Supplementary information

Intercalation vs Adsorption Strategies of Myo-inositol hexakisphosphate into Zn-Fe Layered Double Hydroxide: A tiff between Anion exchange and Co-precipitation

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Table S1. Cartesian coordinates of phytic acid molecule optimized in B3LYP/6-31G(d) level of theory.

Atomic Number	X	Y	Z
6	-0.129230	1.253184	-0.523159
6	-1.251195	0.216859	-0.280950
6	-1.101288	-1.064688	-1.126135
6	0.324678	-1.632100	-1.325499
6	1.363216	-0.511545	-1.476226
6	1.251960	0.567459	-0.387016
1	-1.281139	-0.020776	0.783516
1	-0.228751	1.678979	-1.529669
1	0.313970	-2.214978	-2.250320
1	1.195191	-0.014226	-2.437224
1	1.338577	0.152258	0.618729

1	-1.487842	-0.825587	-2.123296
8	2.674939	-1.078305	-1.642253
8	-1.854980	-2.178799	-0.610729
8	-2.523886	0.751971	-0.723258
8	-0.264357	2.255806	0.464481
8	2.302626	1.496341	-0.643358
15	0.383871	-2.790388	1.222123
15	-3.413790	-2.239301	-0.226049
15	-3.666383	1.514418	0.124846
15	-0.407263	3.884612	0.126916
15	3.294613	2.152370	0.454680
15	3.607549	-1.806045	-0.574036
8	-3.745091	2.986313	-0.008585
8	-3.818896	-1.622600	1.066051
8	0.772258	-2.574700	-0.350673
8	-0.141506	-1.576721	1.881474
8	3.428350	-1.368914	0.856146
8	3.031496	3.578205	0.775461
8	-0.707212	4.576445	1.391689
8	0.899252	4.269952	-0.694040
8	-1.464223	3.946800	-1.071383
8	-4.941874	0.790034	-0.624188
8	-3.621177	0.966739	1.600812
8	-4.230648	-1.753127	-1.500817
8	-3.493760	-3.847687	-0.216812
8	-0.470164	-4.140981	1.252343
8	1.780605	-3.385240	1.744119
8	4.703001	1.930931	-0.304690
8	3.284381	1.190578	1.713609
8	5.009915	-1.489804	-1.259925
8	3.504567	-3.394587	-0.727434
1	-4.223299	-4.153660	0.349844
1	2.843886	-3.767526	-0.107955

1	-1.308968	-4.059180	0.762028
1	2.426387	-2.642909	1.839563
1	-4.629416	-0.860878	-1.344364
1	-5.633570	1.448228	-0.809575
1	5.218241	2.754664	-0.280629
1	-2.378973	3.800591	-0.722739
1	1.712031	4.207697	-0.124219
1	3.461903	0.239072	1.490746
1	5.729500	-2.033730	-0.897921
1	-3.704406	-0.027250	1.625854

Table S2. Optimized bond lengths in Phytic Acid molecule calculated using Gaussian 09 software.

Start C	End C	Bonds	Distance (Å)
C3	C6	O36 - O40	8.66336
		O35 - O40	8.68755
		O36 - O39	10.02931
		O35 - O39	9.73720
C2	C5	O34 - O42	8.67284
		O34 - O41	9.41882
		O33 - O42	9.42677
		O33 - O41	10.22937
C1	C4	O32 - O37	8.47349
		O32 - O38	8.49739
		O31 - O37	8.74114
		O31 - O38	8.08227
C1	C3	O32- O35	6.35033
		O32 - O36	8.09959

		O31 - O35	7.95262
		O31 - O36	9.24242
C3	C4	O36 - O37	3.37440
		O36 - O38	5.64606
		O35 - O37	5.23670
		O35 - O38	7.02343
C1	C6	O32 - O40	6.15647
		O32 - O39	6.53347
		O31 - O40	4.57910
		O31 - O39	4.48231
C5	C6	O40 - O42	5.19913
		O40 - O41	4.35934
		O39 - O42	5.47504
		O39 - O41	3.56484
C4	C6	O40 - O37	6.53719
		O40 - O38	4.81668
		O39 - O37	8.12737
		O38 - O39	6.30410

