Electronic Supplementary Material (ESI) for Materials Advances.

Carbon-layered double hydroxide nanocomposite for efficient removal of inorganic and organic based water contaminants – unravelling the adsorption mechanism

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Synthesis of Porous Carbon Nanospheres

An alkaline solution of phenol (0.6 g) and formaldehyde (2.1 mL) in 15 mL NaOH solution (0.1M) was prepared at 70 ^{o}C under stirring for 30 min. A tri-block copolymers, F108 (15 mL, 0.07 mmol) was introduced into the above solution followed by heating at 65 ^{o}C for 2 h under stirring. It was diluted by adding 50 mL water and stirring was continued for 16 h. 20 mL of the above solution was further diluted with 60 mL of water followed by autoclave heating at 130 ^{o}C for 24 h. The synthesized material was collected by centrifugation, washing and drying. Carbonization of the material was done by heating at 700 ^{o}C for 3h (heating rate 4^{o}C/min) under controlled N_2 atmosphere (flow rate of 40 mL/min). The synthesized porous carbon was designated as CF108.

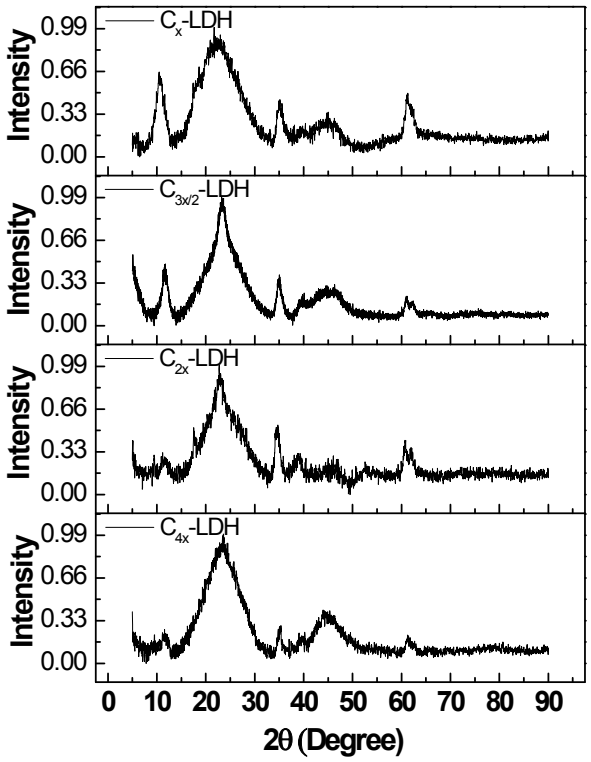

Fig. S1: Plot of normalized intensity vs 2θ (degree)

