Supporting information

Efficient removal of Pb^{2+} and Cd^{2+} using Cu(I)-Br coordination polymer constructed with amino-rich sites ligand

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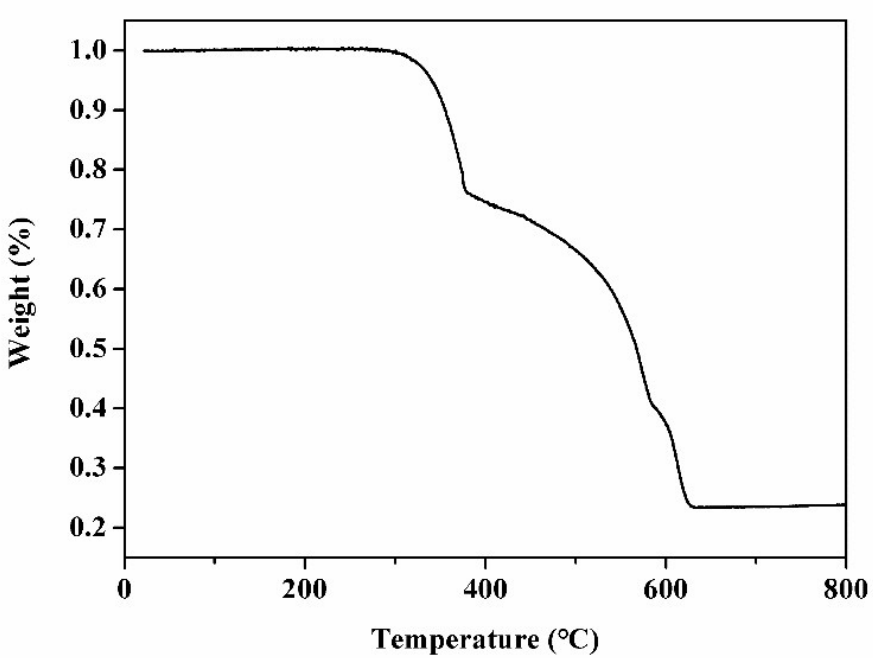

Fig. S1 The TGA curve for compound **1**.

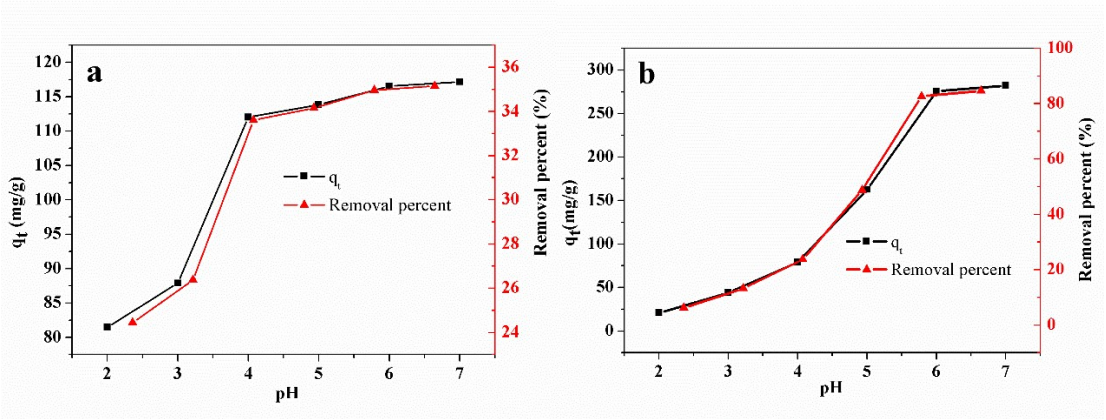

Fig. S2 Effect of the pH on the adsorption of Pb^{2+} (a) and Cd^{2+} (b) on compound **1**.

