Supplementary Materials

Table S1: Developed bentonite-CoAl-LDH Cr(VI) uptake capacity (Qe1) model numerical optimization target objectives and results

Operational parameter	Scenarios target objectives						Scenario optimization results					
	1	2	3	4	5	6	1	2	3	4	5	6
Temperature (ºC)	In range	In range	In range	45	25	25	25	25	25	45	25	25
Initial Cr(IV) conc. (mg/L)	In range	26	76.5	127	26	76.5	126.6	26	76.5	127	26	76.5
Initial pH	In range	In range	In range	2	4	6	2	2	2	2	4	6
Adsorption Capacity	maximize	maximize	maximize	maximize	maximize	maximize	101.4	34.74	83.54	77.07	29.06	19.80
Desirability							1.0	0.224	0.793	0.72	0.158	0.050

Table S2: Thermodynamics Experimental study experimental variables and results

#	Temp oC	Cr(VI) Initial Conc.,mg/L	pH	Cr(VI) uptake capacity mg/g		ANN Predictions		RSM Predictions	
				CoAl-LDH	Bentonite-CoAl	CoAl-LDH	Bentonite-CoAl	CoAl-LDH	Bentonite-CoAl
1	25	49.58	2.00	50.88	57.6	50.26	56.50	64.10	63.12
2	25	76.5	2.00	58.64	86.4	67.61	74.26	82.51	84.56
3	25	107.69	2.00	77.68	96.72	76.76	97.53	85.48	97.26
4	25	26	4.00	30.72	36.48	26.88	35.62	20.71	28.75
5	25	49.58	4.00	44.56	49.92	45.38	49.30	46.90	52.93
6	25	107.69	4.00	71.2	79.36	73.45	79.46	63.38	80.75
7	25	127	4.00	62.8	94.32	71.46	94.45	53.71	79.99
8	25	49.58	6.00	30.16	32.24	29.57	30.86	43.33	39.88
9	25	76.5	6.00	32	36.32	35.58	36.05	57.19	55.46
10	25	107.69	6.00	42.64	60.16	42.67	58.08	54.90	61.38
11	35	26	2.00	25.12	28.16	21.66	27.80	22.55	28.78
12	35	49.58	2.00	34.48	40.56	31.69	39.42	34.60	44.18
13	35	107.69	2.00	51.76	86.08	52.81	85.98	54.11	78.67
14	35	127	2.00	61.84	73.44	59.65	92.67	57.39	89.04
15	35	49.58	4.00	23.28	39.92	21.10	38.82	29.32	38.68
16	35	107.69	4.00	51.92	72.08	48.70	72.09	43.11	66.86
17	35	26	6.00	33.6	23.68	29.11	20.69	30.27	20.04
18	35	49.58	6.00	28.48	29.52	29.50	28.91	37.67	30.32
19	35	107.69	6.00	53.76	53.12	45.19	55.46	45.72	52.18
20	35	127	6.00	45.12	61.76	44.75	59.19	45.19	58.34
21	45	49.58	2.00	28.48	27.68	28.09	28.57	64.10	23.66
22	45	76.5	2.00	34.72	30.72	43.79	29.51	88.95	34.38
23	45	107.69	2.00	60.96	76.96	50.53	75.77	81.93	51.90
24	45	26	4.00	44.56	16.72	40.90	15.67	12.43	19.39
25	45	49.58	4.00	58.56	24.48	58.30	23.00	55.07	22.85
26	45	107.69	4.00	80.96	44.96	70.13	32.98	66.34	44.77
27	45	127	4.00	63.04	47.92	61.00	45.74	40.55	56.27
28	45	49.58	6.00	27.04	20.56	24.21	15.43	59.65	19.18
29	45	76.5	6.00	29.84	25.84	38.61	27.20	78.43	24.04
30	45	107.69	6.00	43.28	43.28	41.21	39.52	64.37	34.78

Table S3: Kinetics study experimental variables and results

SN	Time (min)	Initial Cr(VI) Conc.,mg/l	Average Cr(VI) Uptake capacity		ANN Predictions	
			CoAl-LDH	B-CoAl-LDH	CoAl-LDH	Bentonite-CoAl-LDH
1	5	20	11.36	15.92	12.32	16.27
2	10	20	14.8	17.12	13.22	18.59
3	20	20	16.16	23.28	15.33	23.04
4	30	20	16.48	26.16	17.12	26.46
5	60	20	18.64	31.76	19.01	30.67
6	120	20	20.08	33.68	19.80	33.72
7	180	20	22.4	35.92	21.76	36.23
8	240	20	23.36	37.76	23.15	37.79
9	5	60	8.16	12.48	9.32	13.92
10	10	60	8.08	23.76	10.80	17.29
11	20	60	13.52	26.56	13.70	25.17
12	30	60	16.72	32.88	16.53	33.50
13	60	60	24.4	50.96	24.48	51.02
14	120	60	43.6	66.96	43.29	66.37
15	180	60	53.44	80.08	52.83	79.91
16	240	60	53.2	81.84	53.66	81.81
17	5	100	26.64	68.72	26.65	70.20
18	10	100	43.2	71.36	43.72	71.36
19	20	100	64.16	75.04	64.14	74.63
20	30	100	70	82.4	73.00	79.19
21	60	100	74.64	83.6	78.44	92.33
22	120	100	78.8	95.76	78.81	95.78
23	180	100	79.68	96.4	79.07	96.24
24	240	100	80.72	95.76	84.58	95.60

