

## Supporting Information

### Efficient Removal of Heavy Metals from Polluted Water with High Selectivity for Hg(II) and Pb(II) by 2-imino-4-Thiobiuret Chemically Modified MIL-125 Metal-Organic Framework

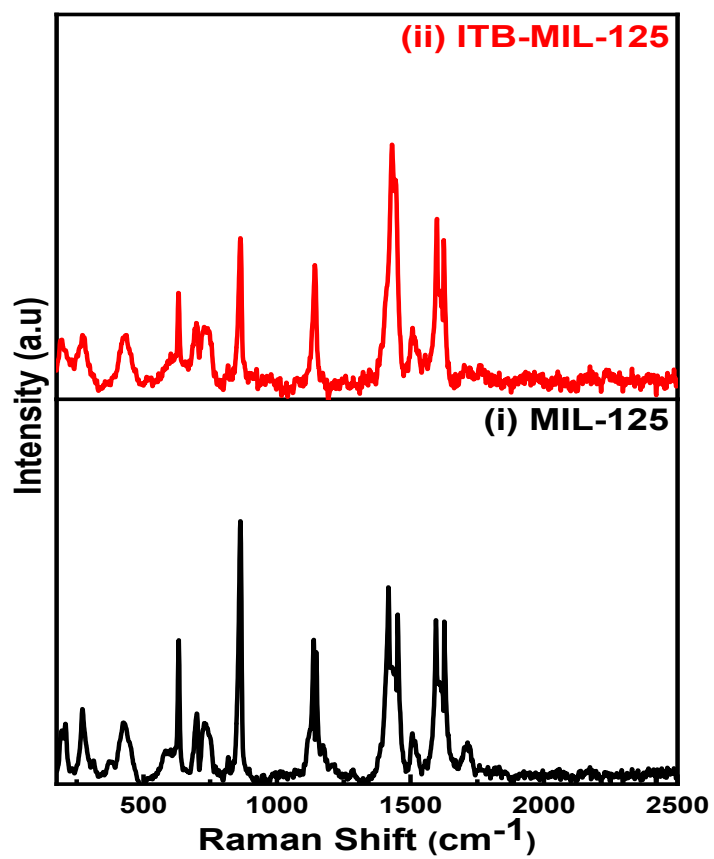
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Fig. S1. Adsorption system.