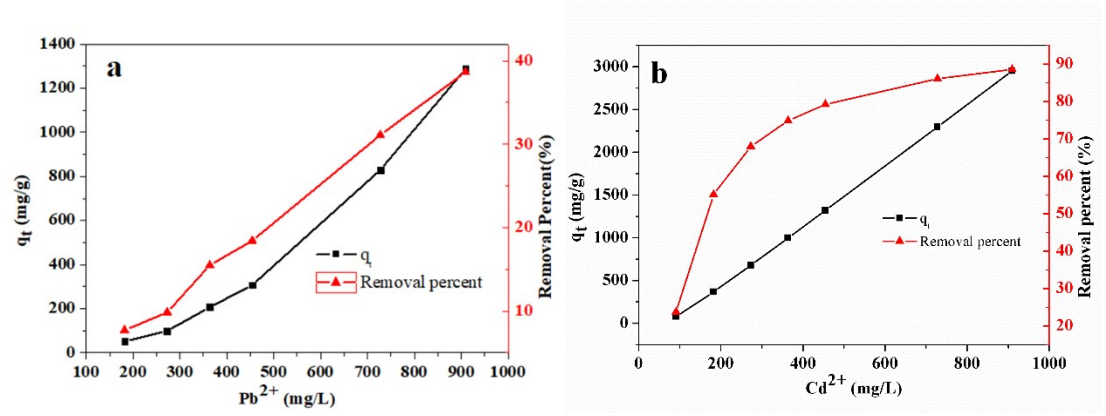

Fig. S3 Effect of initial concentration of Pb^{2+} (a) and Cd^{2+} (b) on the adsorption capacity and removal rate of **1**.

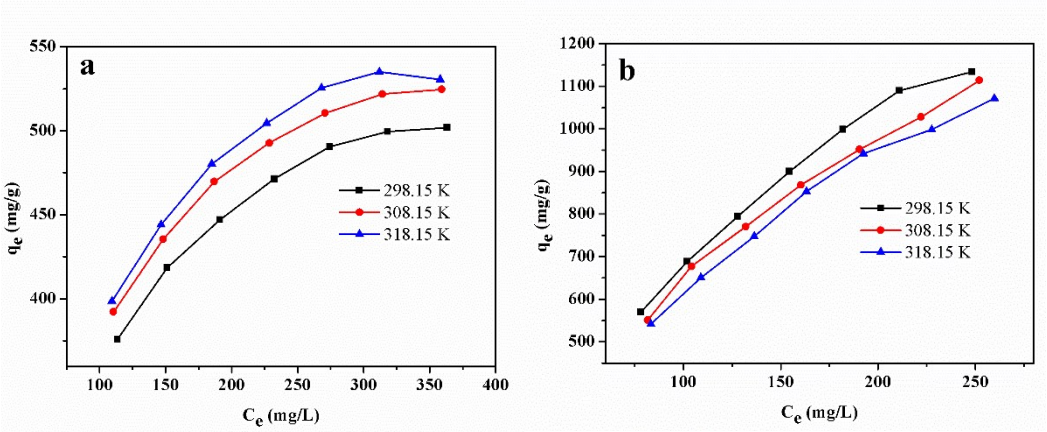

Fig. S4 Adsorption isotherms for Pb^{2+} (a) and Cd^{2+} (b) on compound **1**.

