

# Magnetic functionalized Zr-based MOFs for effective adsorption of Au (III)

## from aqueous solution and mechanism study

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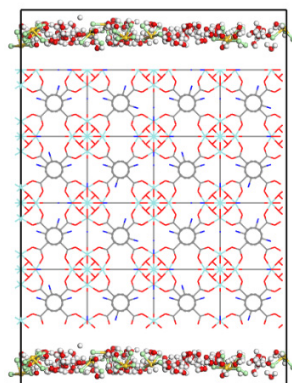
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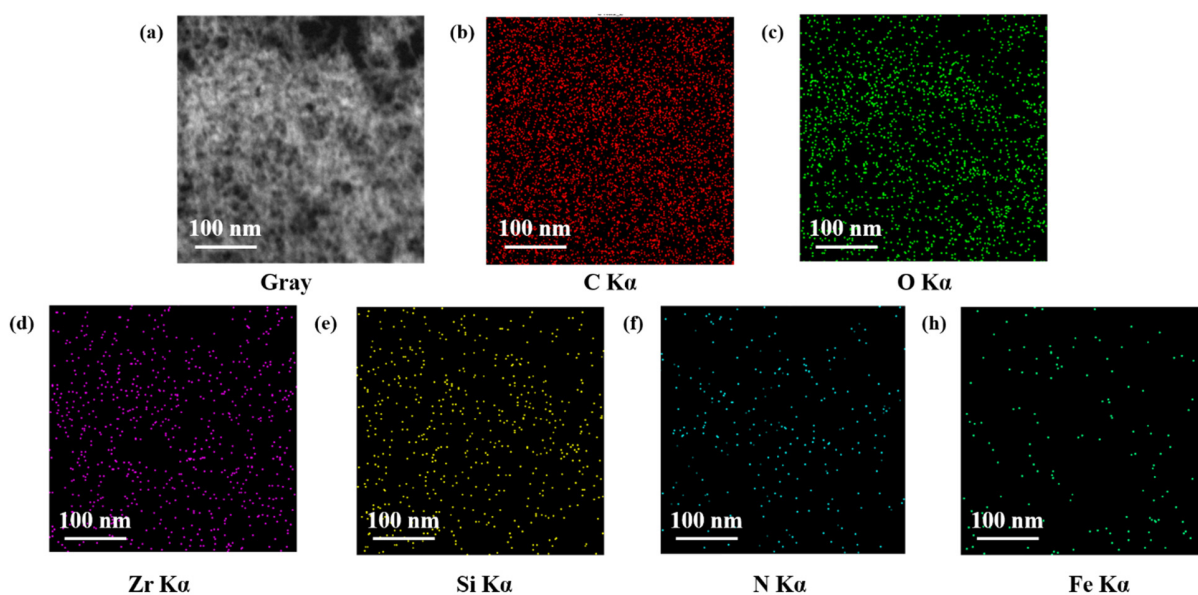
### Materials and instrumentation

Zirconium tetrachloride ( $\text{ZrCl}_4$ ) was purchased from Shanghai Meryer Chemical Technology Co. Ltd., 2-aminoterephthalic acid ( $\text{NH}_2\text{-BDC}$ ),  $\text{N,N}$ -dimethylformamide (DMF) and tetrachloroauric acid trihydrate ( $\text{HAuCl}_4\cdot 3\text{H}_2\text{O}$ ) were supplied by Aladdin Co. Ltd., ferric chloride hexahydrate ( $\text{FeCl}_3\cdot 6\text{H}_2\text{O}$ ), sodium bicarbonate ( $\text{NaHCO}_3$ ), Vitamin C and tetraethyl orthosilicate (TEOS) were provided by J&K Scientific (Beijing) Co. Ltd., glacial acetic acid ( $\text{CH}_3\text{COOH}$ ) and ethanol were supplied by Tongguang Chemical Technology (Beijing) Co. Ltd.. Chemicals used in this work were all used in their as-received states without further purification.

