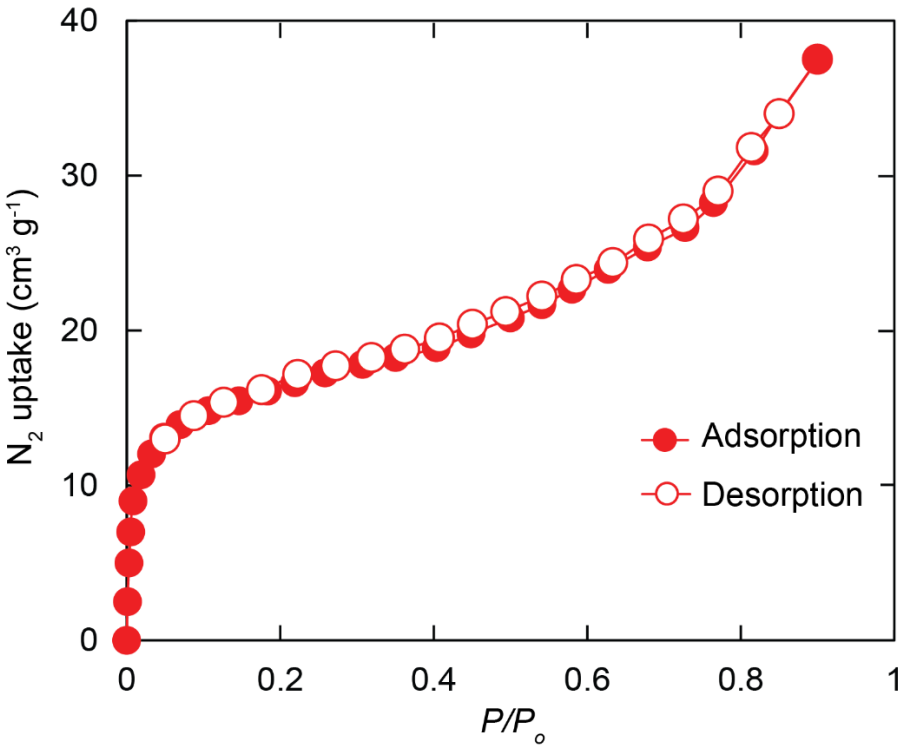
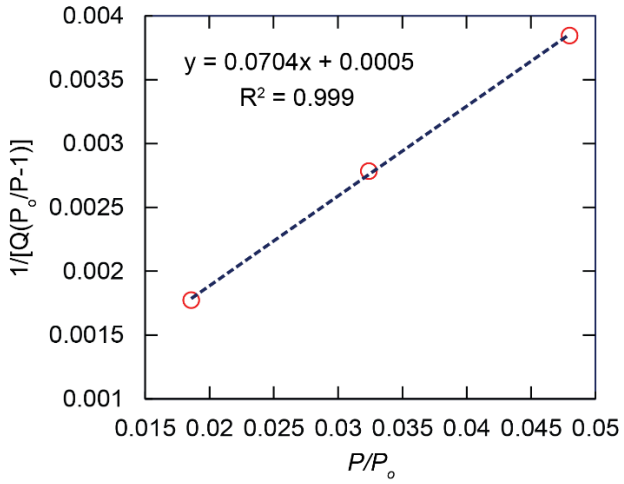
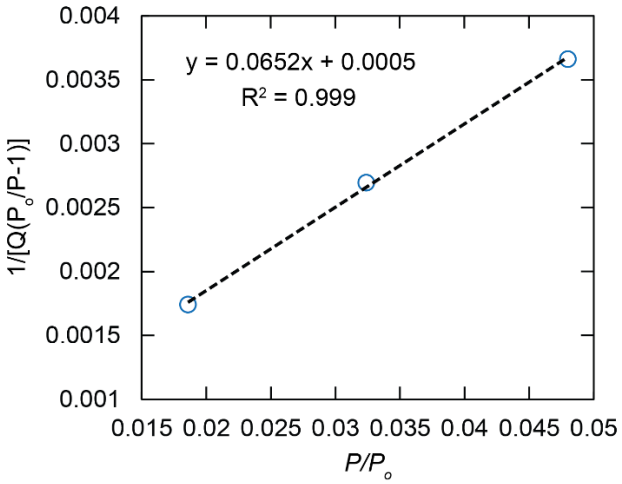


Figure S8. N_2 isotherm of H^+⊂BUT-8(Cr) material at 77 K.