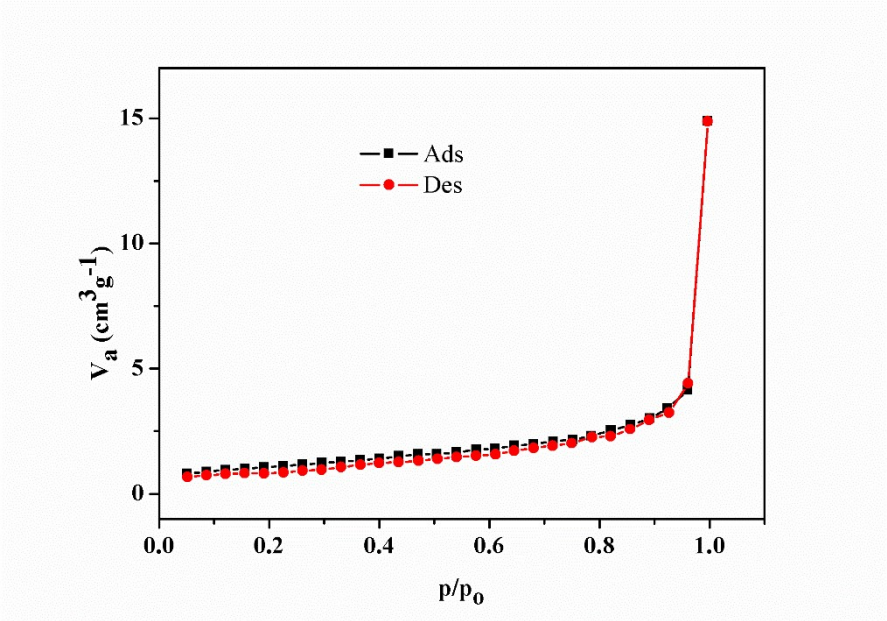

Fig. S5 Adsorption isotherm of N_2 for compound **1**.

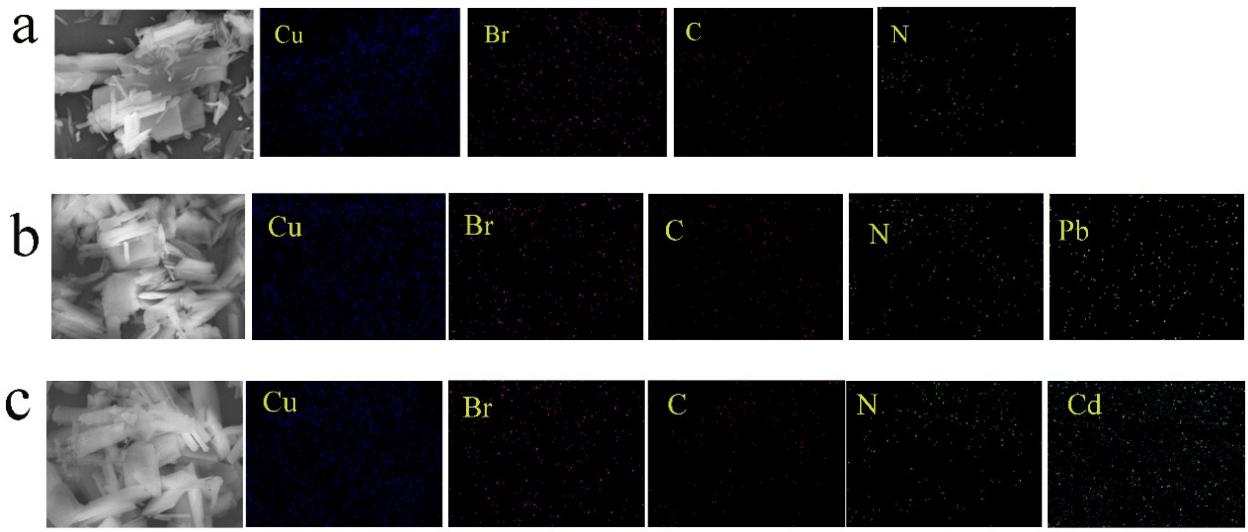

Fig. S6 Elemental SEM mapping images of compound **1**(a); after adsorption of Pb^{2+} and Cd^{2+} (b and c).