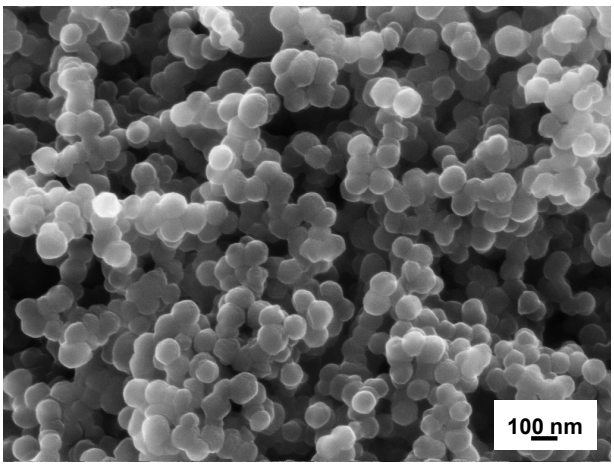

Fig. S2: FESEM image of porous carbon material

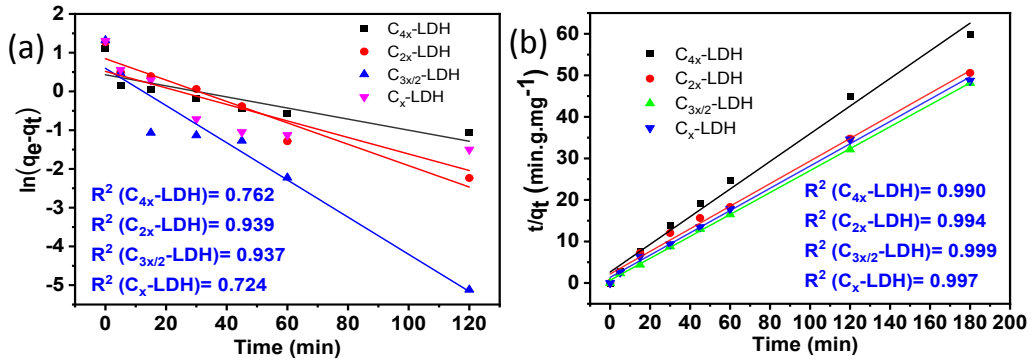

Fig. S3 (a) Pseudo-1st order and (b) Pseudo-2nd order kinetic models of C-LDH for the adsorption of As(V)

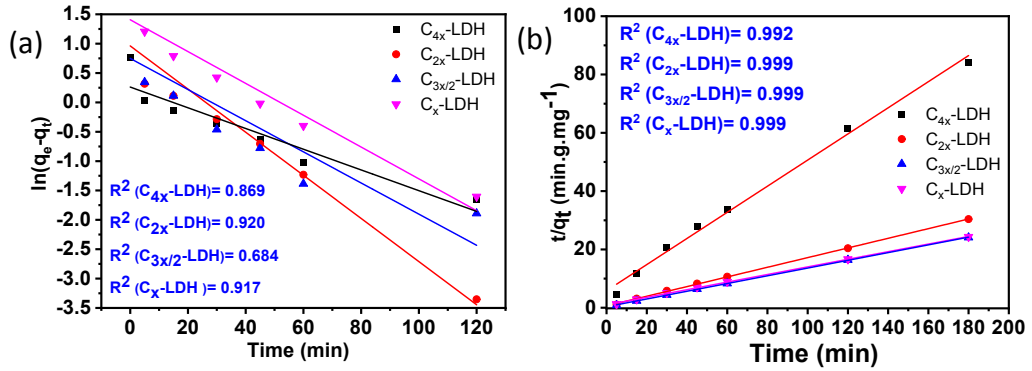

Fig. S4 (a) Pseudo-1st order and (b) Pseudo-2nd order kinetic models of C-LDH for the adsorption of F^-.

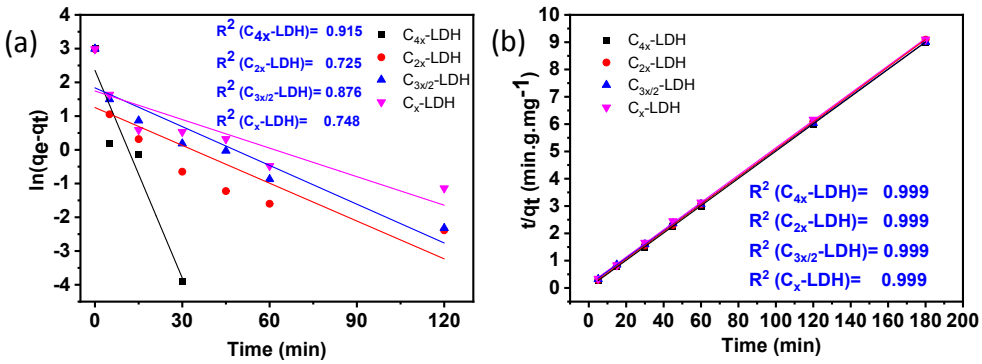

Fig. S5 (a) Pseudo-1st order and (b) Pseudo-2nd order kinetic models of C-LDH for the adsorption of Fe(II)/Fe(III).