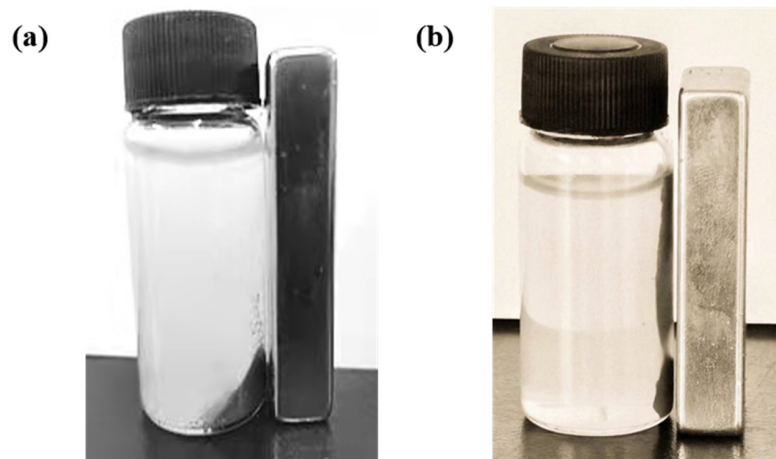
The magnetic functionalized MOFs before and after Au (III) adsorption were characterized by Fourier Transform Infrared Spectroscopy (FTIR, Thermo Nicolet), Malvern Zetasizer Nano ZS90, powder X-ray diffraction analyzer (PXRD, Rigaku Miniflex600,  $\text{Cu K}\alpha$  radiation, 40 kV, 40 mA), transmission electron microscopy (TEM, JEOL, JEM-2200FS) and X-ray photoelectron spectroscopy (XPS, Kratos,  $\text{Al K}\alpha$  radiation). The concentration of Au (III) after adsorption was determined using Inductively Coupled Plasma Optical Emission Spectrometer (ICP-OES, iCAP7000 plus).



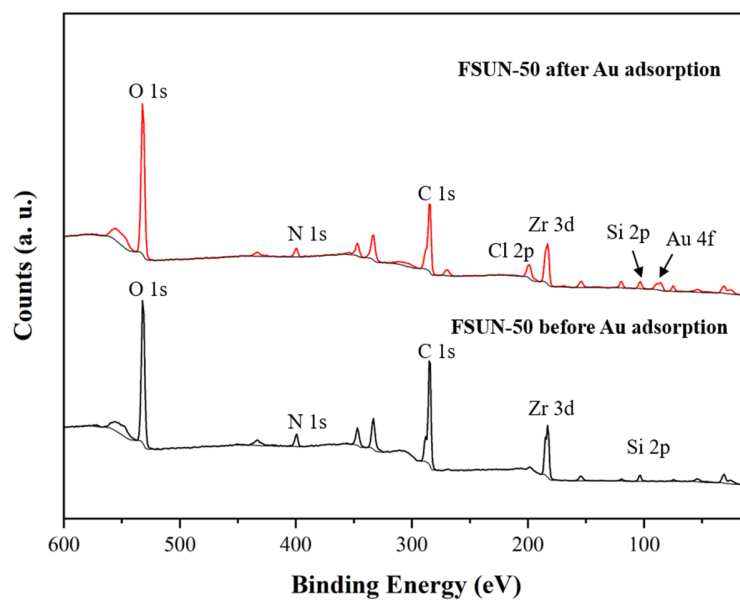
**Figure S1.** The initial configuration of  $\text{AuCl}_4^-$ ,  $\text{H}_2\text{O}$ ,  $\text{H}^+$  and UiO-66- $\text{NH}_2$  before adsorption dynamics simulation. The atoms of hydrogen, oxygen, nitrogen, carbon, zirconium, gold and chloride are colored as white, red, blue, grey, cyan, yellow and green.



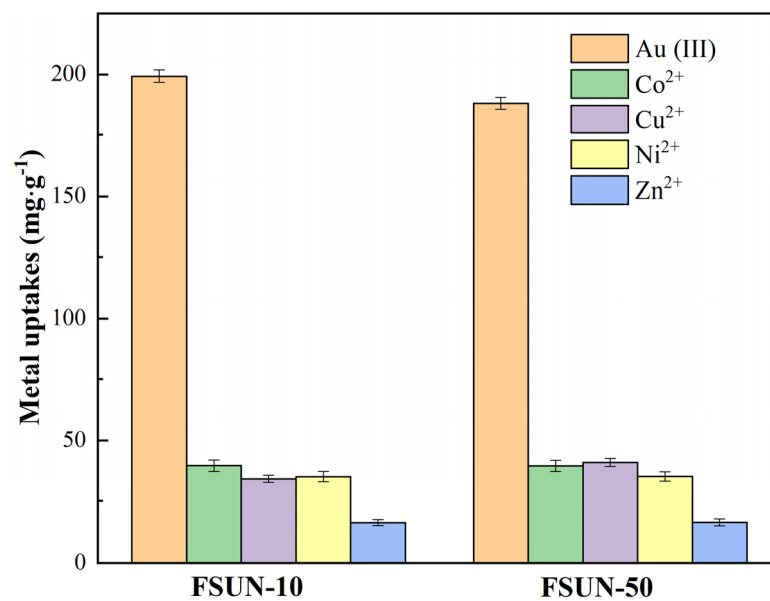
**Figure S2.** (a) EDX elemental mapping background of FSUN-50; (b–h): elemental distribution of C, O, Zr, Si, N of FSUN-50.



