Supplementary information

Intercalation vs Adsorption Strategies of Myoinositol 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	Х	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

8 2.674939 -1.078305 -1.6422 8 -1.854980 -2.178799 -0.610 8 -2.523886 0.751971 -0.7232 8 -0.264357 2.255806 0.4644 8 2.302626 1.496341 -0.6433 15 0.383871 -2.790388 1.2221 15 -3.413790 -2.239301 -0.2269 15 -3.466383 1.514418 0.1248 15 -0.407263 3.884612 0.1269 15 3.294613 2.152370 0.4546 15 3.607549 -1.806045 -0.5740 8 -3.745091 2.986313 -0.0083 8 -3.745091 2.986313 -0.0083 8 -3.818926 -1.576721 1.8814 8 -0.77212 4.576445 1.3916 8 -0.707212 4.576445 1.3916 8 -0.707212 4.576445 1.3916 8 -0.407164 -1.753127 -1.5003 8 -1.464223 3.946800 -1.0717<	1	-1.487842	-0.825587	-2.123296
8 -1.854980 -2.178799 -0.610 8 -2.523886 0.751971 -0.7233 8 -0.264357 2.255806 0.4644 8 2.302626 1.496341 -0.6433 15 0.383871 -2.790388 1.2221 15 -3.413790 -2.239301 -0.266 15 -3.666383 1.514418 0.1248 15 0.407263 3.884612 0.1269 15 3.294613 2.152370 0.4546 15 3.607549 -1.806045 -0.5740 8 -3.745091 2.986313 -0.0083 8 -3.745091 2.986313 -0.0350 8 -3.745091 2.986313 -0.0350 8 -0.141506 -1.576721 1.8814 8 -0.77212 4.576445 1.3916 8 -0.707212 4.576445 1.3916 8 -0.707212 4.576445 1.3916 8 -1.464223 3.946800 -1.0717 8 -1.464223 3.946800 -1.0717 <td>8</td> <td>2.674939</td> <td>-1.078305</td> <td>-1.642253</td>	8	2.674939	-1.078305	-1.642253
8 -2.523886 0.751971 -0.7233 8 -0.264357 2.255806 0.4644 8 2.302626 1.496341 -0.64333 15 0.383871 -2.790388 1.2221 15 -3.413790 -2.239301 -0.2260 15 -3.666383 1.514418 0.1248 15 -0.407263 3.884612 0.1269 15 3.294613 2.152370 0.4546 15 3.607549 -1.806045 -0.5740 8 -3.745091 2.986313 -0.0083 8 -3.745091 2.986313 -0.0083 8 -3.818896 -1.622600 1.0660 8 0.772258 -2.574700 -0.3500 8 0.707212 4.576445 1.3916 8 0.899252 4.269952 -0.6940 8 0.899252 4.269952 -0.6940 8 -1.464223 3.946800 -1.0713 8 -4.230648 -1.753127 -1.5003 8 -3.621177 0.966739 1.6008<	8	-1.854980	-2.178799	-0.610729
8 -0.264357 2.255806 0.4644 8 2.302626 1.496341 -0.6433 15 0.383871 -2.790388 1.2221 15 -3.413790 -2.239301 -0.2260 15 -3.666383 1.514418 0.1248 15 -0.407263 3.884612 0.1269 15 3.294613 2.152370 0.4546 15 3.607549 -1.806045 -0.5740 8 -3.745091 2.986313 -0.0083 8 -3.745091 2.986313 -0.03500 8 -3.745091 2.986313 -0.03500 8 -3.745091 2.986314 0.8561 8 -0.772258 -2.574700 -0.3500 8 -0.141506 -1.576721 1.8814 8 3.031496 3.578205 0.7754 8 -0.707212 4.576445 1.3916 8 -0.69404 -1.464223 3.946800 -1.0712 8 -1.464223 3.946800 -1.0712 8 -3.621177 0.9667	8	-2.523886	0.751971	-0.723258
8 2.302626 1.496341 -0.6433 15 0.383871 -2.790388 1.2221 15 -3.413790 -2.239301 -0.2260 15 -3.666383 1.514418 0.1248 15 -0.407263 3.884612 0.1269 15 3.294613 2.152370 0.4546 15 3.607549 -1.806045 -0.5740 8 -3.745091 2.986313 -0.0083 8 -3.745091 2.986313 -0.0660 8 0.772258 -2.574700 -0.3500 8 -0.141506 -1.576721 1.8814 8 3.031496 3.578205 0.7754 8 -0.707212 4.576445 1.3916 8 -0.707212 4.576445 1.3916 8 -0.707212 4.576445 1.3916 8 -0.4273 3.946800 -1.0711 8 -1.464223 3.946800 -1.0711 8 -4.230648 -1.753127 -1.5000 8 -4.230648 -1.753127 -1.5000 </td <td>8</td> <td>-0.264357</td> <td>2.255806</td> <td>0.464481</td>	8	-0.264357	2.255806	0.464481
15 0.383871 -2.790388 1.2221 15 -3.413790 -2.239301 -0.2261 15 -3.666383 1.514418 0.1248 15 -0.407263 3.884612 0.1269 15 3.294613 2.152370 0.4546 15 3.607549 -1.806045 -0.5740 8 -3.745091 2.986313 -0.0083 8 -3.745091 2.986313 -0.0083 8 -3.745091 2.986313 -0.0083 8 -3.745091 2.986313 -0.0083 8 -3.745091 2.986313 -0.0083 8 -3.745091 2.986313 -0.0083 8 -3.745091 2.986313 -0.0083 8 -3.745091 2.986313 -0.0083 8 -3.745091 2.986313 -0.0083 8 -3.745091 2.986313 -0.0083 8 -0.772258 -2.574700 -0.3500 8 -0.141506 -1.576721 1.8814 8 3.031496 3.578205 0.7754 8 -0.707212 4.576445 1.3916 8 -0.707212 4.576445 1.3916 8 -1.464223 3.946800 -1.0712 8 -3.621177 0.966739 1.6008 8 -3.621177 0.966739 1.6008 8 -3.493760 -3.847687 -0.2166 8 -0.470164 -4.140981 1.2522 8 1.780605 -3.385240 1.744	8	2.302626	1.496341	-0.643358