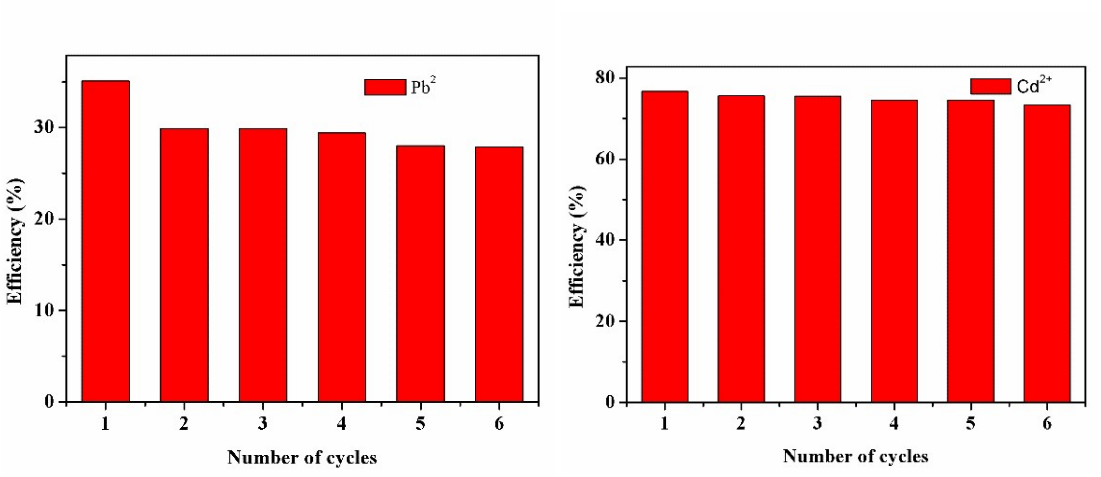

Fig. S7 Reusability of the compound **1** for Pb^{2+} and Cd^{2+} adsorption.

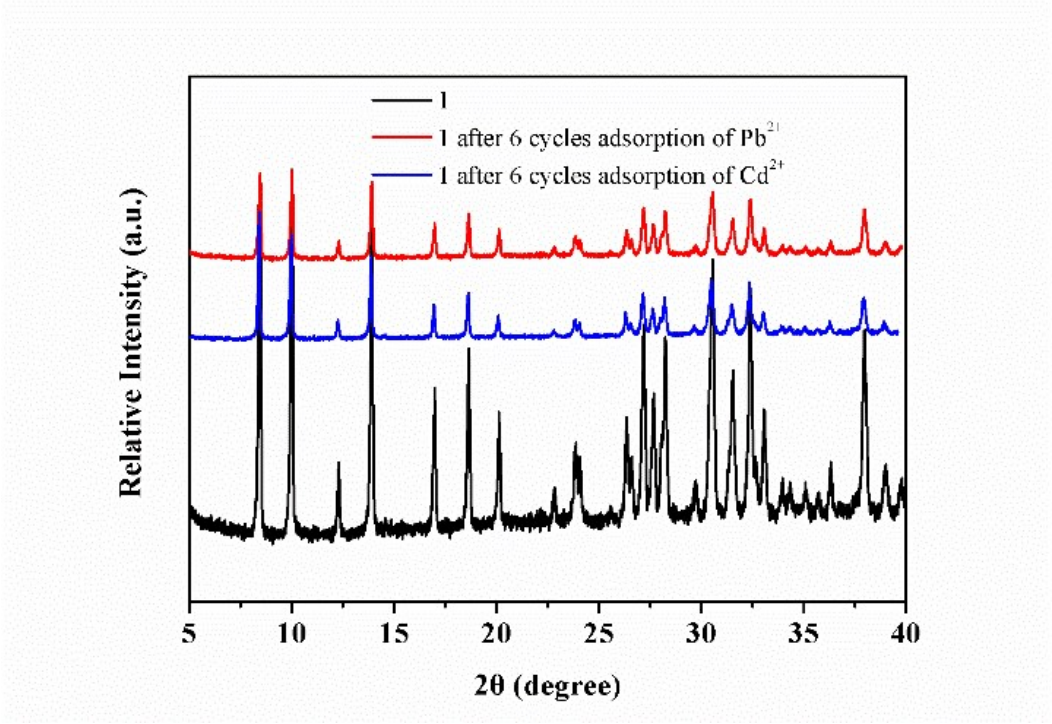

Fig. S8 Powder X-ray diffraction patterns for compound **1** and **1** after 6 adsorption cycles of Pb^{2+} and Cd^{2+}.

Table S1. The detail single crystal data parameters of compound **1**.