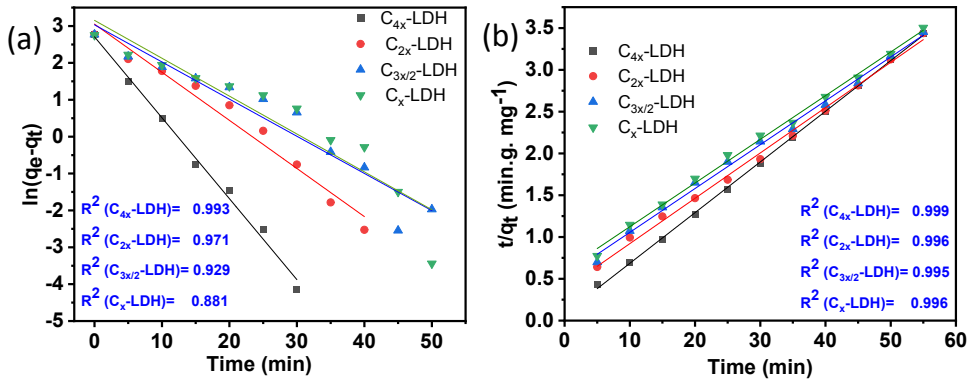

Fig. S6 (a) Pseudo-1st order and (b) Pseudo-2nd order kinetic models of C-LDH for the adsorption of MB.

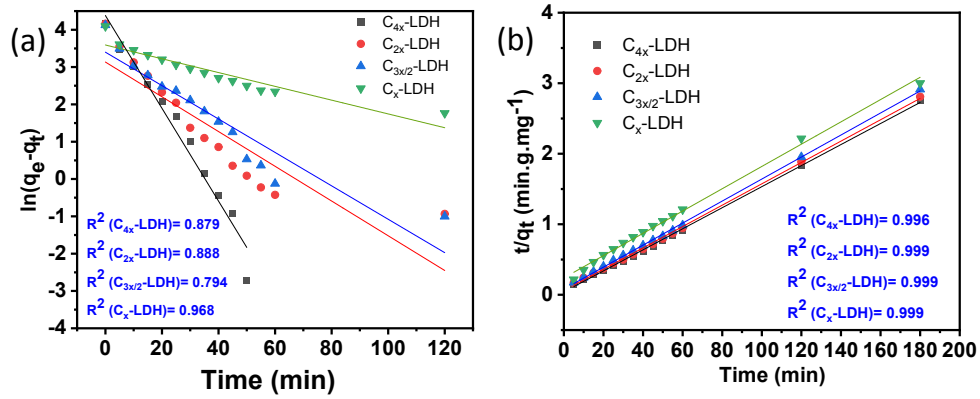

Fig. S7 (a) Pseudo-1st order and (b) Pseudo-2nd order kinetic models of C-LDH for the adsorption of MO.

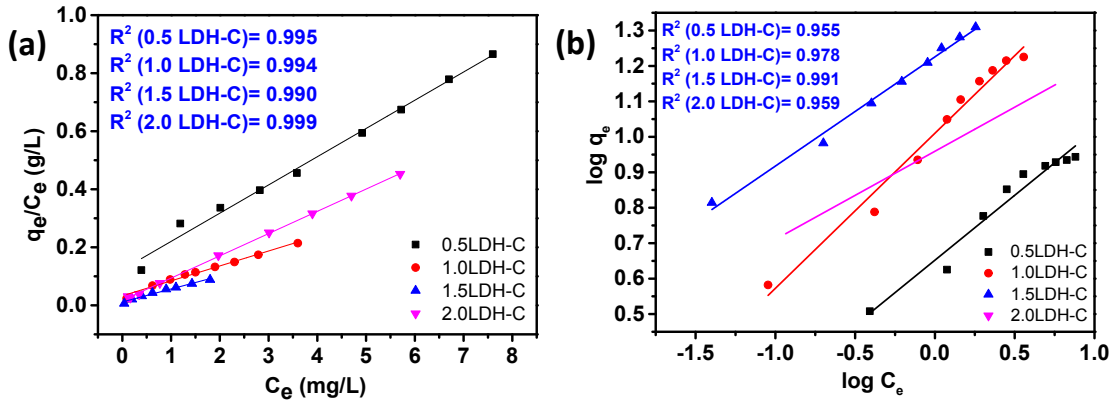

Fig. S8 Plot of (a) Langmuir and (b) Freundlich isotherm model for the adsorption of As(V)

