Supplementary Materials

Adsorption of Pb, Cu and Cd from Water on Coal Fly Ash-Red Mud Modified Composite Material: Characterization and Mechanism

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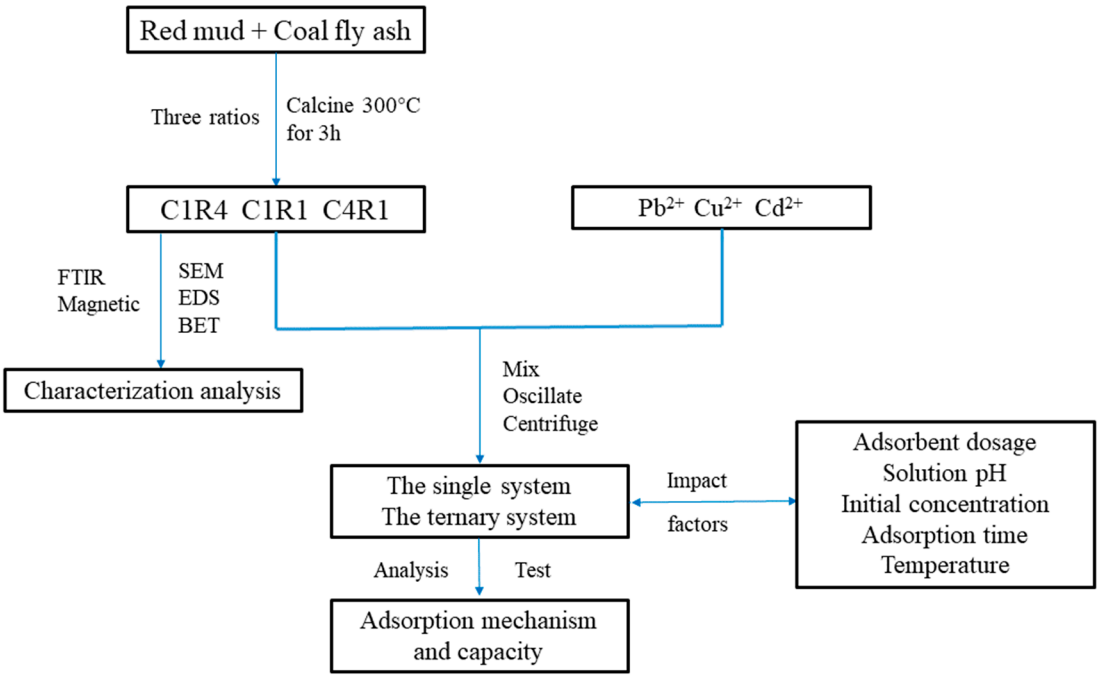

Figure S2. Pore size distribution of CFA, RM, C4R1, C1R1, and C1R4.

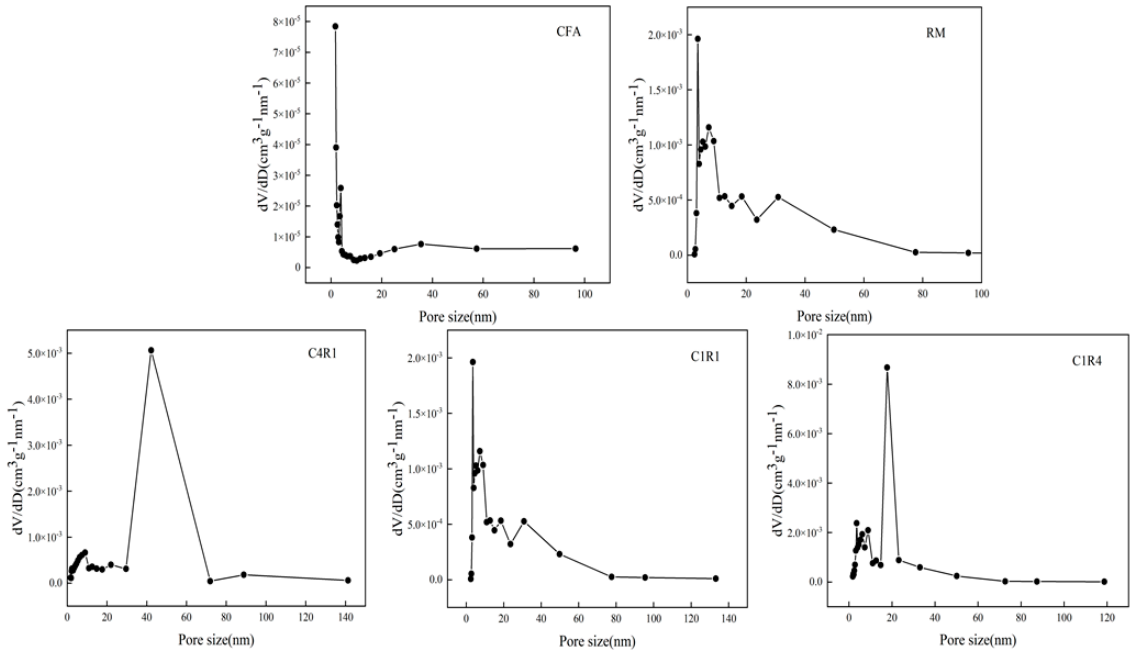

Table S1. Percentage of each element for CFA, RM, C4R1, C1R1, and C1R4 in EDS analysis.