**Fig. S2.** Raman spectra of MIL-125 and ITB-MIL-125.

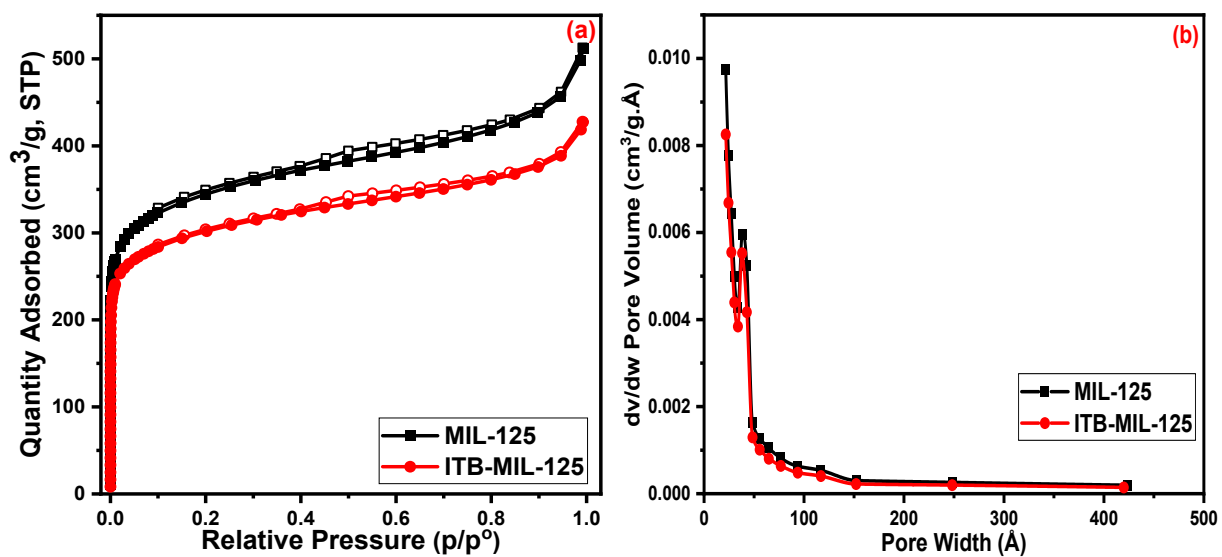
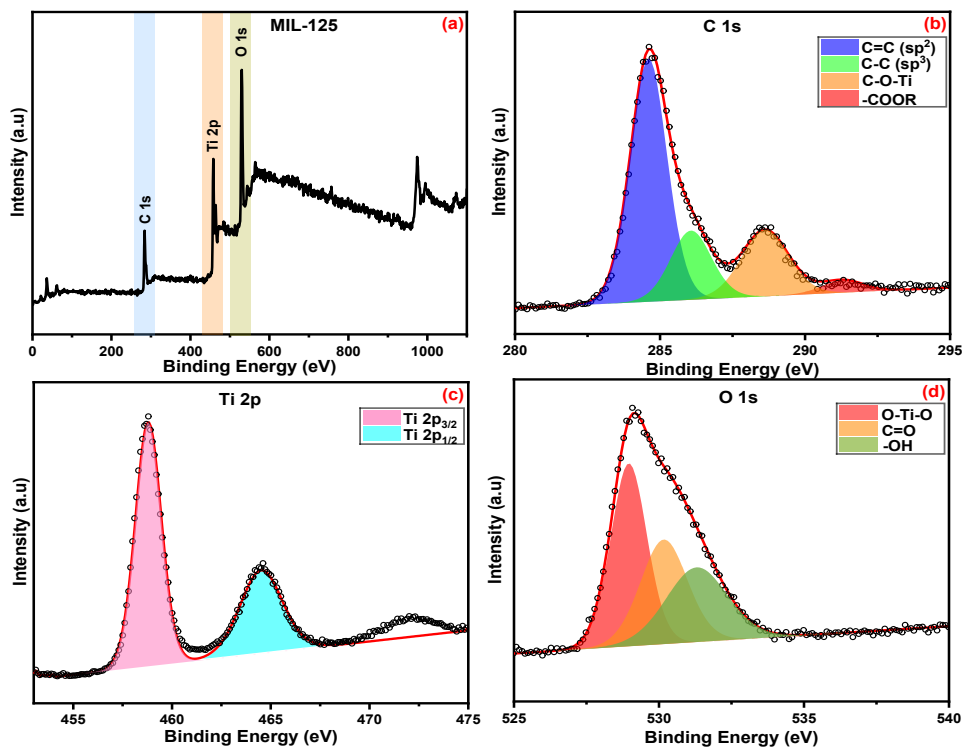
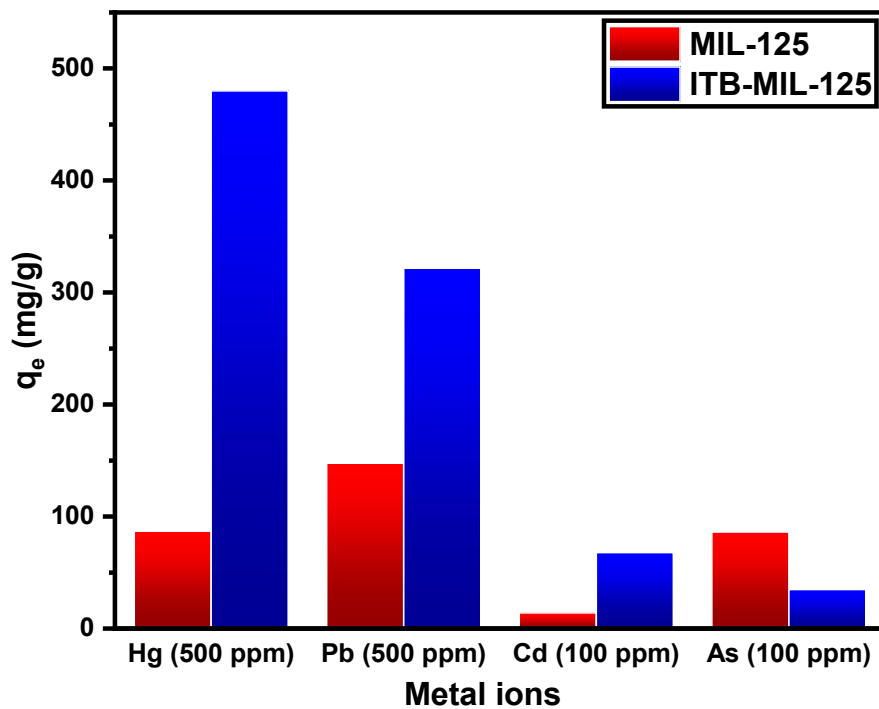


