Supporting Information (SI) on

Efficient removal of Pb^{2+} by Tb-MOFs: Identifying the adsorption mechanism through experimental and theoretical investigations

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Supplemental Information, 6 pages, 4 figures and 4 tables.

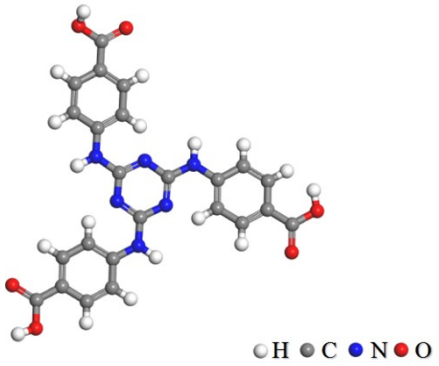

Figure S1. The structure of H_3TATAB.

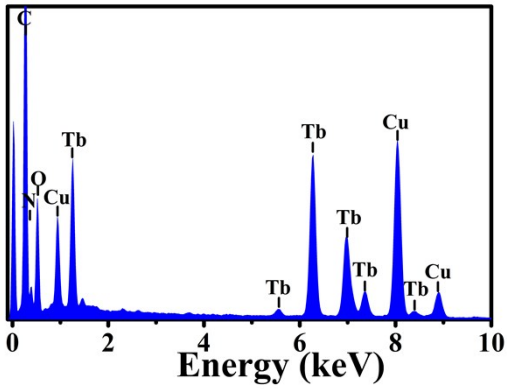

Figure S2. EDS spectrum for Tb-MOFs.

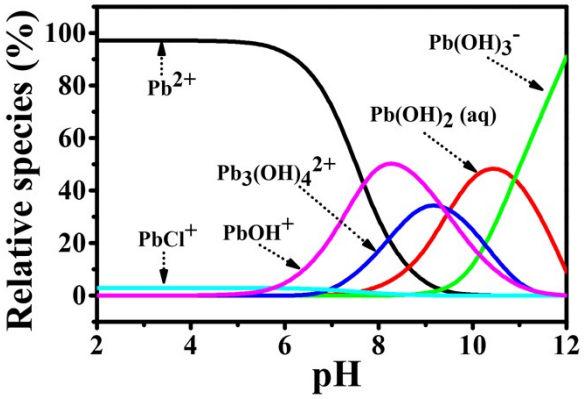

Figure S3. The distribution of Pb^{2+} species in aqueous solutions.

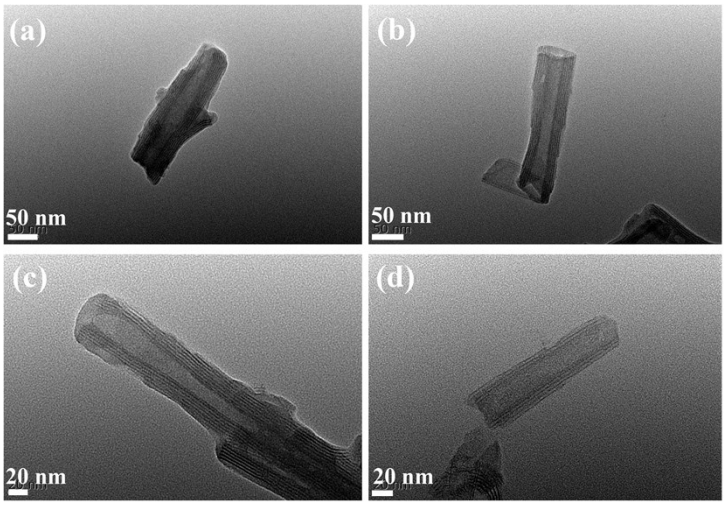

Figure S4. TEM images of Tb-MOFs after fifth cycle of regeneration (a-d).

Table S1 Parameters obtained from different kinetic model.

Equations					
Pseudo second order			Intraparticle diffusion		
$\frac{t}{C_t}=\frac{1}{k_2C_e^2}+\frac{t}{C_e}$			$C_t=k_{id}t^{1/2}+A$		
k_2 (g/(mg·min))	C_e (mg/g)	R^2	k_{id} (g/(mg·min))	A(mg/g)	R^2_{id}
0.002	380	0.999	the first stage		
			100	7.69	0.999
			the second stage		
			12.93	266	0.980
			the third stage		
			4.30	312	0.997
			the fourth stage		
			0	343	1

k_2, k_{id}, and A represent the kinetic constants. C_e and C_t are the mass of Pb^{2+} adsorbed on Tb-MOFs at equilibrium and at time.

Table S2 Thermodynamic parameters for Pb^{2+} removal onto Tb-MOFs.

T (K)	ΔG^0 (kJ/mol)	ΔS^0 (J/(mol·K))	ΔH^0 (kJ/mol)
298	-22.76		
308	-24.33	157.32	24.12
318	-25.91		

Table S3 The concentration of Tb in solution after adsorption in regeneration cycles.

pH = 5.5, m/V= 0.15 g/L.

Number of cycles	0	1	2	3	4	5
[Tb] (μg/mL)	0.095	0.088	0.075	0.083	0.077	0.072
ω([Tb(g)]/[MOFs(g)])	0.63 ‰	0.59 ‰	0.50 ‰	0.55 ‰	0.51 ‰	0.48 ‰
ω([Tb(g)]/[Tb in MOFs (g)])	2.5 ‰	2.4 ‰	2.0 ‰	2.2 ‰	2.1 ‰	1.9 ‰

[Tb] is the concentration of Tb released in solution; ω([Tb]/[MOFs]) is the weight ratio of released Tb and Tb-MOFs in solution; ω([Tb]/[Tb in MOFs]) is the weight ratio of released Tb and the total Tb of Tb-MOFs in solution.

Table S4 The calculated binding energies (E_b) between Pb^{2+} and Tb-MOFs by DFT calculations

Binding mode	E_b (eV)	Binding distance (Å)	Description
[Single-Tb-MOFs...Pb]$^{2+}$	5.99	2.36/2.24 (Pb-N1/N2)	Single ligand binding with Pb^{2+}
[Single(-H)-Tb-MOFs...Pb]$^{+}$	20.66	2.12/2.29 (Pb-N1/N2)	Single ligand binding (N1 removed a proton) with Pb^{2+}
[Double-Tb-MOFs...Pb]$^{2+}$	7.78	2.44/2.53/2.54/2.71 (Pb-N1/N2/N3/N4)	Double ligands binding with Pb^{2+}
[Double(-H)-Tb-MOFs...Pb]$^{+}$	14.95	2.25/2.31 (Pb-N3/N4)	Double ligands binding (N3 removed a proton)
[Double(-2H)-Tb-MOFs...Pb]	20.78	2.27/2.26/2.36 (Pb-N1/N3/N4)	Double ligands binding (N1 and N3 removed two protons)