Material	Element	Wt%	Wt% Sigma	Atomic percentage
CFA	C	5.39	0.50	9.00
	O	46.40	0.33	58.10
	Na	1.45	0.06	1.27
	Mg	0.57	0.04	0.47
	Al	17.27	0.15	12.82
	Si	22.77	0.18	16.24
	K	1.09	0.05	0.56
	Ca	0.48	0.04	0.24
	Ti	0.27	0.05	0.11
	Fe	1.04	0.09	0.37
	Cu	1.02	0.16	0.32
	Zr	3.55	0.14	0.82
	Total	100.00		100.00
RM	C	9.14	0.58	15.42
	O	48.17	0.40	60.99
	Na	5.04	0.14	4.44
	Al	9.88	0.13	7.41
	Si	3.45	0.07	2.48
	S	0.27	0.03	0.17
	K	0.16	0.03	0.08
	Ca	2.08	0.05	1.05
	Ti	1.85	0.06	0.78
	Fe	18.34	0.21	6.65
	Cu	0.97	0.09	0.31
	Zn	0.65	0.10	0.20
	Total	100.00		100.00
C4R1	C	25.44	3.57	37.08
	O	39.19	1.90	42.89
	Na	6.72	0.35	5.12
	Mg	0.23	0.05	0.16
	Al	8.52	0.42	5.53
	Si	11.06	0.54	6.89
	K	0.42	0.05	0.19
	Ca	1.46	0.09	0.64
	Ti	0.28	0.05	0.10
	Fe	1.93	0.13	0.60
	Cu	0.95	0.11	0.26
	Zn	0.83	0.13	0.22
	Pd	0.46	0.09	0.08
	Pt	2.52	0.22	0.23
	Total	100.00		100.00
C1R1	O	49.55	0.26	64.66

	Na	12.42	0.16	11.28
	Mg	1.01	0.06	0.86
	Al	12.30	0.12	9.52
	Si	13.39	0.12	9.96
	K	0.31	0.03	0.17
	Ca	0.80	0.04	0.41
	Ti	0.98	0.05	0.43
	Fe	5.20	0.10	1.94
	Cu	0.76	0.08	0.25
	Zn	0.60	0.09	0.19
	Pd	0.47	0.08	0.09
	Pt	2.22	0.17	0.24
	Total	100.00		100.00
C1R4	C	12.99	2.69	21.15
	O	43.83	1.38	53.58
	Na	8.65	0.30	7.36
	Al	8.67	0.28	6.29
	Si	9.02	0.29	6.28
	K	0.14	0.03	0.07
	Ca	0.76	0.04	0.37
	Ti	0.85	0.05	0.35
	Fe	10.76	0.36	3.77
	Cu	0.83	0.08	0.25
	Zn	0.67	0.09	0.20
	Pd	0.52	0.07	0.10
	Pt	2.29	0.16	0.23
	Total	100.00		100.00

Table S2. Physical properties of CFA, RM, C4R1, C1R1, and C1R4.

Property	**CFA**	**RM**	**C4R1**	**C1R1**	**C1R4**
Specific surface area (m^2/g)	0.6828	33.0184	29.6572	32.5141	63.8254
External surface area (m^2/g)	0.0068	28.9177	27.6757	30.7317	61.9258
Micropore area (m^2/g)	0.6869	4.1007	1.9815	1.7824	1.8996
Micropore volume (cm^3/g)	0.0004	0.0020	0.0009	0.0007	0.0005
Pore volume (cm^3/g)	0.0023	0.0902	0.1110	0.1138	0.1821
Average particle diameter (nm)	13.6887	10.7782	14.9773	14.0113	11.3385

Table S3. Adsorption isothermal parameters of Pb, Cu, and Cd by C4R1, C1R1, and C1R4.

