

Magnetic functionalized Zr-based MOFs for effective adsorption of Au (III) from aqueous solution and mechanism study

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Materials and instrumentation

Zirconium tetrachloride ($ZrCl_4$) was purchased from Shanghai Meryer Chemical Technology Co. Ltd., 2-aminoterephthalic acid (NH_2 -BDC), N,N-dimethylformamide (DMF) and tetrachloroauric acid trihydrate ($HAuCl_4 \cdot 3H_2O$) were supplied by Aladdin Co. Ltd., ferric chloride hexahydrate ($FeCl_3 \cdot 6H_2O$), sodium bicarbonate ($NaHCO_3$), Vitamin C and tetraethyl orthosilicate (TEOS) were provided by J&K Scientific (Beijing) Co. Ltd., glacial acetic acid (CH_3COOH) 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, Cu $K\alpha$ radiation, 40 kV, 40 mA), transmission electron microscopy (TEM, JEOL, JEM-2200FS) and X-ray photoelectron spectroscopy (XPS, Kratos, Al $K\alpha$ radiation). The concentration of Au (III) after adsorption was determined using Inductively Coupled Plasma Optical Emission Spectrometer (ICP-OES, iCAP7000 plus).

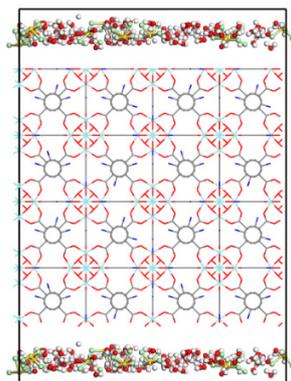


Figure S1. The initial configuration of AuCl_4^- , H_2O , H^+ and UiO-66- NH_2 before adsorption dynamics simulation. The atoms of hydrogen, oxygen, nitrogen, carbon, zirconium, gold and chloride are colored as white, red, blue, grey, cyan, yellow and green.

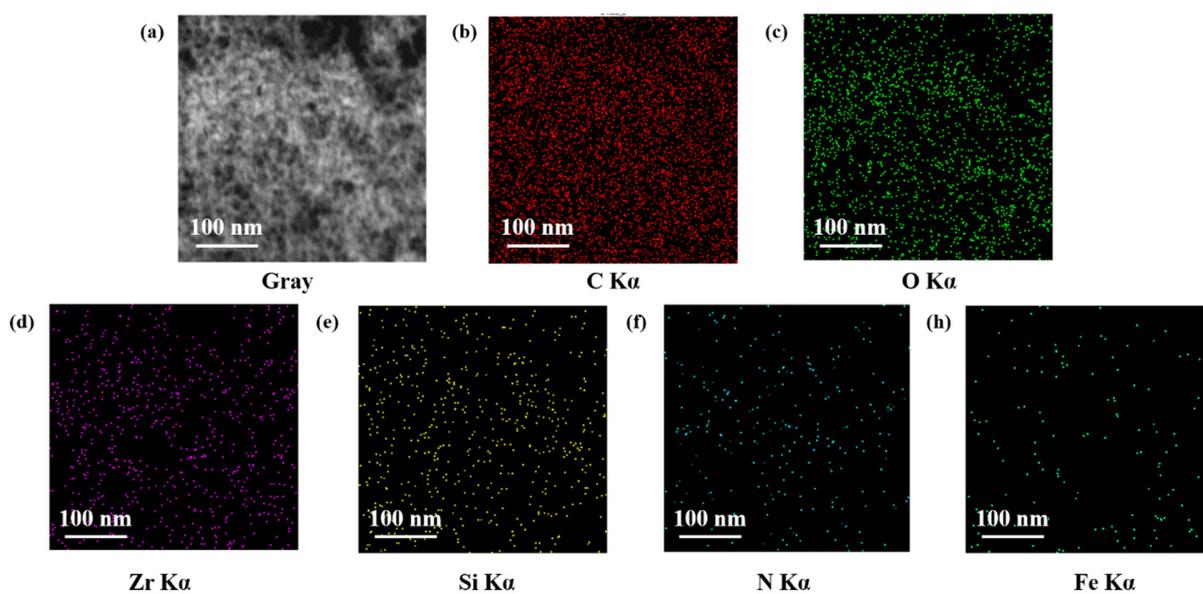


Figure S2. (a) EDX elemental mapping background of FSUN-50; (b–h): elemental distribution of C, O, Zr, Si, N of FSUN-50.