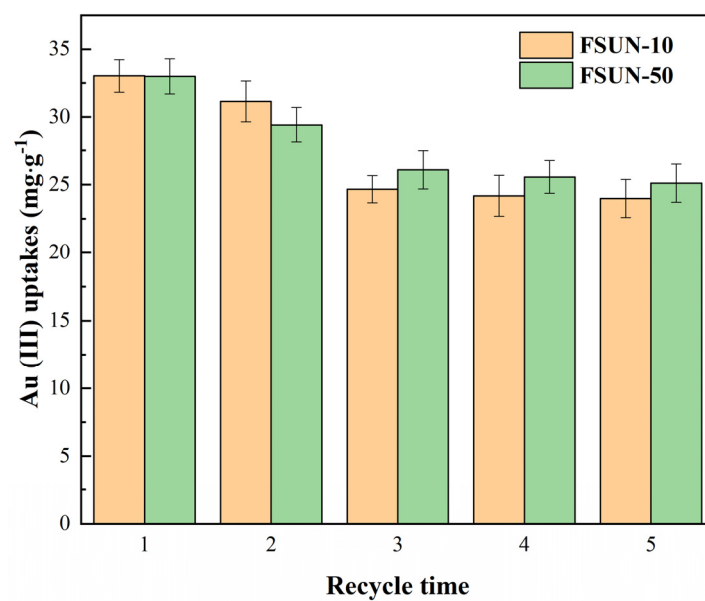
**Figure S3.** Magnetic separation of FSUN-10 (a) and FSUN-50 (b) by external magnet.



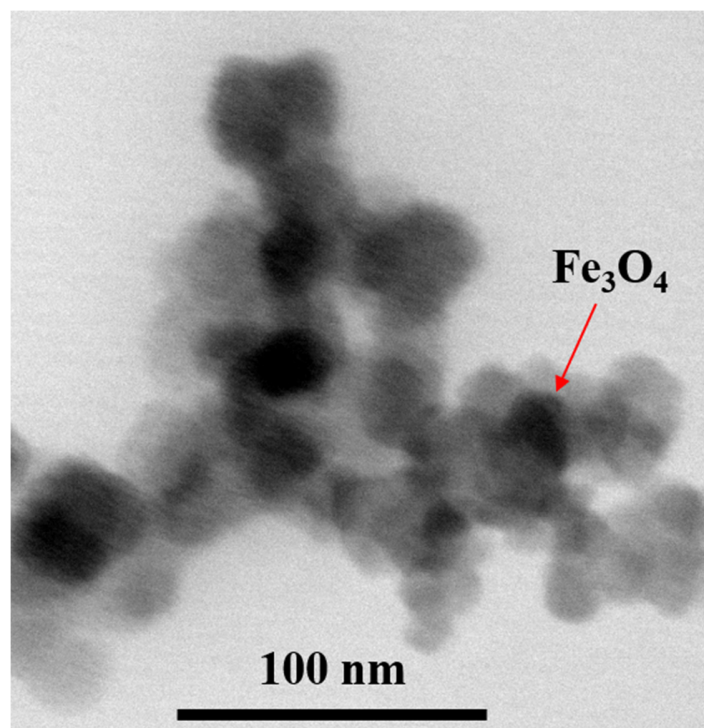
**Figure S4.** XPS survey scan of FSUN-50 before and after Au (III) adsorption.



**Figure S5.** Adsorption of Au (III), Co<sup>2+</sup>, Cu<sup>2+</sup>, Ni<sup>2+</sup> and Zn<sup>2+</sup> by FSUN-10 and FSUN-50.



**Figure S6.** Au (III) uptakes by FSUN-10 and FSUN-50 as a function of recycling time ( $m = 30$  mg,  $V = 10$  mL,  $C_0 = 100$  mg·L<sup>-1</sup>).



**Figure S7.** TEM image of the regenerated FSUN-50.