Empirical formula	$C_6H_{12}N_{12}Br_2Cu_2$ (**1**)
Formula weight	539.18
T (K)	296.15
Crystal system	*P*-1
Space group	triclinic
a/Å	3.849(6)
b/Å	9.074(15)
c/Å	10.642(17)
V/Å^3	354.9(10)
Z	2
*D*c/Mg mm^{-3}	2.523
μ/mm-1	8.643
F(000)	260
Radiation	MoKα (λ = 0.71073)
Reflections collected	1723
Independent reflections	1235 [R_{int} = 0.0504, R_{sigma} = 0.1048]
Data/restraints/parameters	1235/0/102
Goodness-of-fit on F2	0.985
Final R indexes [I>=2σ (I)]	R_1[a] = 0.0686, wR_2[b] = 0.1737
Final R indexes [all data]	R_1 = 0.0985, wR_2 = 0.1887
[a] $R_1 = \Sigma\|\|Fo\| - \|Fc\|\|/\Sigma\|Fo\|$. [b] $wR^2 = \|\Sigma w(\|Fo\|^2 - \|Fc\|^2)^2/\Sigma\|w(Fo^2)^2\|^{1/2}$	

Table S2 The kinetic parameters of pseudo-first-order and pseudo-second-order kinetic models for Pb^{2+} and Cd^{2+} on compound **1**.

	Initial concentration (mg/L)	Pseudo-first order model			Pseudo-second order model		
		q_e (mg/g)	k_1 (1/min)	R^2	q_e (mg/g)	k_2 (g/mg · min)	R^2
Pb^{2+}	300	361	0.1085	0.99747	394	0.0004327	0.99619
	500	878	0.2173	0.98836	787	0.001047	0.99932
	800	1519	0.2649	0.99346	1667	0.0008438	0.99993
	1000	2063	0.2009	0.9862	2274	0.0002969	0.99989
Cd^{2+}	300	1023	0.1925	0.98833	1067	0.001028	0.9998
	500	1735	0.234	0.97872	1993	0.0008426	0.99993
	800	2830	0.3519	0.98136	3450	0.001612	0.99998
	1000	3170	0.3045	0.9365	4436	0.001055	0.99998

Table S3 The Langmuir and Freundlich isotherm parameters of Pb^{2+} and Cd^{2+} on compound **1** under different temperatures.

Metal ions	T (K)	Langmuir constants			Freundlich constants		
		q_m (mg/g)	K_L (L/mg)	R^2	K_F (L/g)	$1/n$	R^2
Pb^{2+}	298.15	598.8	0.01551	0.9986	116.8	0.2525	0.9542
	308.15	621	0.01609	0.9988	124.1	0.2502	0.9529
	318.15	633	0.01663	0.9987	126.6	0.2507	0.9292
Cd^{2+}	298.15	2175	0.004559	0.9900	40.13	0.6137	0.9892
	308.15	2078	0.004486	0.9943	39.82	0.6042	0.9921
	318.15	2007	0.004432	0.9939	38.20	0.6041	0.9908

Table S4 Comparison of the adsorption capacity of Pb^{2+} and Cd^{2+} by various adsorbents.

Adsorbent	Metal ion	Adsorption capacity (mg/g)	Reference
nFe_3O_4 @MIL-88A(Fe)/APTMS	Pb^{2+}	536.22	22
	Cd^{2+}	693	22
Fe_3O_4 -HBPA-ASA	Pb^{2+}	88.36	23
	Cd^{2+}	165.46	23
melamine modified Zr-MOFs	Pb^{2+}	205	27
Urea-based MOFs	Pb^{2+}	909	37
UiO-66-NH_2 MOF	Pb^{2+}	441.2	17
	Cd^{2+}	415.6	17
$Cu_2Br_2(MA)_2$	Pb^{2+}	598.8	this work
	Cd^{2+}	2175	this work

Table S5 Thermodynamic parameters for the adsorption of Pb^{2+} and Cd^{2+} on compound **1**.

Ion	T (K)	ΔG^0 (kJ/mol)	ΔH^0 (kJ/mol)	ΔS^0 (J/mol·K)
Pb^{2+}	298.15	-29.97	2.75	109.75
	308.15	-31.07		
	318.15	-32.17		
Cd^{2+}	298.15	-25.42	-1.12	81.52
	308.15	-26.23		
	318.15	-27.05		