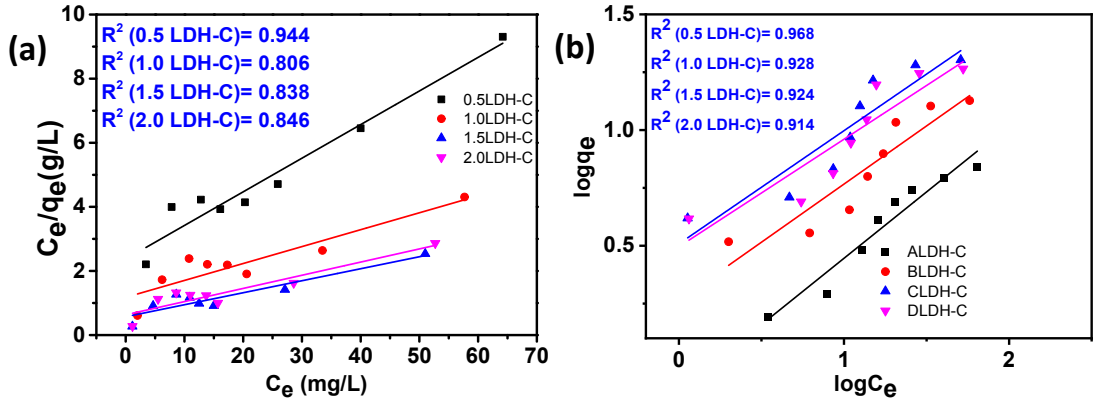

Fig. S9 Plot of (a) Langmuir and (b) Freundlich isotherm model for the adsorption of F^-.

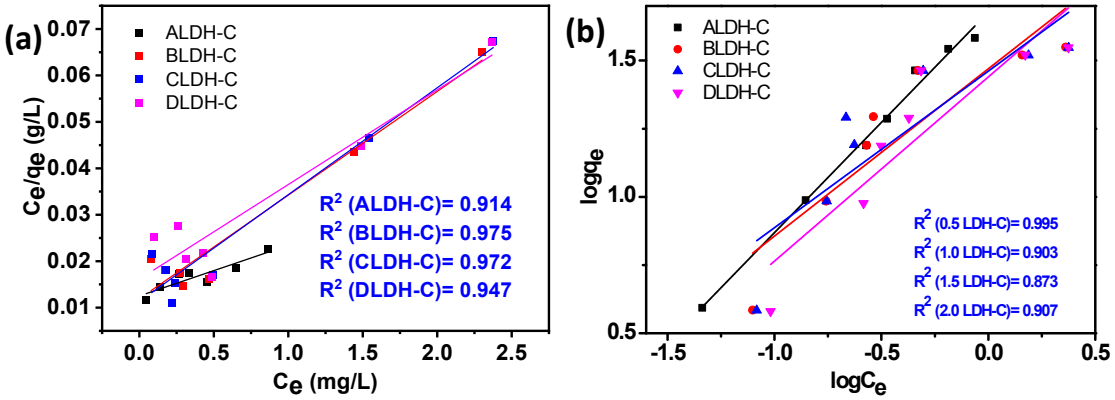

Fig. S10 Plot of (a) Langmuir and (b) Freundlich isotherm model for the adsorption of Fe(II)/Fe(III).

