

## Supporting Information

### **Fine tuning of pore size in metal-organic frameworks for superior removal of U(VI) from aqueous solution**

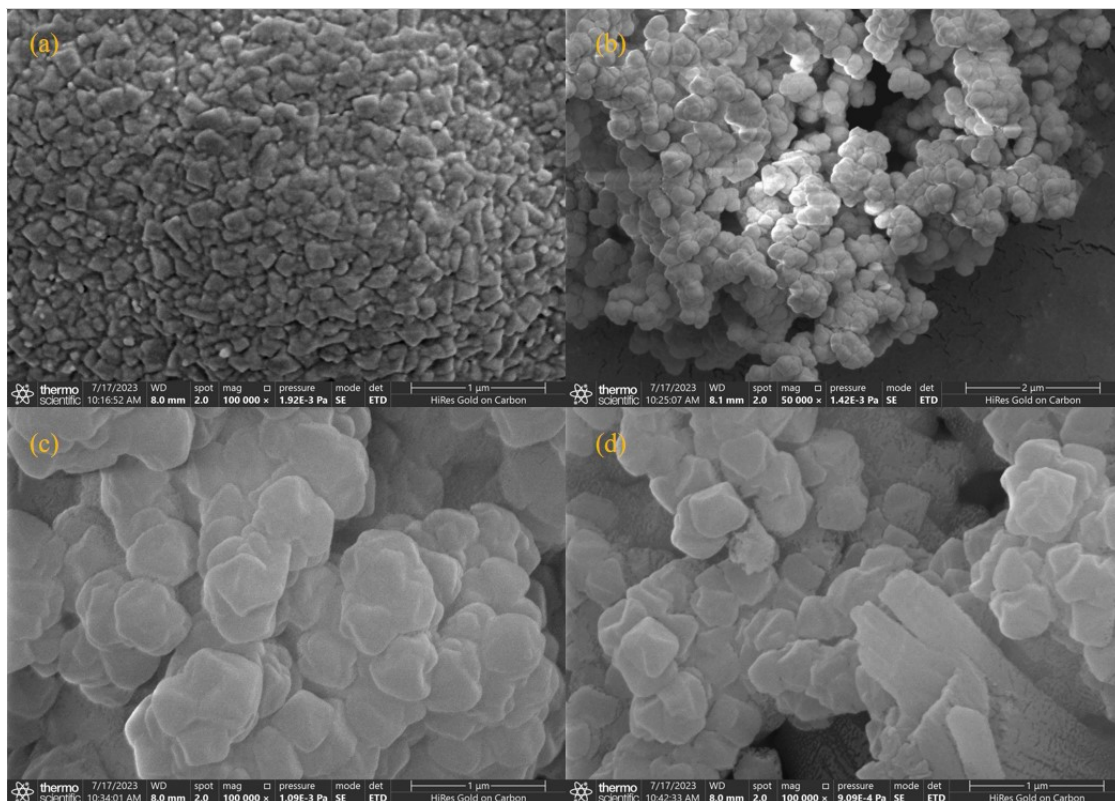
Tianyu Fu<sup>a</sup>, Hongjuan Liu<sup>a,c\*</sup>, Xinyi Wang<sup>a</sup> and Yingjiu Liu<sup>b</sup>

<sup>a</sup>*School of Nuclear Science and Technology, University of South China, Hengyang, 421001, China*