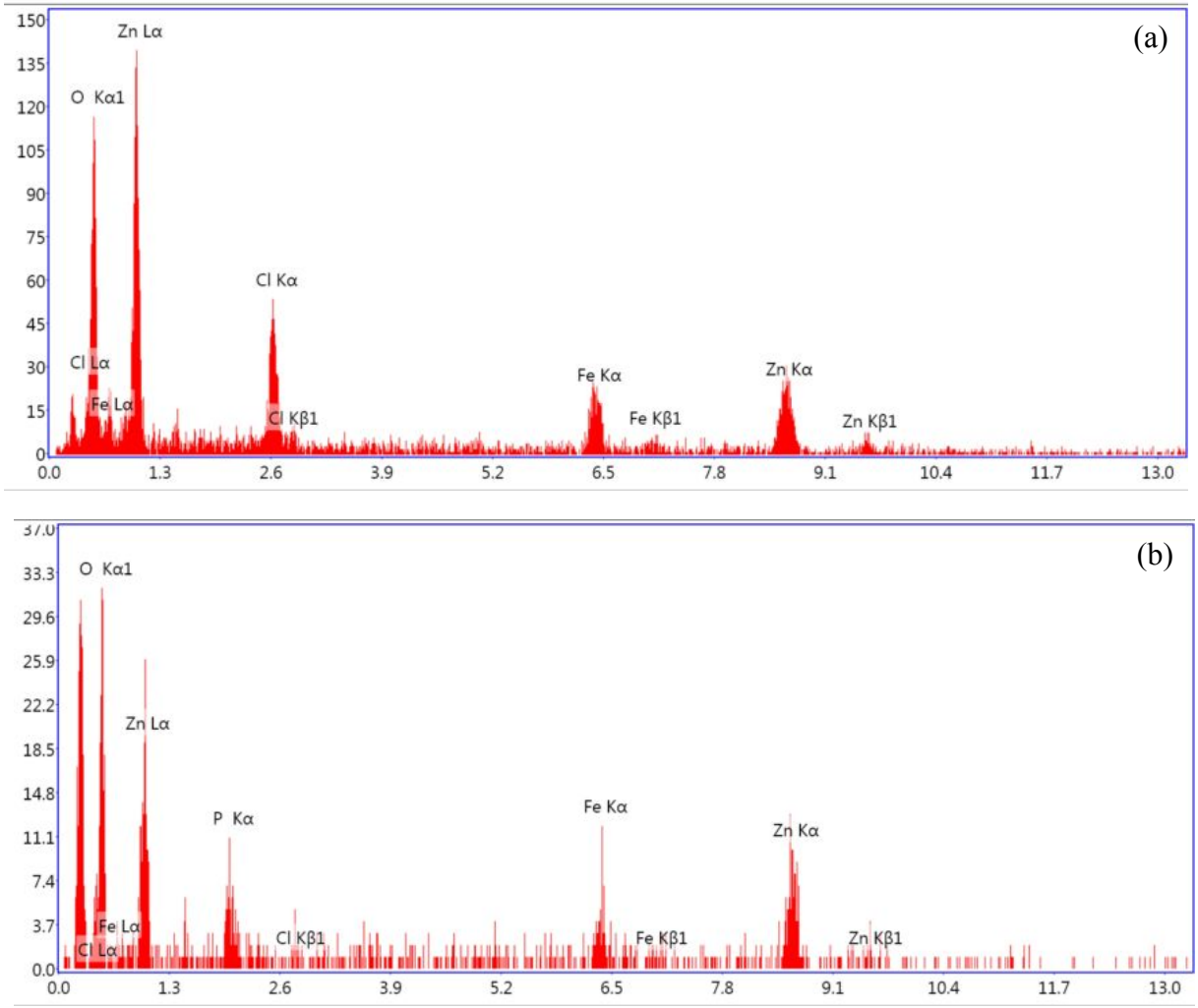

Fig. S1. EDX spectra for (a) ZLDH and (b) Z1.

Table S3. Elemental composition of ZLDH and Z1 obtained from EDX analysis.