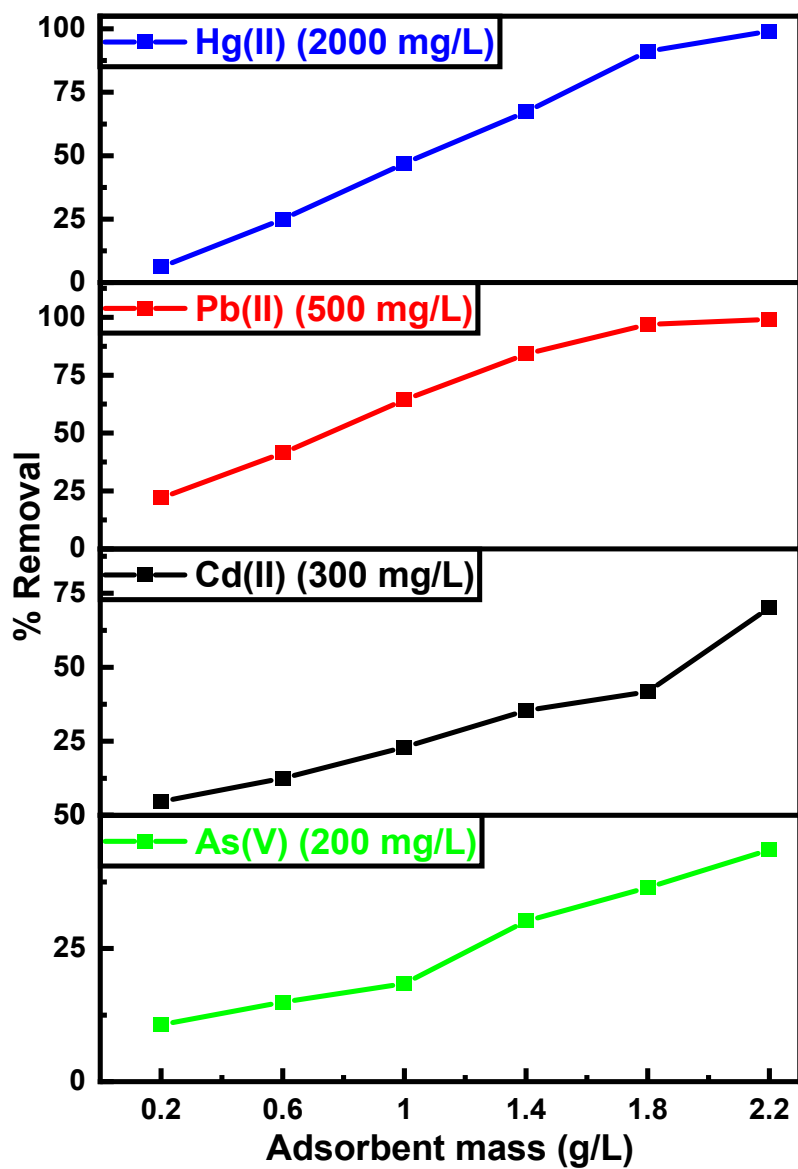
Fig. S3. (a)  $N_2$  adsorption-desorption isotherms and (b) Estimated BJH pore size distribution for MIL-125 and ITB-MIL-125.