(a)



(b)



(c)

Parameters	BET model	Langmuir model
P/P_o range	0.01858 - 0.04799	0.01858 - 0.04799
Correlation Coefficient	0.999	0.999
C	141.8	130.4
Q_m ($cm^3\ g^{-1}$ STP)	14.104	15.337
Molecular cross-sectional area (S / nm^2)	0.1620	0.1620
Surface area ($m^2\ g^{-1}$)	61.41	66.77

$$S = \frac{Q_m \times N_A \times A}{V}$$

Where S and Q_m are the BET or Langmuir surface area and quantity adsorbed. N_A is Avogrado'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 $Å^2$. This data was converted into the surface area per gram, leading to a theoretical surface area of 2751 $m^2\ g^{-1}$.

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

H^+⊂BUT-8(Cr)	
Crystal density (g cm^{-3})	0.707 [1]
Accessible solvent surface per cell ($Å^2$)	3482
Calculated SA ($m^2\ g^{-1}$)	2751
Unit cell volume ($Å^3$)	17903 [1]

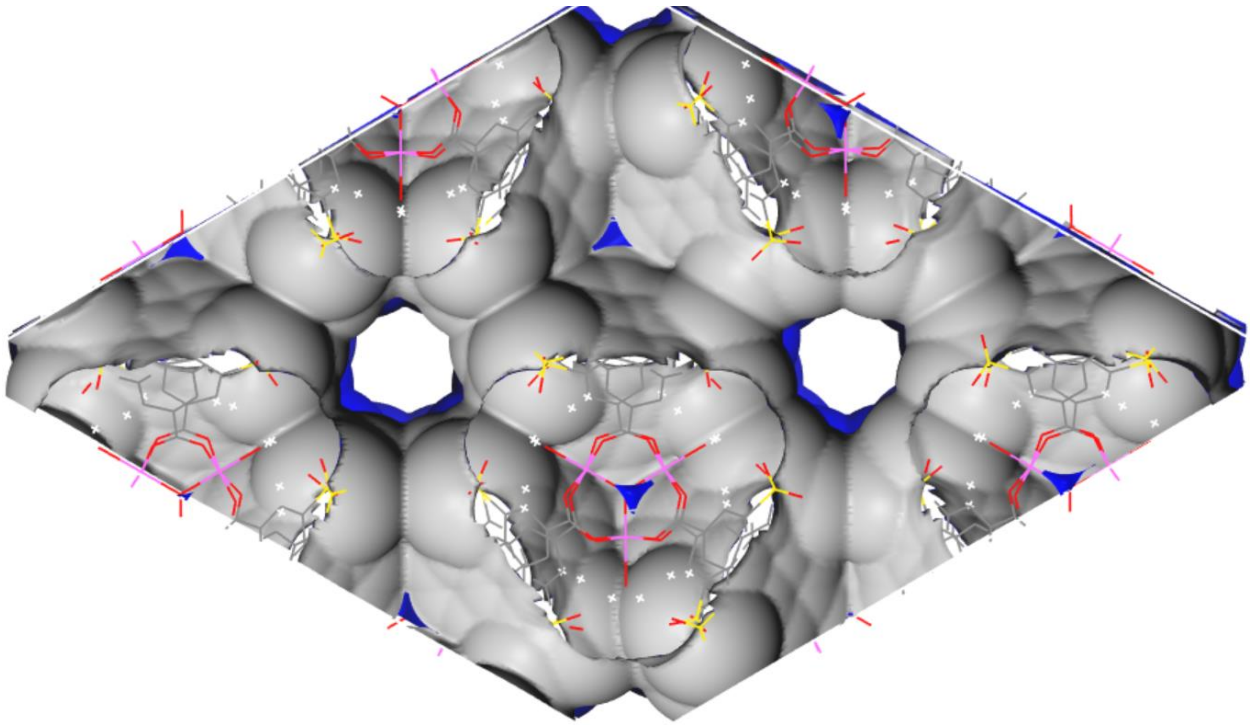


Figure S10. Accessible solvent surface and van der Waals surface of H^+⊂BUT-8(Cr).