Elements	**Atomic %**	
	ZLDH	**Z1**
Zn	22.26	24.62
Fe	8.65	8.78
Cl	9.48	0.14
P	0.00	6.12
O	60.50	56.33

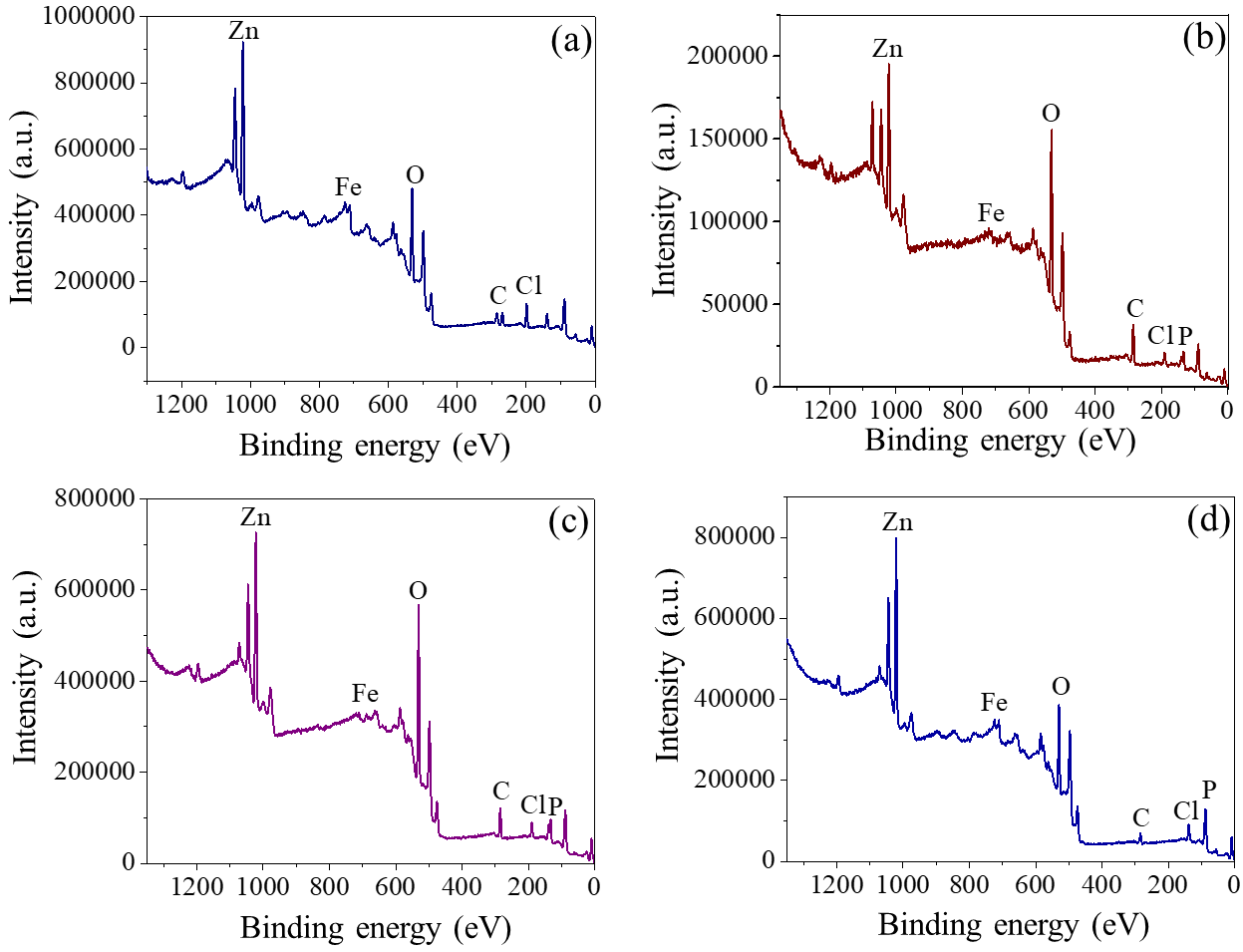

Fig. S2. XPS survey spectra for (a) ZLDH, (b) Z1, (c) ZAP1 and (d) ZAP5.