**Fig. S4.** XPS survey spectrum of MIL-125 (a) and XPS high-resolution spectra of (b) C 1s, (c) Ti 2p and (d) O 1s.

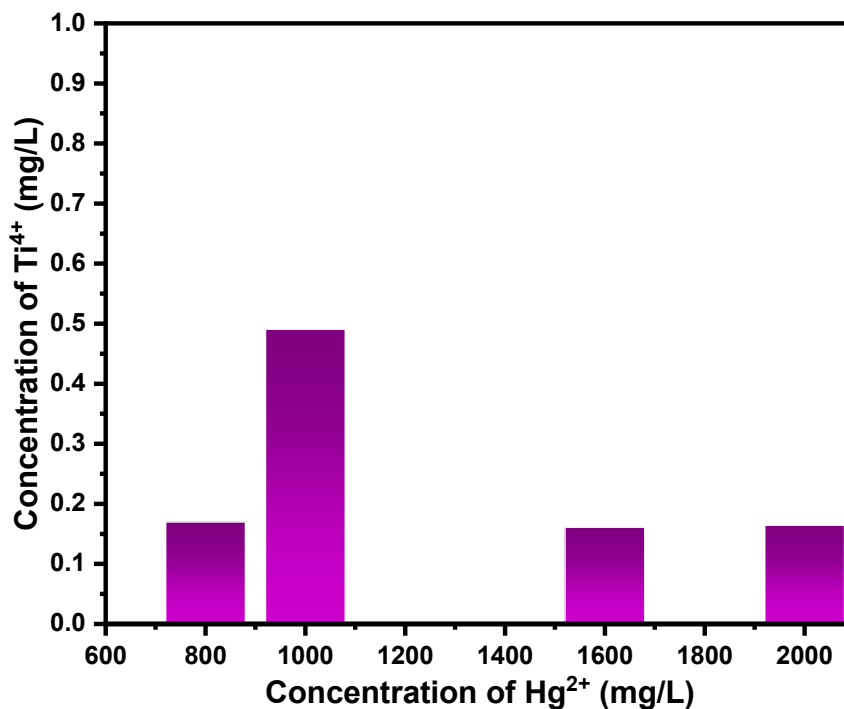


**Fig. S5.** Comparison of adsorption capacities of MIL-125 and ITB-MIL-125 adsorbents at pH 6 for Hg(II), Pb(II) and Cd(II); and at pH 2 for As(V). [Conditions: adsorbent mass = 0.005 g, volume = 5 mL and T = 298 K].

