

# High-performance $\text{Hg}^{2+}$ removal from ultra-low-concentration aqueous solution using both acylamide- and hydroxyl-functionalized metal-organic framework

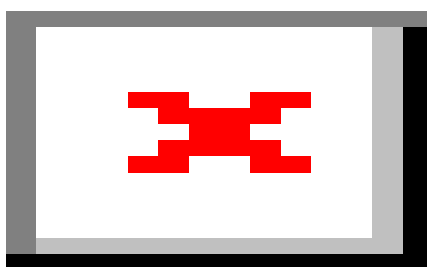
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**Table S1** Adsorption isotherm constants for  $\text{Hg}^{2+}$  onto MOF material.

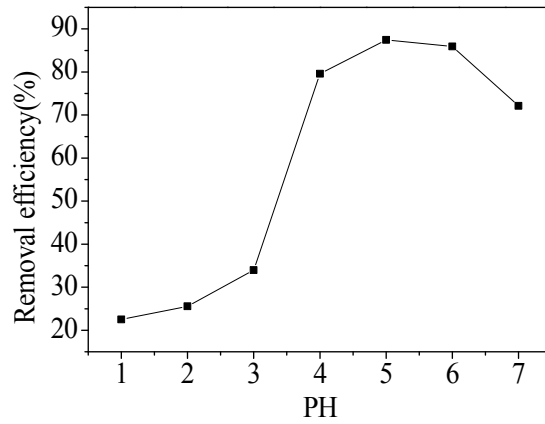
Langmuir isotherm			Freundlich isotherm		
$q_{max}$	$K_L$	$R^2$	$K_F$	$1/n$	$R^2$
$\text{mg g}^{-1}$	$\text{mg L}^{-1}$		$\text{mg g}^{-1}$		
333.33	2.776	0.9145	71.593	0.671	0.816

**Table S2** Thermodynamic parameters for sorption of  $\text{Hg}^{2+}$ .

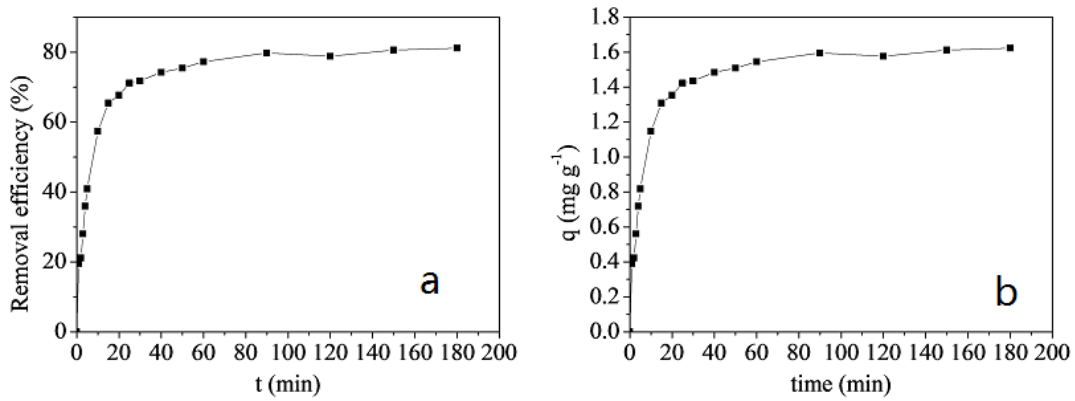
$\Delta H^0$ ( $\text{kJ mol}^{-1} \text{ k}^{-1}$ )	$\Delta S^0$ ( $\text{J mol}^{-1} \text{ k}^{-1}$ )	$\Delta G^0$ ( $\text{kJ mol}^{-1}$ )		
		298.15	308.15	318.15
-3.93	67.33	-24.01	-24.68	-25.35



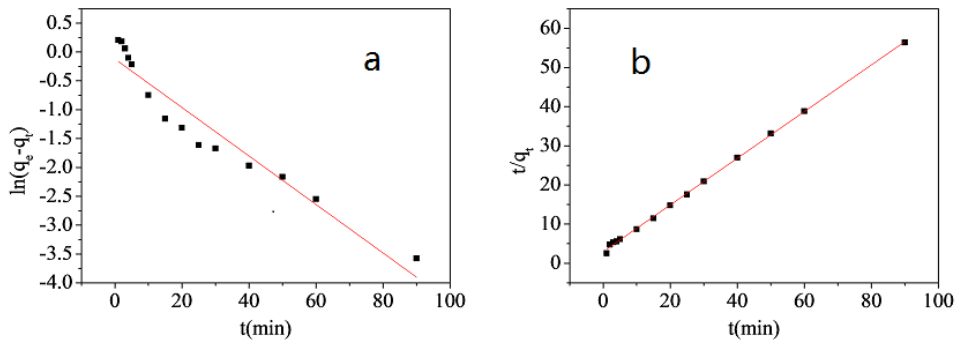
**Fig. S1** PXRD patterns simulated from single crystal data, of synthesized samples and  $\text{Hg}^{2+}$  loaded samples.