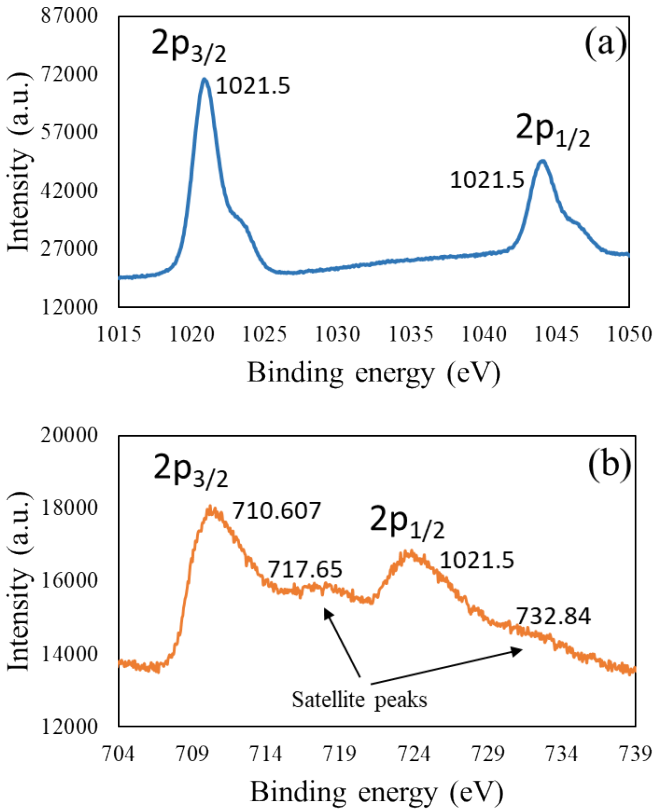

Fig. S3. XPS spectra for (a) Zn and (b) Fe in Zn-Fe-Cl LDH (ZLDH).

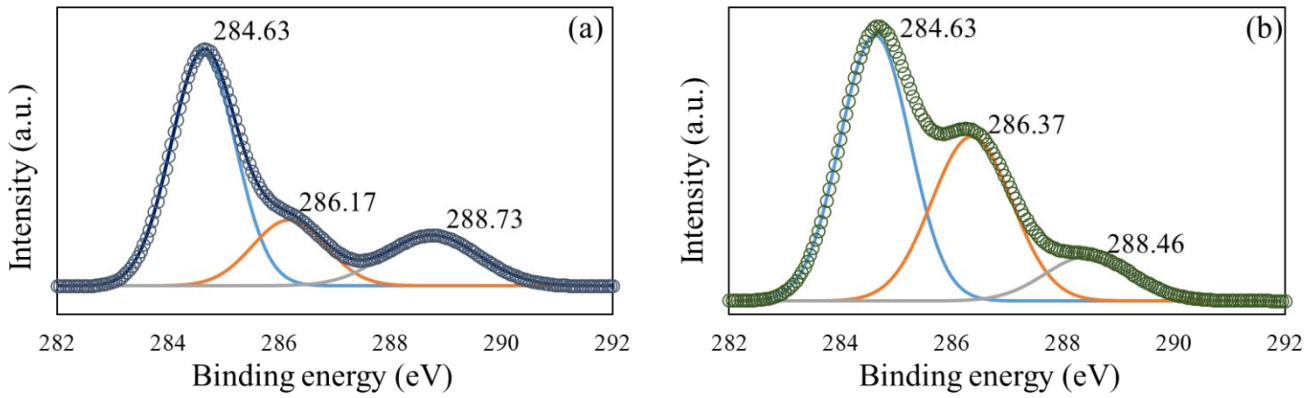

Fig. S4. Deconvoluted C 1s XPS spectra for (a) ZLDH and (b) Z1.