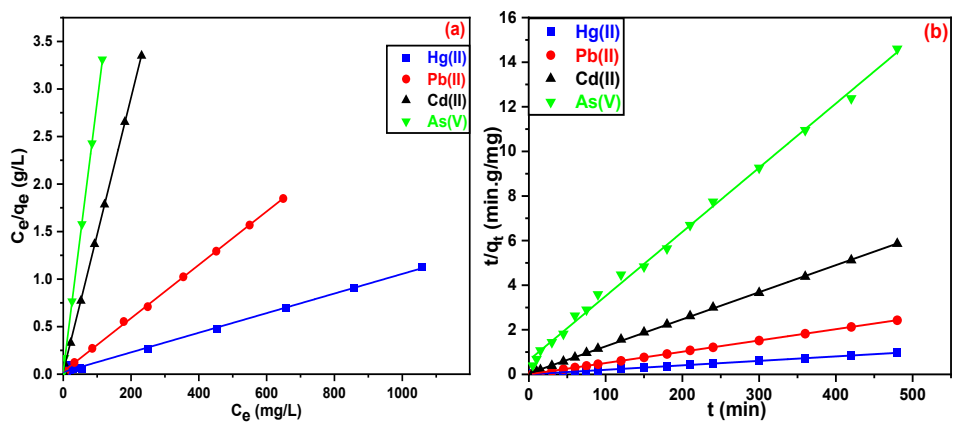


**Fig. S6.** Effect of adsorbent mass (g/L) on the removal efficiency as at pH 6 for Hg(II), Pb(II) and Cd(II); and at pH 2 for As(V). [Conditions:  $C_o = 2000$  mg/L Hg(II), 500 mg/L Pb(II), 300 mg/L Cd(II), 200 mg/L As(V), adsorbent mass = 0.2-2.2 g/L, volume = 5 mL and  $T = 298$  K].

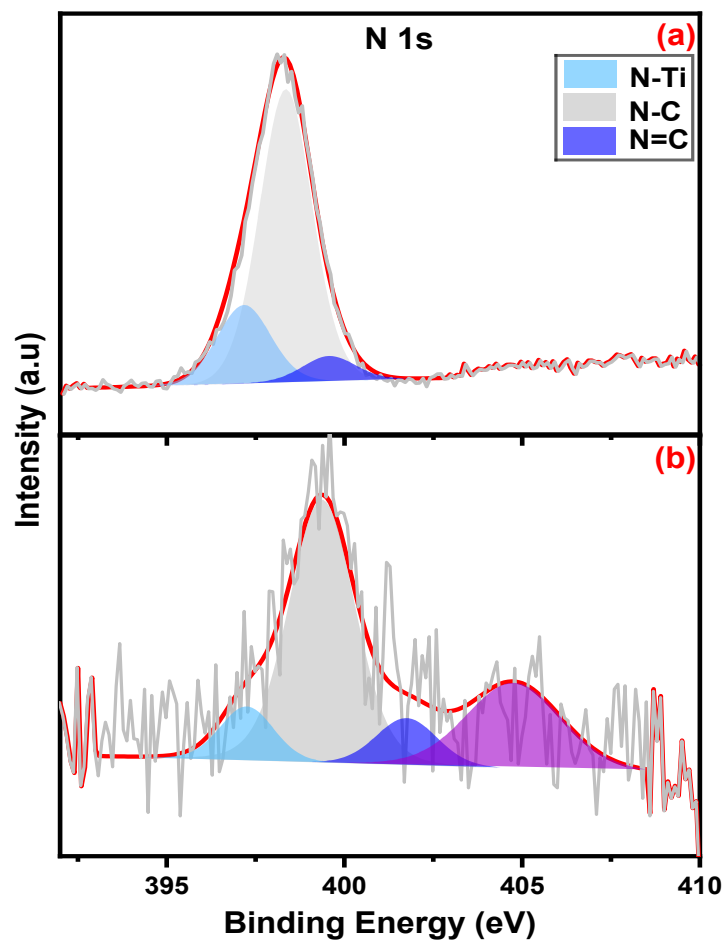
Experiments were conducted to evaluate the extent of ion exchange between Hg(II) from aqueous solution and Ti(IV) from MIL-125 frameworks. The adsorption experiment was carried out at room temperature under the same condition of adsorbent dose (0.005 g) and volume of Hg(II) solution (5 mL) for 24 hrs. The concentrations were measured by ICP-OES before and after the adsorption process. Fig. S7 shows the concentration of  $\text{Ti}^{4+}$  is less than 0.5 mg/L, which confirms the adsorption of Hg(II) without significant ion exchange with Ti(IV).



**Fig. S7.** Ion exchange study at pH 6 for Hg(II). [Conditions:  $C_0 = 800, 1000, 1600$  and  $2000$  mg/L, adsorbent mass = 0.005 g, volume = 5 mL and  $T = 298$  K].



**Fig. S8.** (a) Langmuir adsorption isotherm and (b) Pseudo-second order for adsorption of Hg(II), Pb(II), Cd(II) and As(V) on the ITB-MIL-125 adsorbent.



**Fig. S9.** XPS high-resolution of N1s (a) before adsorption and (b) after adsorption of Hg(II) ions.