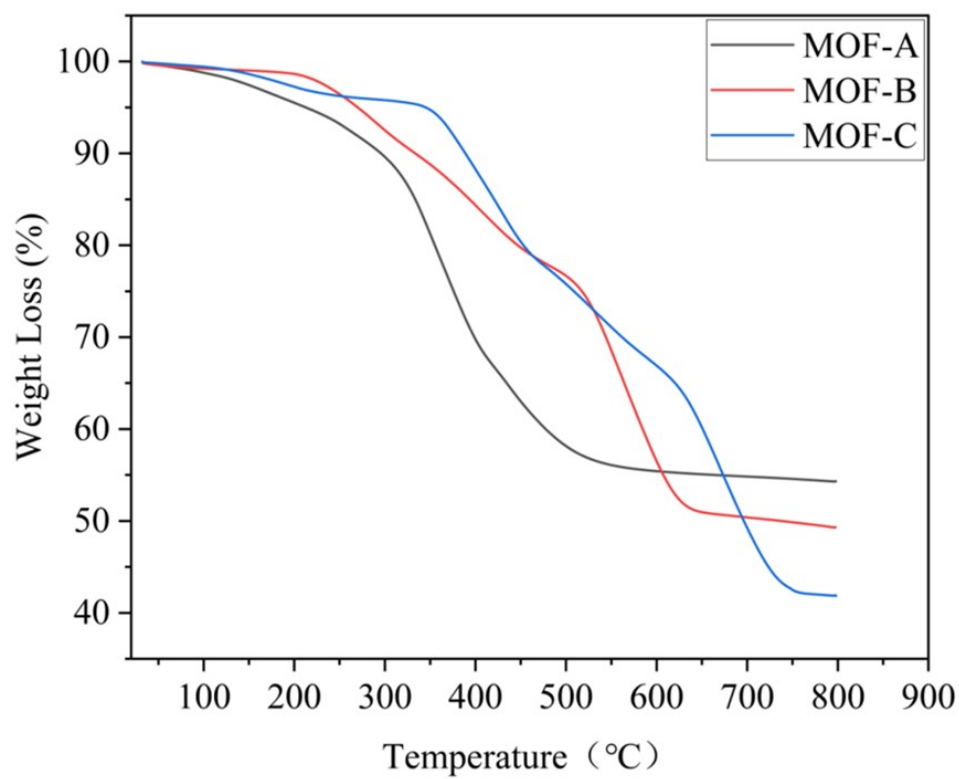
<sup>b</sup>*Hunan Province Key Laboratory of Pollution Control and Resources Reuse Technology, University of South China, Hengyang 421001, PR China*

<sup>c</sup>*Key Discipline Laboratory for National Defense for Biotechnology in Uranium Mining and Hydrometallurgy, University of South China, Hengyang 421001, PR China*

\*To whom correspondence should be addressed. Electronic mail: [l\\_ruyue@126.com](mailto:l_ruyue@126.com) (Hongjuan Liu).