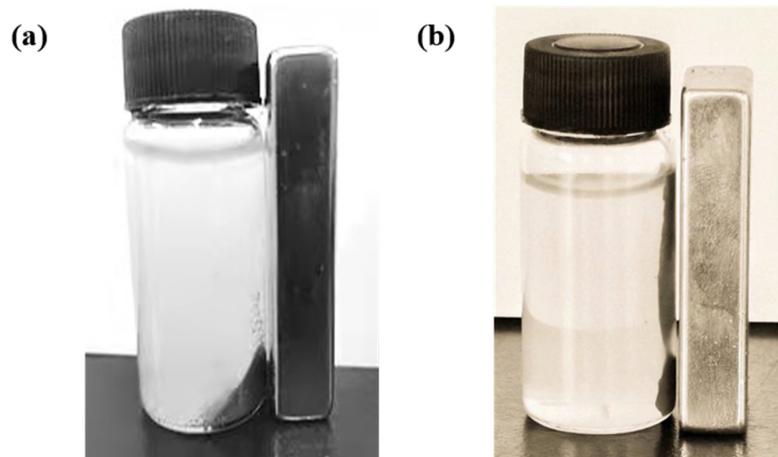


Figure S3. Magnetic separation of FSUN-10 (a) and FSUN-50 (b) by external magnet.

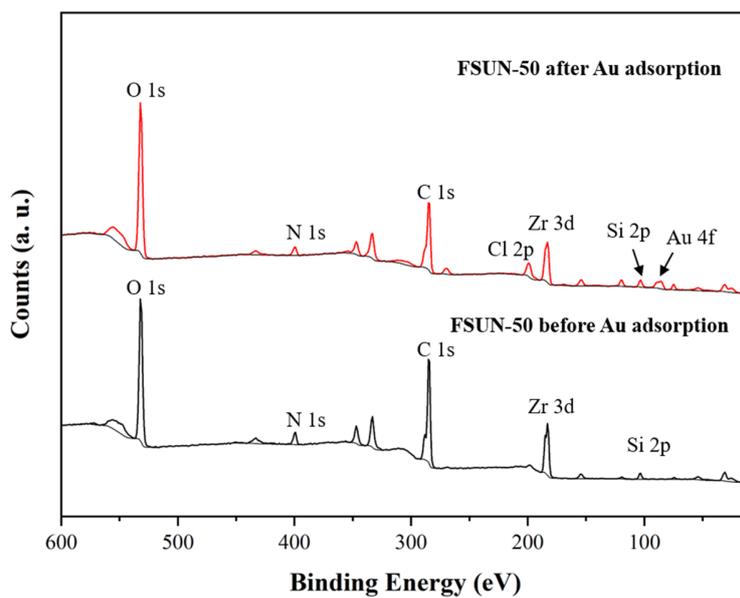


Figure S4. XPS survey scan of FSUN-50 before and after Au (III) adsorption.