Table S4. Linear equilibrium models fittings parameters CoAl-LDH and bentonite-CoAl-LDH for Cr(VI) uptake

Model	Mathematical representation	Temp	Parameter	CoAl-LDH			B-CoAl-LDH		
				EXP	ANN	RSM	EXP	ANN	RSM
Langmuir	$\frac{C_e}{q_e} = \frac{1}{b} q_m + \frac{C_e}{q_m}$	25°C	R^2	0.9542	0.9836	0.9850	0.8449	0.8445	0.9850
			RMSE	0.0931	0.0352	0.0309	0.0675	0.0752	0.0309
			q_{max}, mg/g	107.1126	109.4092	164.5945	184.4272	183.7434	164.5945
			K_L , L/mg	0.0305	0.0218	0.0140	0.0118	0.0116	0.0140
Freundlich	$\ln q_e = \ln K_f + \frac{1}{n} \ln C_e$		R^2	0.8355	0.9852	0.9671	0.9330	0.9213	0.9671
			RMSE	0.0564	0.0151	0.0294	0.0468	0.0509	0.0294
			K_F	9.2766	8.9310	5.9676	4.8747	4.7094	5.9676
			1/n	0.4795	0.4625	0.6074	0.6625	0.6675	0.6074
Langmuir	$\frac{C_e}{q_e} = \frac{1}{b} q_m + \frac{C_e}{q_m}$	35°C	R^2	0.9699	0.9330	0.9989	0.7099	0.7322	0.9723
			RMSE	0.6090	0.5250	0.7342	0.3825	0.3527	0.2527
			q_{max}, mg/g	99.4079	105.7050	92.9946	167.9892	180.9617	185.4516
			K_L , L/mg	0.0117	0.0103	0.0133	0.0076	0.0068	0.0074
Freundlich	$\ln q_e = \ln K_f + \frac{1}{n} \ln C_e$		R^2	0.9917	0.9872	0.9962	0.9445	0.9767	0.9977
			RMSE	0.2269	0.1859	0.2595	0.1662	0.1558	0.1167
			K_F	3.2461	3.0066	3.7738	2.5087	2.5797	3.3205
			1/n	0.6091	0.6253	0.5739	0.7355	0.7285	0.6858
Langmuir	$\frac{C_e}{q_e} = \frac{1}{b} q_m + \frac{C_e}{q_m}$	45°C	R^2	0.7852	0.9212	0.4175	0.2482	0.5373	0.2491
			RMSE	0.6720	0.6591	0.5124	0.7421	0.6028	1.0119
			q_{max}, mg/g	152.6126	126.5626	111.2150	236.0006	196.1880	253.5690
			K_L , L/mg	0.0056	0.0068	0.0161	0.0034	0.0047	0.0025
Freundlich	$\ln q_e = \ln K_f + \frac{1}{n} \ln C_e$		R^2	0.9771	0.9899	0.5794	0.8950	0.9515	0.9424
			RMSE	0.2535	0.2276	0.1994	0.2758	0.2344	0.3402
			K_F	1.7252	1.9486	2.8292	1.5103	1.9273	1.2393
			1/n	0.7521	0.7087	0.7227	0.7990	0.7560	0.8015

Table S5. CoAl-LDH and B-CoAl-LDH for Cr(VI) uptake thermodynamic parameters

Using Linear Langmuir models fittings parameters

Adsorbent	**Temp**	ΔG (kJ/mol)			Kd (L/**m**mol)			ΔH (kJ/mol)			ΔS (kJ/mol K)		
		EXP	ANN	RSM	EXP	ANN	RSM	EXP	ANN	RSM	EXP	ANN	RSM
							Linear model						
Co-Al-LDH	25ºC	-18.259	-17.424	-16.320	0.0305	0.0218	0.0140	-66.565	-46.033	5.553	-0.162	-0.096	0.073
	35ºC	-16.414	-16.097	-16.747	0.0117	0.0103	0.0133						
	45ºC	-15.022	-15.512	-17.795	0.0056	0.0068	0.0161						
B-Co-Al-LDH	25ºC	-15.896	-15.858	-16.320	0.0118	0.0116	0.0140	-48.584	-35.214	-67.398	-0.109	-0.065	-0.171
	35ºC	-15.314	-15.041	-15.236	0.0076	0.0068	0.0074						
	45ºC	-13.691	-14.562	-12.878	0.0034	0.0047	0.0025						