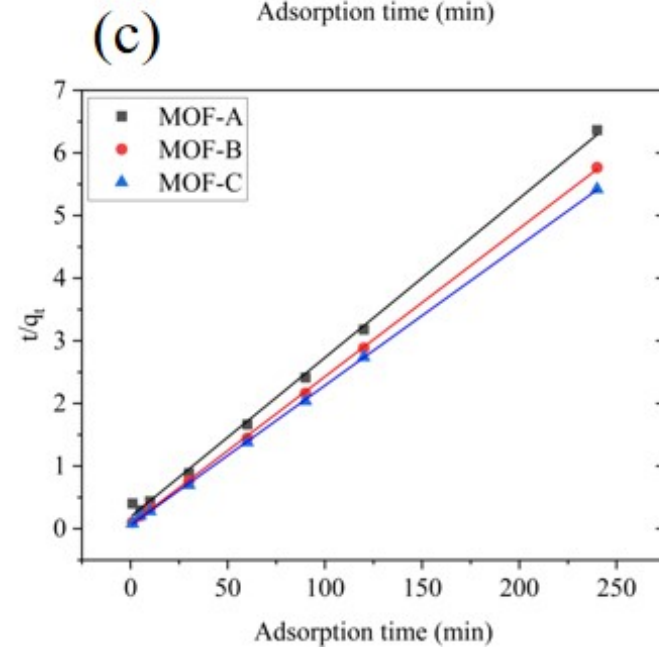
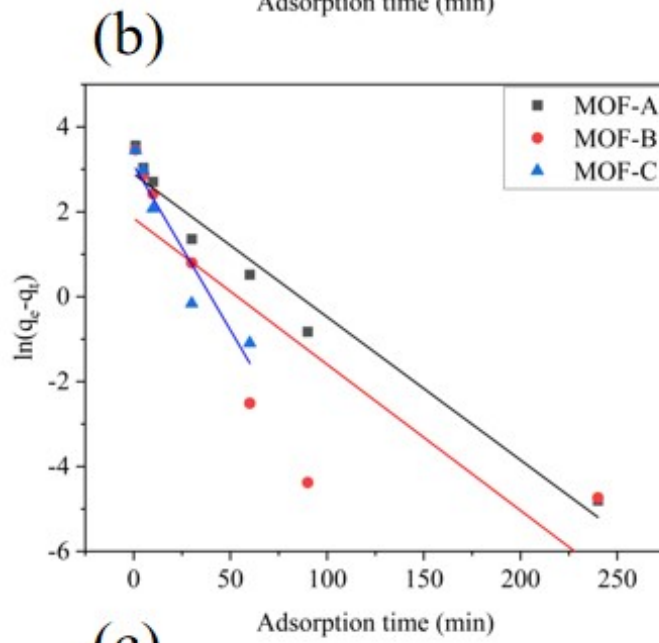
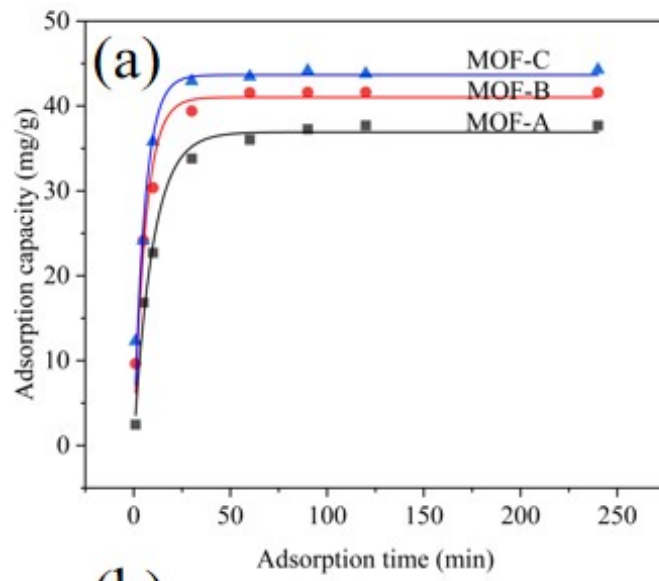
**Fig. S1.** SEM images of (a) MOF-A, (b) MOF-B, (c) MOF-C, (d) MOF-C with U.



**Fig. S2.** The thermogravimetric curves of three MOFs.

**Table S1** Kinetic parameters for the U(VI) adsorption of MOFs

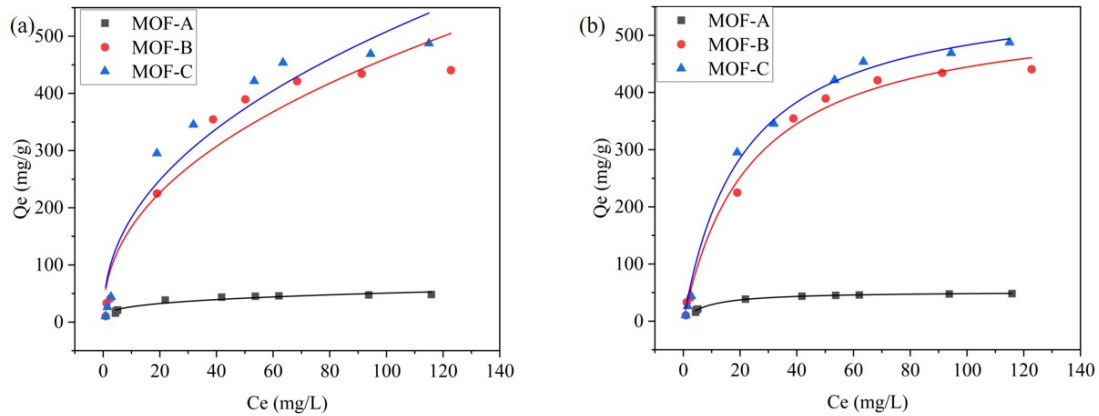
Adsorbents	Pseudo-first-order kinetics			Pseudo-second-order kinetics		
	$Q_e(\text{mg}\cdot\text{g}^{-1})$	$K_1(\text{min}^{-1})$	$R^2$	$Q_e(\text{mg}/\text{g})$	$K_2(\text{min}^{-1})$	$R^2$
MOF-A	18.08	0.0777	0.968	39.34	0.0034	0.998
MOF-B	6.34	0.0792	0.691	42.30	0.0087	0.999
MOF-C	22.18	0.1579	0.882	43.29	0.0090	0.999