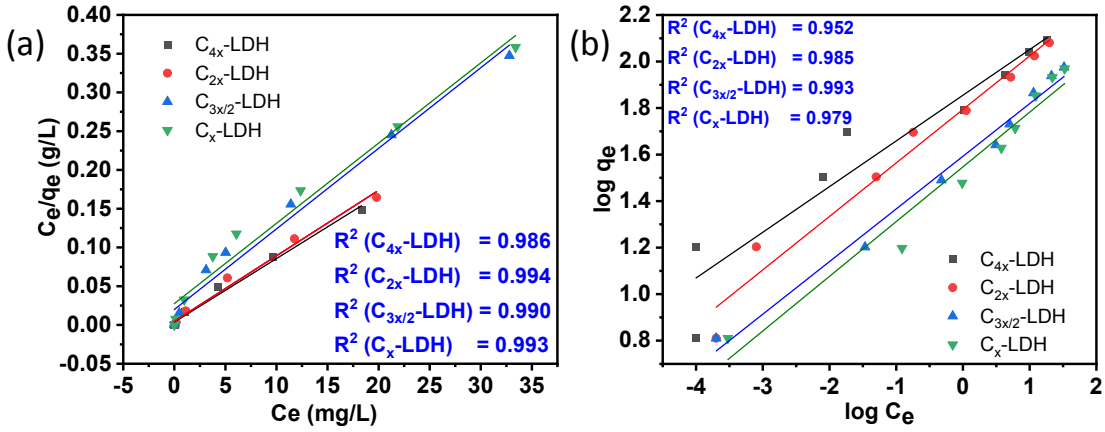

Fig. S11 Plot of (a) Langmuir and (b) Freundlich isotherm model for the adsorption of MB.

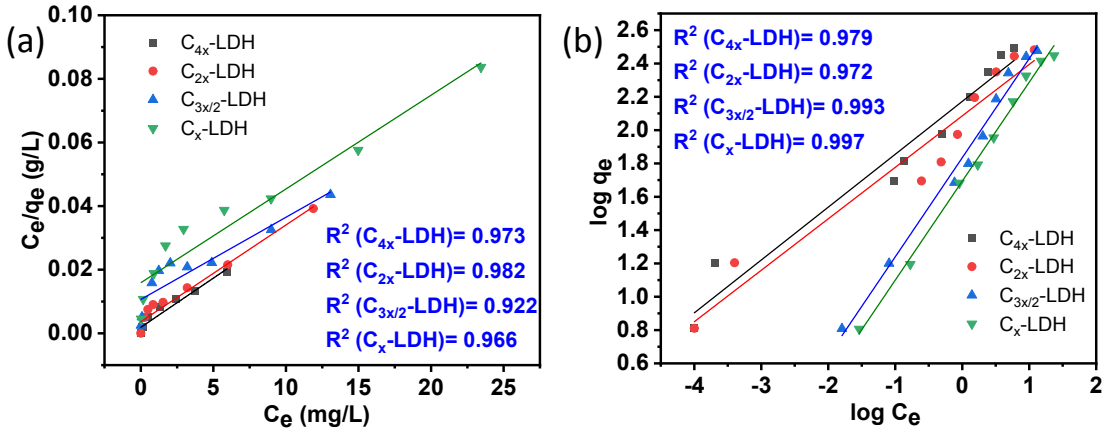

Fig. S12 Plot of (a) Langmuir and (b) Freundlich isotherm model for the adsorption of MO.

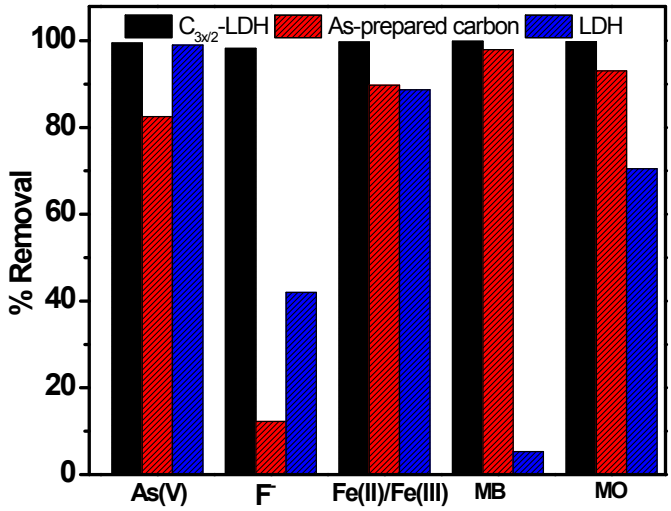

Fig. S13 Plot of comparative study on removal of pollutants by $C_{3x/2}$-LDH, As-prepared carbon and LDH.