[1] F. Yang, G. Xu, Y. Dou, B. Wang, H. Zhang, H. Wu, W. Zhou, J. Li and B. Chen, A flexible metal–organic framework with a high density of sulfonic acid sites for proton conduction, *Nature Energy*, 2017, **2**, 877–883.

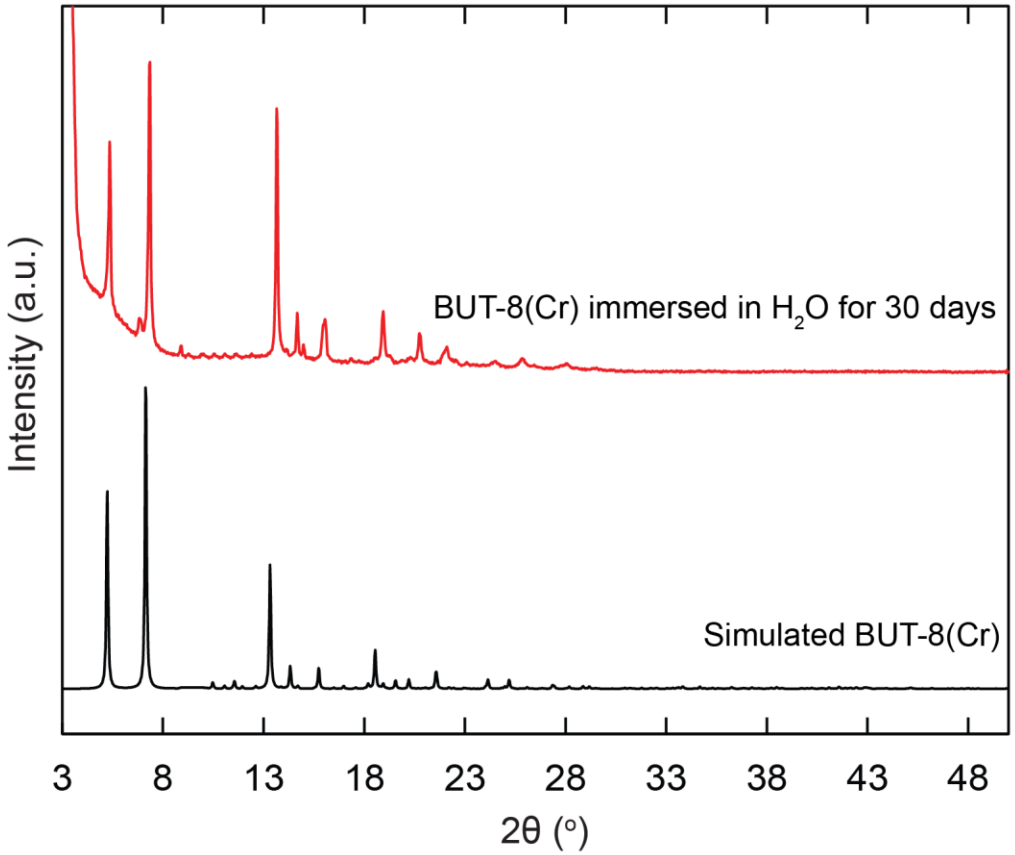


Figure S11. PXRD pattern of BUT-8(Cr) immersed in water for 30 days in comparison with the simulated structure