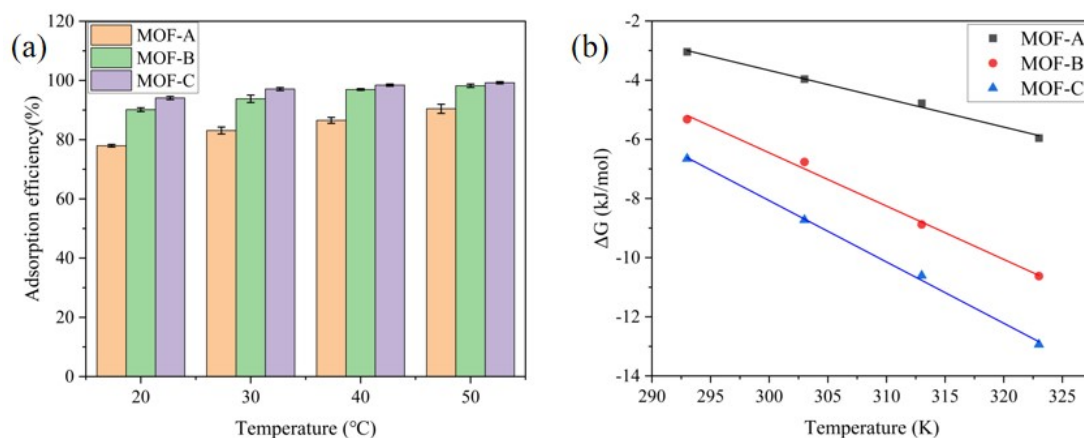
**Fig. S3.** (a) Effect of contact time on the U(VI) adsorption by MOF-A, MOF-B, and MOF-C (m=10 mg, pH=11 (MOF-A), pH=5 (MOF-B and MOF-C), T=308 K,  $C_0=20$  mg·L<sup>-1</sup>); (b) Pseudo-first-order kinetics fitting and (c) pseudo-first-order kinetics fitting for the three MOFs.

**Table S2** Parameters of Langmuir and Freundlich isotherm models of the U(VI) adsorption on three MOFs

Adsorbents	Langmuir model			Freundlich model		
	$Q_m(\text{mg}\cdot\text{g}^{-1})$	$K_l(\text{L}\cdot\text{mg}^{-1})$	$R^2$	$K_f(\text{L}\cdot\text{mg}^{-1})$	$1/n$	$R^2$
MOF-A	51.91	0.12576	0.993	14.14	0.27717	0.943
MOF-B	550.03	0.04212	0.993	60.04	0.44265	0.942
MOF-C	584.13	0.04679	0.995	65.67	0.44778	0.931



**Fig. S4.** Adsorption isotherms of U(VI) on MOF-A, MOF-B and MOF-C (adsorbent amount: 10 mg; pH: 11 (MOF-A), 5 (MOF-B and MOF-C); temperature: 308 K; contact time: 90 min); (a) Freundlich model fitting; (b) Langmuir model fitting.



**Fig. S5.** (a) Effect of temperature on the U (VI) adsorption performance of MOF-A, MOF-B and MOF-C (adsorbent amount: 10 mg; pH: 11 (MOF-A), 5 (MOF-B and MOF-C); initial U (VI) concentration: 20 mg·L<sup>-1</sup>; contact time: 90 min); (b)

Thermodynamic fitting of three MOFs.

**Table S3** Thermodynamic parameters of uranium adsorption by MOFs

Adsorbents	$\Delta G$ (kJ/mol)				$\Delta H$ (kJ/mol)	$\Delta S$ (kJ/mol)	$R^2$
	293 K	303 K	313 K	323 K			
MOF-A	-3.04	-3.96	-4.78	-5.96	25.04	0.095	0.994
MOF-B	-5.32	-6.76	-8.88	-10.62	47.60	0.18	0.995
MOF-C	-6.65	-8.72	-10.61	-12.94	54.12	0.21	0.998