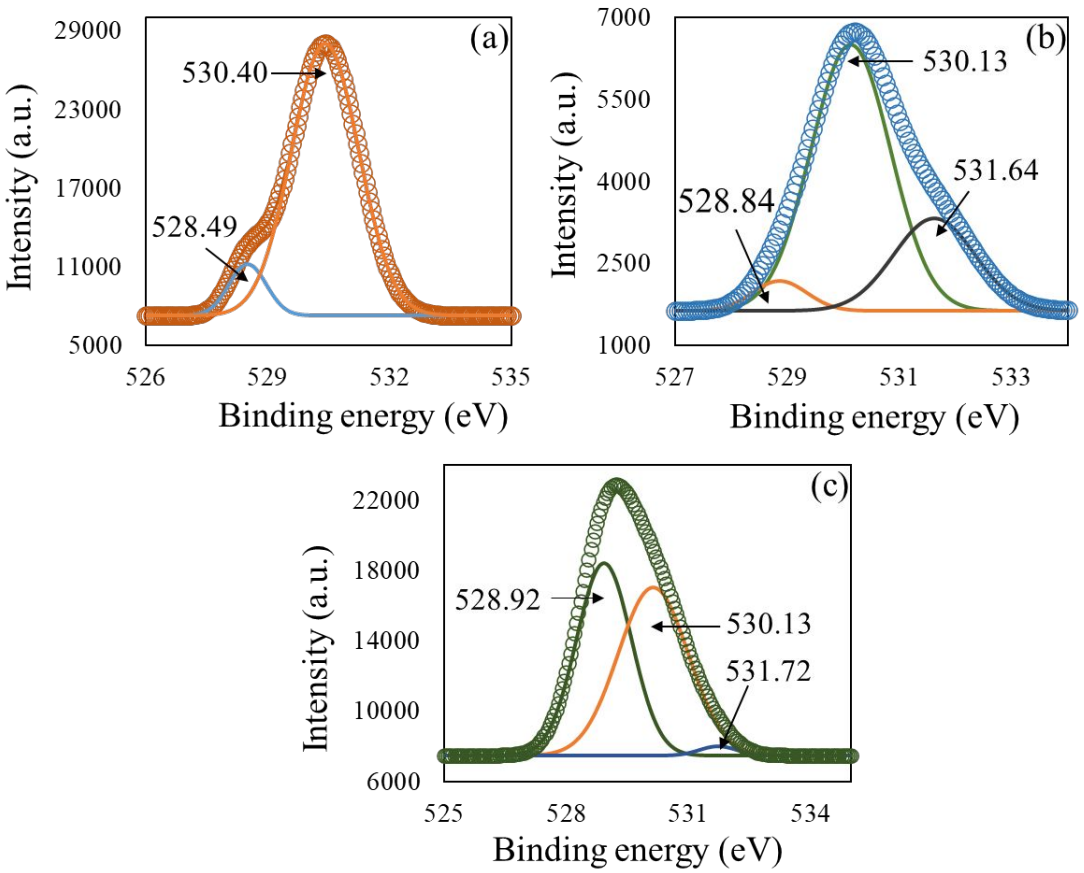

Fig. S5. Deconvoluted O 1s XPS spectra of (a) ZLDH, (b) Z1 and (c) ZAP5.