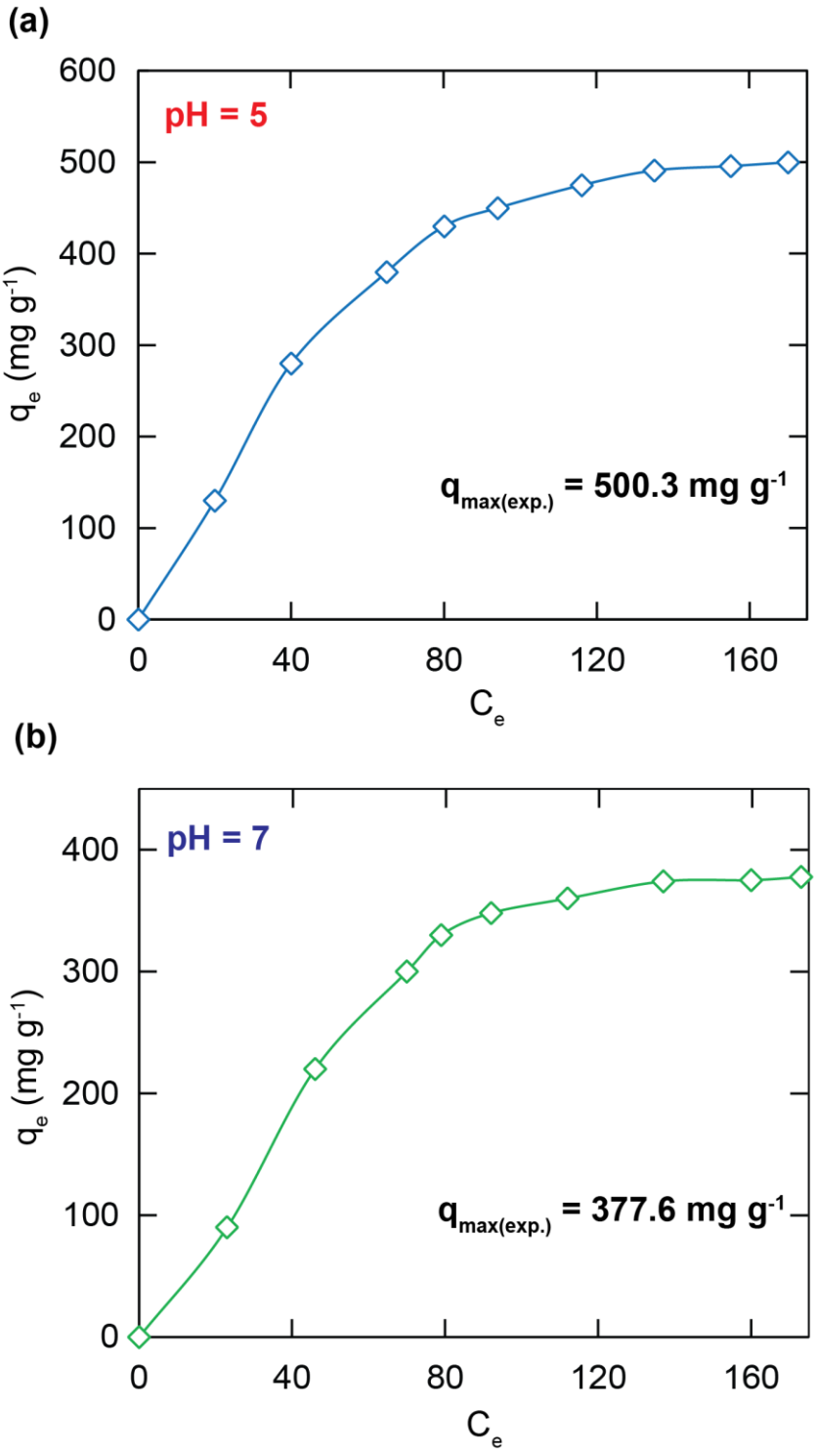


Figure S12. Effect of the concentration of RhB on the adsorption capacity of H^+⊂BUT-8(Cr) [m = 10 mg, V_{RhB} = 100 mL, C_o: 25-175 mg L^{-1}, t = 24 h] at pH = 5 (a); pH = 7 (b).

Adsorption isothermal models

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

$$\frac{C_e}{q_e} = \frac{1}{K_L q_m} + \frac{C_e}{q_m} \quad \text{(S1)}$$

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

$$q_e = \frac{RT}{b} \ln(k_T C_e) \quad \text{(S3)}$$

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, β 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):

$$R_L = \frac{1}{1 + K_L C_o} \quad \text{(S4)}$$

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