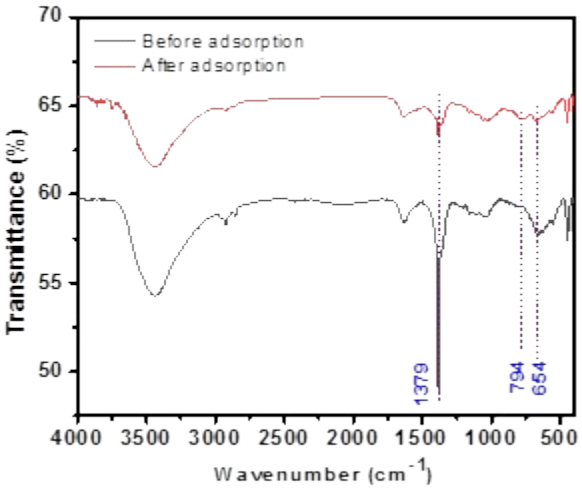

Fig. S14 FTIR plot of $C_{3x/2}$-LDH before and after adsorption of water pollutants

Table S1: Quantitative estimation of C1s, O1s, Al2p, Mg2p and Ca2p for C-LDH from XPS study

Sample ID	C1s	O1s	Al2p	Mg2p	Ca2p
C_{4x}-LDH	75.82	18.12	2.26	2.75	1.05
C_{2x}-LDH	65.24	26.29	3.88	3.16	1.43
$C_{3x/2}$-LDH	57.45	30.33	5.25	4.92	2.05
C_x-LDH	52.61	33.10	5.25	6.72	2.32

Table S2: Quantitative estimation (atomic%) of C (from carbon analyzer) and Al, Mg and Ca (from ICP-AES) of C-LDH

Sample ID	C	Al	Mg	Ca	Al:Mg:Ca
C_{4x}-LDH	57.50	2.45	3.33	1.95	1:1.36:0.79
C_{2x}-LDH	40.50	4.99	6.90	3.64	1:1.38:0.73
$C_{3x/2}$-LDH	38.10	5.52	7.23	3.92	1:1.31:0.71
C_x-LDH	30.30	6.07	8.28	3.99	1:1.36:0.66

Table S3: Percentage removal of As(V), F^-, Fe(II)/Fe(III), MB and MO at different times using different C-LDH composites.

Sample ID	% Removal of different water contaminants at 5 min/60 min/180 min				
	As(V)	F^-	Fe(II)/Fe(III)	MB	MO
C_{4x}-LDH	49.2/65.2/80.5	10.4/16.8/20.2	93.8/99.9/99.9	71.7/100/100	50.7/100/100
C_{2x}-LDH	51.1/87.7/95.1	45.4/56.3/59.2	84.6/97.9/98.9	48.8/100/100	44.9/96.9/97.9
$C_{3x/2}$-LDH	57.1/97.0/99.9	60.6/72.2/74.7	77.5/97.8/99.9	44.7/99.8/100	44.1/93.1/94.5
C_x-LDH	52.0/90.1/98.7	40.6/67.3/74.0	73.2/95.8/98.9	40.4/98.5/100	35.3/75.8/91.7

Table S4: Kinetics data for the adsorption of As(V), F^-, Fe(II)/Fe(III), MB and MO on C-LDH composites

Contaminant	Sample ID	Pseudo-1st order equation: $\ln (q_e-q_t) = -k_1 t + \ln q_e$			Pseudo-2nd order equation: $t/q_t = 1/k_2 q_e^2 + (1/q_e)t$		
		k_1 (min^{-1})	q_e (mg/g)	R^2	k_2 ($g.mg^{-1}min^{-1}$)	q_e (mg/g)	R^2
As(V)	C_{4x}-LDH	0.014	1.537	0.762	0.042	3.004	0.990
	C_{2x}-LDH	0.027	2.327	0.939	0.033	3.677	0.994
	$C_{3x/2}$-LDH	0.048	1.816	0.937	0.106	3.787	0.999
	C_x-LDH	0.021	1.678	0.724	0.053	3.729	0.997
F^-	C_{4x}-LDH	0.017	1.298	0.869	0.034	2.232	0.992
	C_{2x}-LDH	0.036	2.616	0.613	0.043	6.038	0.999
	$C_{3x/2}$-LDH	0.026	2.114	0.814	0.049	7.544	0.999
	C_x-LDH	0.027	4.083	0.877	0.018	7.663	0.999
Fe(II)/Fe(III)	C_{4x}-LDH	0.205	10.51	0.915	0.135	20.41	0.999
	C_{2x}-LDH	0.037	3.50	0.725	0.054	19.86	0.999
	$C_{3x/2}$-LDH	0.038	6.276	0.876	0.024	19.92	0.999
	C_x-LDH	0.028	5.716	0.748	0.023	19.76	0.999
MB	C_{4x}-LDH	0.219	14.99	0.993	0.046	16.493	0.999