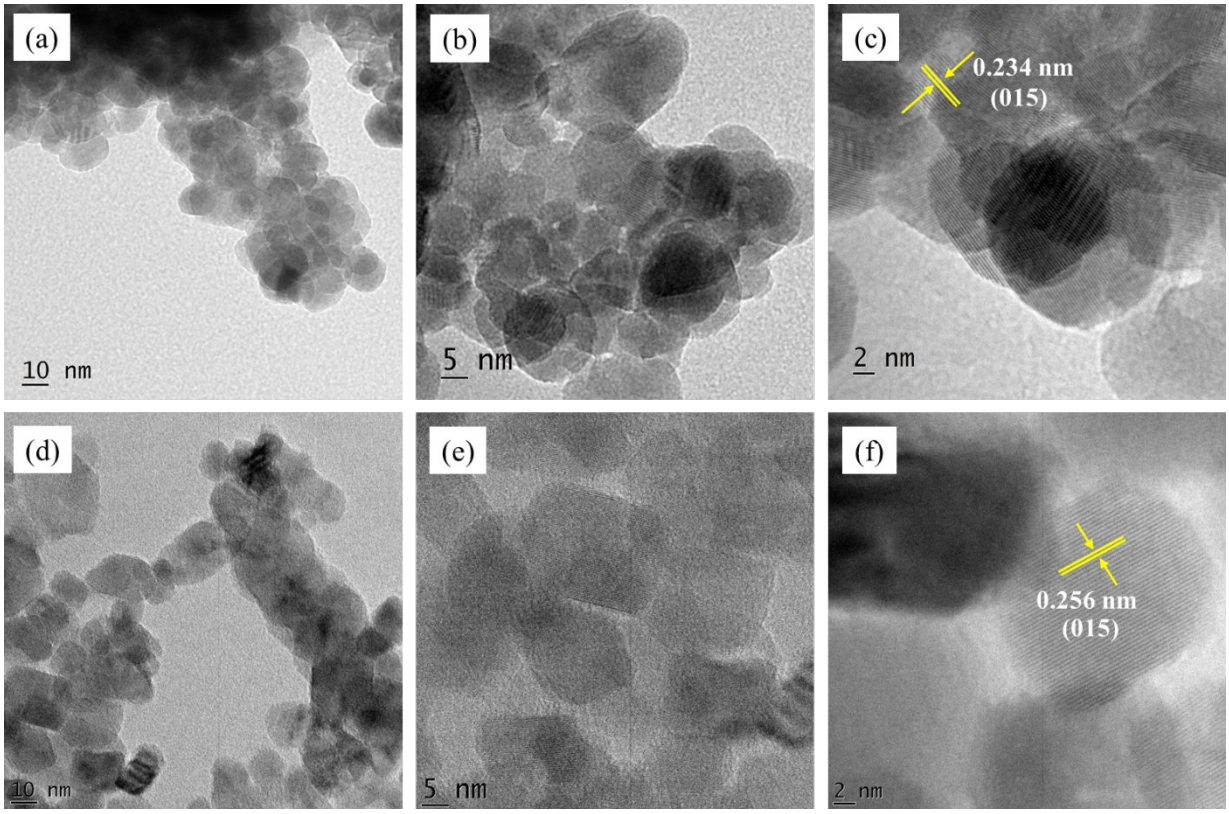

Fig. S6. HRTEM images for (a), (b), (c) ZLDH and (d), (e), (f) Z1.