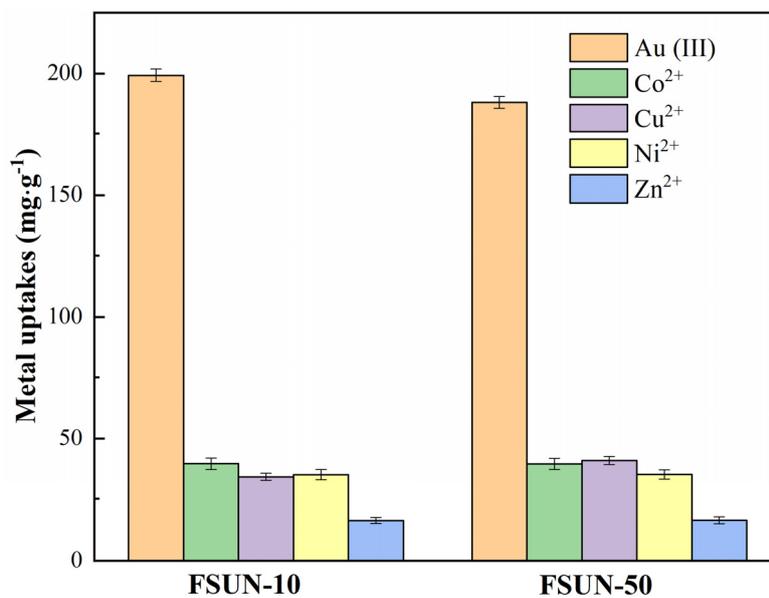


Figure S5. Adsorption of Au (III), Co²⁺, Cu²⁺, Ni²⁺ and Zn²⁺ by FSUN-10 and FSUN-50.

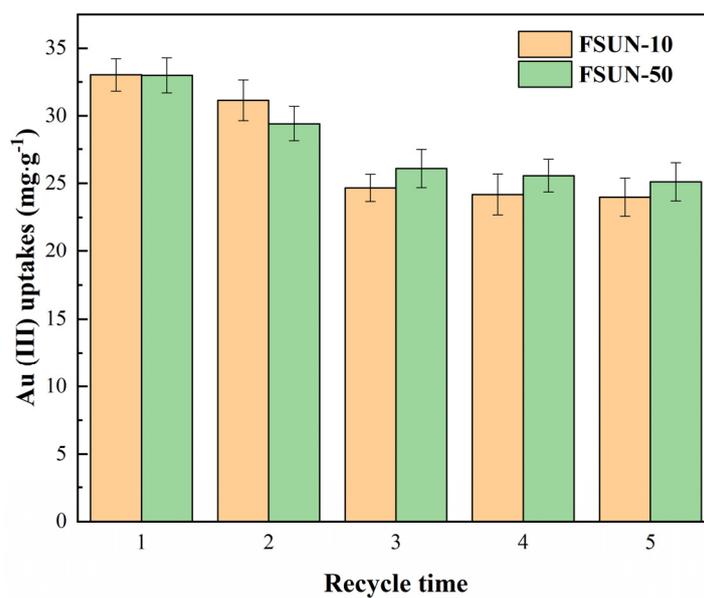


Figure S6. Au (III) uptakes by FSUN-10 and FSUN-50 as a function of recycling time ($m = 30$ mg, $V = 10$ mL, $C_0 = 100$ mg·L⁻¹).

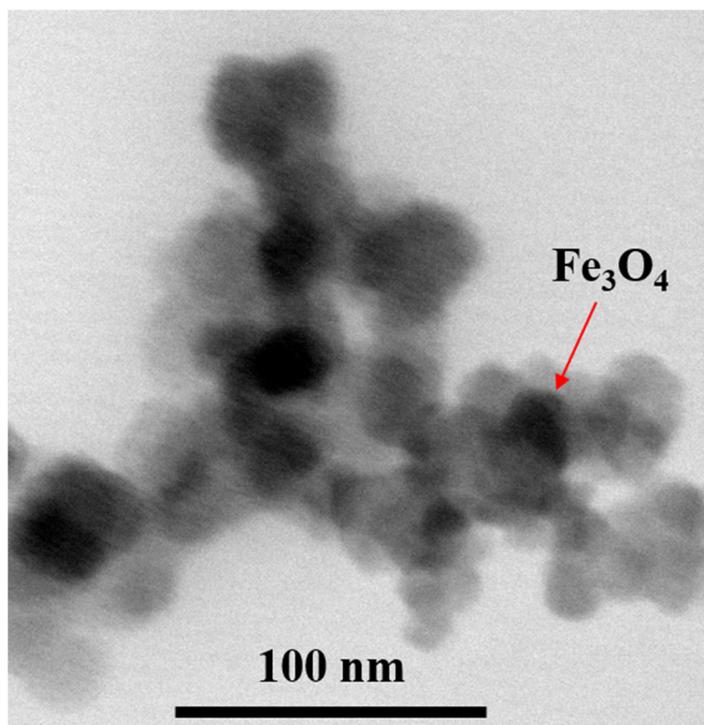


Figure S7. TEM image of the regenerated FSUN-50.