Isotherm model	Absorbent	Heavy metal	Parameter	Temperature		
				25°C	35°C	45°C
Langmuir	C4R1	Pb	q_m	126.58	133.33	135.14
			K_L	4.16	3.95	3.89
			R^2	0.9682	0.9643	0.9698
Freundlich	C4R1	Pb	K_F	43.40	59.16	66.09
			1/n	0.3316	0.2604	0.261
			R^2	0.9377	0.9473	0.9496
Sips	C4R1	Pb	K_S	0.9216	0.8601	0.8456
			n_s	0.0570	0.0636	0.0681
			R^2	0.4065	0.3212	0.2666
Langmuir	C4R1	Cu	q_m	111.11	114.94	119.05
			K_L	1.18	1.14	1.11
			R^2	0.9563	0.9601	0.9691
Freundlich	C4R1	Cu	K_F	26.79	27.61	28.64
			1/n	0.3445	0.3535	0.3647
			R^2	0.9285	0.9271	0.9267
Sips	C4R1	Cu	K_S	0.0237	0.0284	0.0430
			n_s	0.4380	0.4544	0.4805
			R^2	0.9501	0.9522	0.9589
Langmuir	C4R1	Cd	q_m	106.38	111.11	120.49
			K_L	1.25	1.18	1.09
			R^2	0.9562	0.9595	0.9639
Freundlich	C4R1	Cd	K_F	25.61	26.60	28.49
			1/n	0.3304	0.3424	0.3566
			R^2	0.9448	0.9518	0.9517
Sips	C4R1	Cd	K_S	0.0146	0.0162	0.0192
			n_s	0.4090	0.4089	0.3938
			R^2	0.9398	0.9444	0.9522
Langmuir	C1R1	Pb	q_m	135.14	140.21	144.52
			K_L	3.89	3.76	3.64
			R^2	0.9707	0.9481	0.9554
Freundlich	C1R1	Pb	K_F	62.39	38.36	40.69
			1/n	0.2673	0.4273	0.4348
			R^2	0.9322	0.9360	0.9489
Sips	C1R1	Pb	K_S	0.1299	0.2318	0.3615
			n_s	0.3824	0.5472	0.6224
			R^2	0.9731	0.9487	0.9495
Langmuir	C1R1	Cu	q_m	114.94	117.64	126.58
			K_L	1.14	1.12	1.04
			R^2	0.9657	0.9686	0.9682
Freundlich	C1R1	Cu	K_F	27.53	28.42	30.00
			1/n	0.3516	0.3609	0.3747

			R^2	0.9376	0.9330	0.9629
Sips	C1R1	Cu	K_S	0.0274	0.0337	0.0260
			n_s	0.4446	0.4651	0.4234
			R^2	0.9522	0.9527	0.9689
Langmuir	C1R1	Cd	q_m	108.70	113.64	129.87
			K_L	1.23	1.16	1.02
			R^2	0.9558	0.9554	0.9455
Freundlich	C1R1	Cd	K_F	25.94	27.22	34.44
			1/n	0.3354	0.3529	0.3496
			R^2	0.9566	0.9562	0.9243
Sips	C1R1	Cd	K_S	0.0127	0.0142	0.0526
			n_s	0.3856	0.4021	0.3885
			R^2	0.9522	0.9538	0.9655
Langmuir	C1R4	Pb	q_m	142.85	149.25	155.67
			K_L	3.68	3.53	3.41
			R^2	0.9749	0.9742	0.9773
Freundlich	C1R4	Pb	K_F	65.40	68.83	74.09
			1/n	0.2734	0.2815	0.2871
			R^2	0.9307	0.9282	0.9206
Sips	C1R4	Pb	K_S	0.1466	0.1545	0.2723
			n_s	0.3789	0.3829	0.3962
			R^2	0.9702	0.9711	0.9803
Langmuir	C1R4	Cu	q_m	119.05	123.46	138.89
			K_L	1.11	1.07	0.94
			R^2	0.9681	0.9711	0.9753
Freundlich	C1R4	Cu	K_F	28.65	62.47	32.46
			1/n	0.3605	0.2634	0.382
			R^2	0.9431	0.9415	0.9300
Sips	C1R4	Cu	K_S	0.0325	0.0398	0.7115
			n_s	0.4446	0.4583	0.4955
			R^2	0.9698	0.9722	0.9743
Langmuir	C1R4	Cd	q_m	112.36	116.27	128.21
			K_L	1.17	1.13	1.03
			R^2	0.9603	0.9641	0.9685
Freundlich	C1R4	Cd	K_F	26.77	49.89	30.25
			1/n	0.3456	0.2706	0.3683
			R^2	0.9492	0.9568	0.9609
Sips	C1R4	Cd	K_S	0.0150	0.0172	0.0331
			n_s	0.3981	0.3980	0.4206
			R^2	0.9544	0.9598	0.9676

Where q_m (mg/g) is the saturated adsorption capacity, K_L (L/mg) is the equilibrium constant of Langmuir, K_F (L/mg) is the equilibrium constant of Freundlich, 1/n is a value about the priority of the adsorption process, K_S (L/mg) is the equilibrium constant of Sips, n_s is the heterogeneity of the adsorbent surface, R^2 is correlation coefficient of the curve. The adsorbent dosage was 0.1 g, the initial heavy metal concentration was 100 mg/L, pH=6 and adsorption time was 90 min.