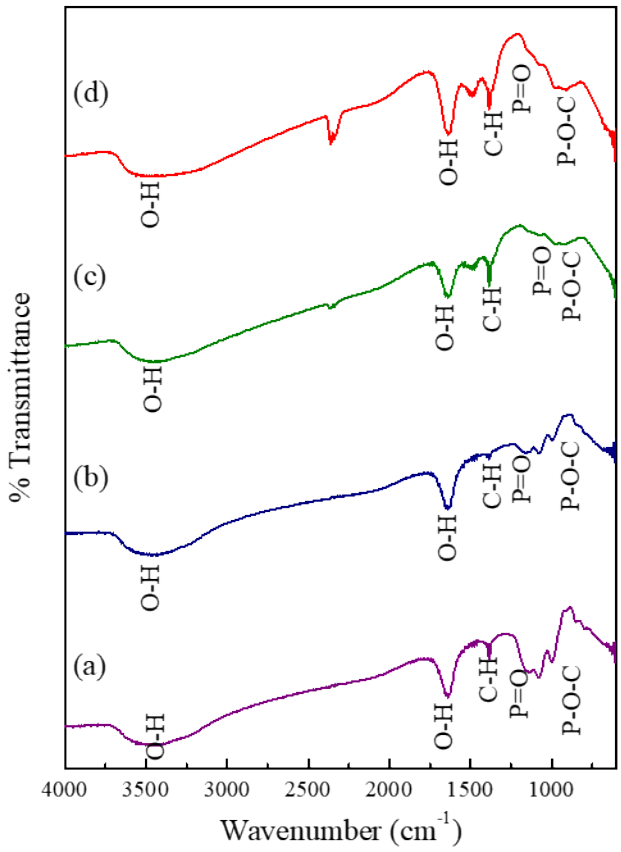

Fig. S7. FTIR spectra for (a) Z2, (b) Z3, (c) Z4 and (d) Z5

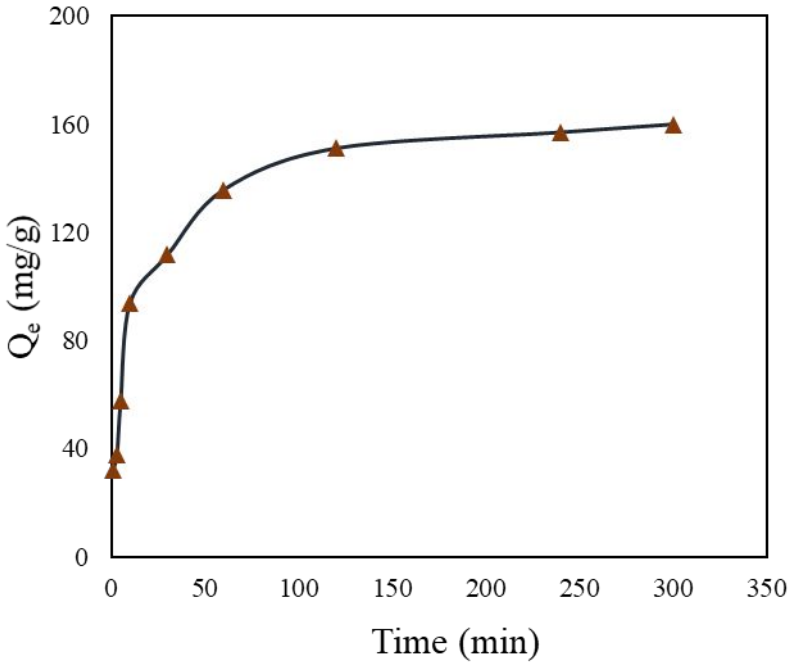

Fig. S8. Variation of adsorption capacity with time.

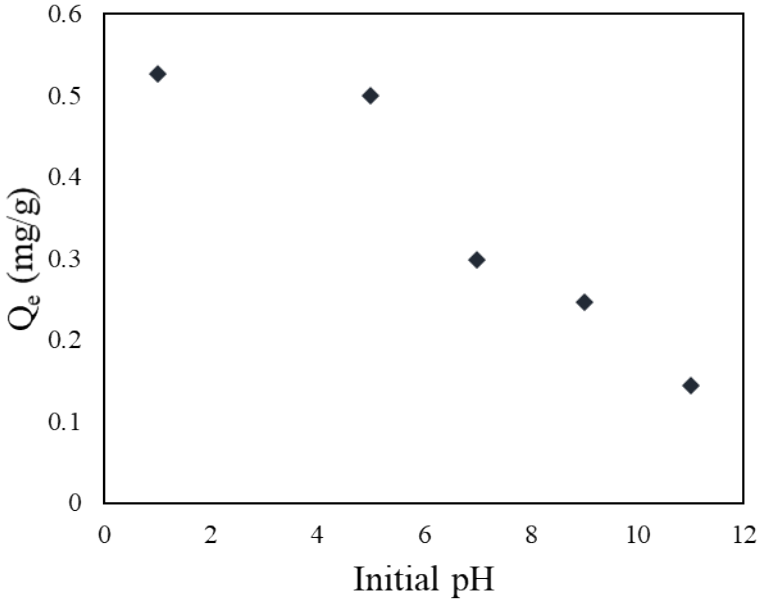

Fig. S9. Variation of adsorption capacity with pH of solution.

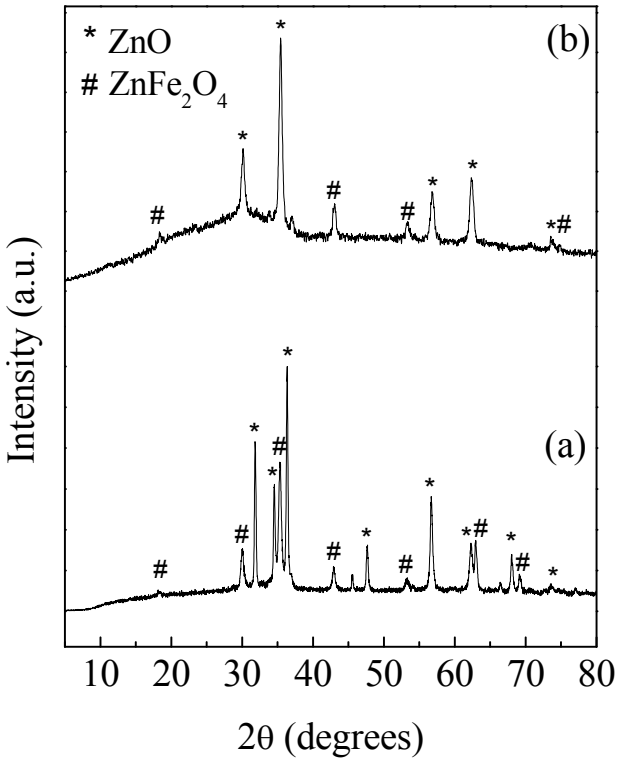

Fig. S10. PXRD pattern for (a) Calcined ZLDH (b) Product formed after reconstruction with sodium phytate solution. From the PXRD reflections, formation of mixed metal oxide phase is observed, instead of formation of phytate intercalated LDH structure.