	C_{2x}-LDH	0.130	21.14	0.971	0.007	18.436	0.996
	$C_{3x/2}$-LDH	0.101	20.76	0.929	0.005	19.066	0.995
	C_x-LDH	0.103	23.42	0.881	0.004	19.157	0.996
MO	C_{4x}-LDH	0.018	36.30	0.879	0.0009	66.98	0.996
	C_{2x}-LDH	0.044	29.95	0.888	0.0028	66.05	0.999
	$C_{3x/2}$-LDH	0.046	22.98	0.794	0.004	64.10	0.999
	C_x-LDH	0.124	79.95	0.968	0.006	63.29	0.999

Table S5: Parameters of adsorption isotherm models for the adsorption of As(V), F^-, Fe(II)/Fe(III), MB and MO.

Contaminants Name	Sample ID	Langmuir isotherm: $C_e/q_e = C_e/q_m + 1/K_L.q_m$				Freundlich isotherm: $\log q_e = \log K_F + 1/n_F \log C_e$		
		K_L (L/mg)	q_m (mg/g)	R_L	R^2	K_F (g.mg^{-1}min^{-1})	n_F (mg/g)	R^2
As(V)	C_{4x}-LDH	0.792	10.28	0.386	0.995	4.487	2.7	0.955
	C_{2x}-LDH	4.512	13.04	0.099	0.992	10.237	2.3	0.978
	$C_{3x/2}$-LDH	3.853	22.37	0.114	0.990	15.713	3.2	0.991
	C_x-LDH	1.574	19.42	0.241	0.999	9.105	4.0	0.794

F^-	C_{4x}-LDH	0.072	8.07	0.819	0.969	0.975	1.9	0.982
	C_{2x}-LDH	0.265	16.34	0.416	0.999	5.082	2.9	0.968
	$C_{3x/2}$-LDH	0.424	20.40	0.308	0.998	8.082	3.1	0.921
	C_x-LDH	0.488	18.40	0.279	0.998	7.825	3.3	0.931
Fe(II)/Fe(III)	C_{4x}-LDH	1.146	80.00	0.080	0.914	47.56	1.2	0.995
	C_{2x}-LDH	1.889	44.84	0.050	0.975	29.44	1.6	0.903
	$C_{3x/2}$-LDH	2.035	43.48	0.046	0.972	28.90	1.7	0.873
	C_x-LDH	1.262	49.09	0.073	0.947	27.53	1.5	0.907
MB	C_{4x}-LDH	2.28	122.1	0.119	0.986	71.63	5.1	0.952
	C_{2x}-LDH	1.78	118.34	0.147	0.994	62.24	4.3	0.985
	$C_{3x/2}$-LDH	0.37	96.15	0.451	0.990	39.15	4.4	0.993
	C_x-LDH	0.51	97.08	0.375	0.993	35.24	4.2	0.979
MO	C_{4x}-LDH	1.62	328.9	0.160	0.973	148.6	3.1	0.979
	C_{2x}-LDH	0.84	323.6	0.268	0.982	121.7	3.2	0.972
	$C_{3x/2}$-LDH	0.31	299.0	0.496	0.922	68.2	1.7	0.993
	C_x-LDH	0.22	280.1	0.579	0.966	49.3	1.7	0.997