Table S4. Kinetic fitting parameters of C4R1, C1R1, and C1R4 in the single system.

Kinetic model	Adsorbent	Parameter	Pb	Cu	Cd
Pseudo-first-order	C4R1	q_e	48.12	45.24	43.20
		K_1	1.352	0.457	0.317
		R^2	0.9296	0.8376	0.8446
Pseudo-second-order	C4R1	q_e	50.14	47.98	46.07
		K_2	1.854	0.524	0.378
		R^2	0.9844	0.9712	0.9670
Elovich	C4R1	A	132761	121	66
		B	0.3006	0.1531	0.1408
		R^2	0.7506	0.9395	0.9217
Pseudo-first-order	C1R1	q_e	48.25	46.42	46.06
		K_1	1.476	0.523	0.397
		R^2	0.9240	0.8306	0.8521
Pseudo-second-order	C1R1	q_e	50.20	49.05	48.21
		K_2	1.862	0.563	0.422
		R^2	0.9832	0.9667	0.9710
Elovich	C1R1	A	37427	152	111
		B	0.1292	0.0732	0.0736
		R^2	0.7571	0.9745	0.9503
Pseudo-first-order	C1R4	q_e	48.59	47.14	46.43
		K_1	1.483	0.512	0.402
		R^2	0.8860	0.8479	0.9245
Pseudo-second-order	C1R4	q_e	50.36	50.19	49.52
		K_2	1.964	0.574	0.517
		R^2	0.9822	0.9788	0.9886
Elovich	C1R4	A	54627	171	85
		B	0.1332	0.0726	0.0657
		R^2	0.7842	0.9497	0.9569

Where q_e (mg/g) is the theoretical adsorption capacity at equilibrium, K_1 and K_2 are separately the rate constants for pseudo-first-order and pseudo-second-order kinetic models, A [mg/(g· min)] is the initial adsorption rate for Elovich kinetic model, B (g/mg) is the Elovich adsorption constant, R^2 is correlation coefficient of the curve. The temperature was 25 °C, the adsorbent dosage was 0.1 g, pH=6 and the initial heavy metal concentration was 100 mg/L.

Table S5. Kinetic fitting parameters of C4R1, C1R1, and C1R4 in the ternary system.

Kinetic model	Adsorbent	Parameter	Pb	Cu	Cd
Pseudo-first-order	C4R1	q_e	43.16	39.88	29.76
		K_1	1.473	0.673	0.511
		R^2	0.9131	0.9876	0.9735
Pseudo-second-order	C4R1	q_e	46.02	42.79	35.21
		K_2	1.976	0.702	0.628
		R^2	0.9480	0.9913	0.9918
Elovich	C4R1	A	43.97	4.27	3.49
		B	0.1427	0.0873	0.1214
		R^2	0.9199	0.9707	0.9810
Pseudo-first-order	C1R1	q_e	48.84	43.89	33.54
		K_1	1.476	0.694	0.517
		R^2	0.8900	0.9865	0.9674
Pseudo-second-order	C1R1	q_e	45.21	47.04	36.12
		K_2	2.083	0.744	0.622
		R^2	0.9427	0.9920	0.9895
Elovich	C1R1	A	44.56	4.25	3.41
		B	0.1372	0.0829	0.1112
		R^2	0.9450	0.9762	0.9869
Pseudo-first-order	C1R4	q_e	46.21	45.89	36.25
		K_1	1.397	0.698	0.564
		R^2	0.8794	0.9745	0.9761
Pseudo-second-order	C1R4	q_e	49.40	48.52	40.12
		K_2	2.165	0.802	0.671
		R^2	0.9333	0.9864	0.9952
Elovich	C1R4	A	50.61	4.79	4.86
		B	0.1365	0.083	0.111
		R^2	0.9327	0.9765	0.9811

Where q_e (mg/g) is the theoretical adsorption capacity at equilibrium, K_1 and K_2 are separately the rate constants for pseudo-first-order and pseudo-second-order kinetic models, A [mg/(g· min)] is the initial adsorption rate for Elovich kinetic model, B (g/mg) is the Elovich adsorption constant, R^2 is correlation coefficient of the curve. The temperature was 25 °C, the adsorbent dosage was 0.1 g/L, pH=5 and the initial heavy metal concentration was 100 mg/L.