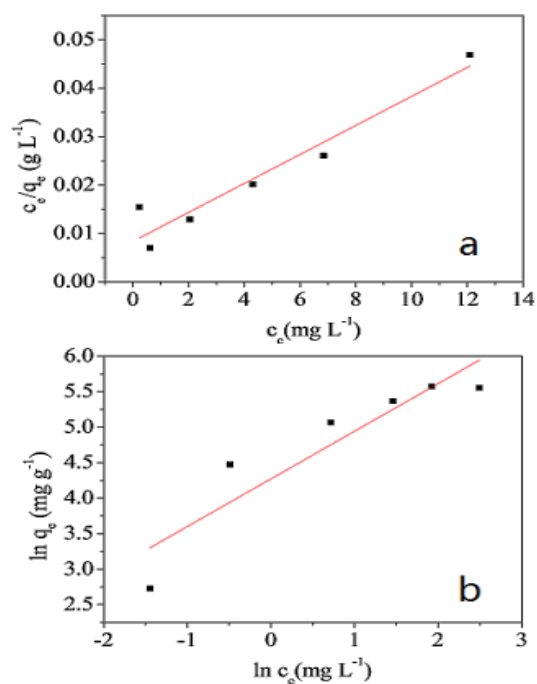
**Fig. S2** pH effect on the adsorption of  $\text{Hg}^{2+}$  ( $C_0(\text{Hg}^{2+})=100$  ppb,  $v=40$  mL,  $m(\text{adsorbent})=2$  mg,  $T=25^\circ\text{C}$ ,  $t=2$  h).



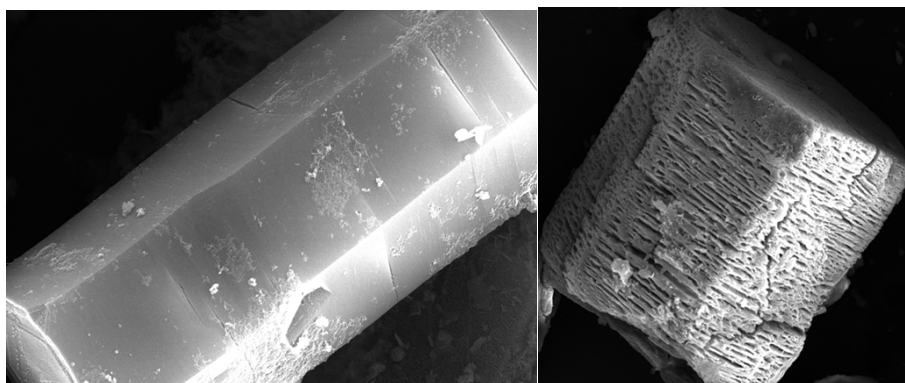
**Fig. S3** Effect of contact time on  $\text{Hg}(\text{II})$  removal ( $C_0(\text{Hg}^{2+})=100$  ppb,  $v=40$  mL,  $m(\text{adsorbent})=2$  mg,  $T=25^\circ\text{C}$ ,  $\text{pH}=5$ )



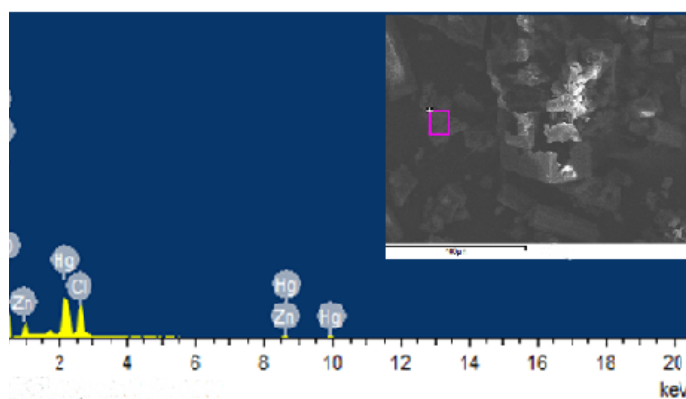
**Fig. S4** Pseudo-first-order kinetic plot (a) and pseudo-second-order kinetic plot (b) for the adsorption of  $\text{Hg}(\text{II})$  onto adsorbent.



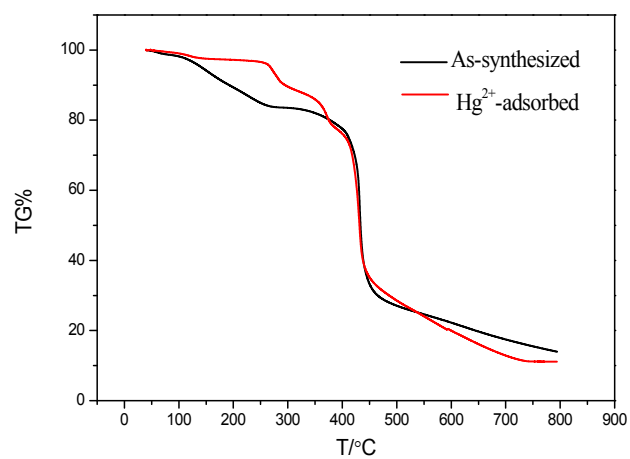
**Fig. S5** Adsorption isotherms fitted by the Langmuir (a) and Freundlich (b) models ( $c^0(\text{Hg}^{2+})=100$  ppb,  $v=40$  mL,  $m(\text{adsorbent})=2$  mg,  $T=25^\circ\text{C}$ ,  $t=1$  h).



**Fig. S6** The TEM image of the MOF material before and after the adsorption of Hg(II).



**Fig. S7** SEM and EXD spectra of the MOF material after loading Hg<sup>2+</sup>.



**Fig. S8** TG curves of as-synthesized and Hg<sup>2+</sup>-adsorbed MOF sample.