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8 -3.818896 -1.622600 1.0660 8 0.772258 -2.574700 -0.3500 8 -0.141506 -1.576721 1.8814 8 3.428350 -1.368914 0.8561 8 3.031496 3.578205 0.7754 8 3.031496 3.578205 0.7754 8 -0.707212 4.576445 1.3916 8 -0.707212 4.576445 1.3916 8 -0.707212 4.576445 1.3916 8 -0.707212 4.576445 1.3916 8 -0.707212 4.576445 1.3916 8 -1.464223 3.946800 -1.0713 8 -1.464223 3.946800 -1.0713 8 -3.621177 0.966739 1.6008 8 -3.621177 0.966739 1.6008 8 -3.493760 -3.847687 -0.2163 8 -3.493760 -3.847687 -0.2163 8 -0.470164 -4.140981 1.2523 8 3.284381 1.190578 1.7136	8	-3.745091	2.986313	-0.008585
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$\begin{array}{cccccccccccccccccccccccccccccccccccc$	8	3.031496	3.578205	0.775461
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	8	-0.707212	4.576445	1.391689
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	8	0.899252	4.269952	-0.694040
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	8	-1.464223	3.946800	-1.071383
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	8	-4.941874	0.790034	-0.624188
8 -4.230648 -1.753127 -1.5007 8 -3.493760 -3.847687 -0.2167 8 -0.470164 -4.140981 1.2527 8 1.780605 -3.385240 1.7441 8 4.703001 1.930931 -0.3046 8 3.284381 1.190578 1.7136 8 5.009915 -1.489804 -1.2599 8 3.504567 -3.394587 -0.7274 1 -4.223299 -4.153660 0.3498 1 2.843886 -3.767526 -0.1079	8	-3.621177	0.966739	1.600812
8 -3.493760 -3.847687 -0.2163 8 -0.470164 -4.140981 1.2523 8 1.780605 -3.385240 1.7441 8 4.703001 1.930931 -0.3046 8 3.284381 1.190578 1.7136 8 5.009915 -1.489804 -1.2599 8 3.504567 -3.394587 -0.7274 1 -4.223299 -4.153660 0.3498 1 2.843886 -3.767526 -0.1079	8	-4.230648	-1.753127	-1.500817
8 -0.470164 -4.140981 1.2523 8 1.780605 -3.385240 1.7441 8 4.703001 1.930931 -0.3046 8 3.284381 1.190578 1.7136 8 5.009915 -1.489804 -1.2599 8 3.504567 -3.394587 -0.7274 1 -4.223299 -4.153660 0.3498 1 2.843886 -3.767526 -0.1079	8	-3.493760	-3.847687	-0.216812
8 1.780605 -3.385240 1.7441 8 4.703001 1.930931 -0.3046 8 3.284381 1.190578 1.7136 8 5.009915 -1.489804 -1.2599 8 3.504567 -3.394587 -0.7274 1 -4.223299 -4.153660 0.3498 1 2.843886 -3.767526 -0.1079	8	-0.470164	-4.140981	1.252343
8 4.703001 1.930931 -0.3046 8 3.284381 1.190578 1.7136 8 5.009915 -1.489804 -1.2599 8 3.504567 -3.394587 -0.7274 1 -4.223299 -4.153660 0.3498 1 2.843886 -3.767526 -0.1079	8	1.780605	-3.385240	1.744119
8 3.284381 1.190578 1.7136 8 5.009915 -1.489804 -1.2599 8 3.504567 -3.394587 -0.7274 1 -4.223299 -4.153660 0.3498 1 2.843886 -3.767526 -0.1079	8	4.703001	1.930931	-0.304690
8 5.009915 -1.489804 -1.2599 8 3.504567 -3.394587 -0.7274 1 -4.223299 -4.153660 0.3498 1 2.843886 -3.767526 -0.1079	8	3.284381	1.190578	1.713609
8 3.504567 -3.394587 -0.7274 1 -4.223299 -4.153660 0.3498 1 2.843886 -3.767526 -0.1079	8	5.009915	-1.489804	-1.259925
1 -4.223299 -4.153660 0.3498 1 2.843886 -3.767526 -0.1079	8	3.504567	-3.394587	-0.727434
1 2.843886 -3.767526 -0.1079	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)
		O36 - O40	8.66336
C3	C6	O35 - O40	8.68755
		036 - 039	10.02931
		035 - 039	9.73720
		034 - 042	8.67284
C2	C5	O34 - O41	9.41882
		033 - 042	9.42677
		033 - 041	10.22937
		032 - 037	8.47349
C1	C4	032 - 038	8.49739
		031 - 037	8.74114
		O31 - O38	8.08227
		O32- O35	6.35033
C1	C3	032 - 036	8.09959

		O31 - O35	7.95262
		O31 - O36	9.24242
		036 - 037	3.37440
C3	C4	O36 - O38	5.64606
		035 - 037	5.23670
		035 - 038	7.02343
		032 - 040	6.15647
C1	C6	032 - 039	6.53347
		O31 - O40	4.57910
		031 - 039	4.48231
		O40 - O42	5.19913
C5	C6	O40 - O41	4.35934
		039 - 042	5.47504
		039 - 041	3.56484
		040 - 037	6.53719
C4	C6	O40 - O38	4.81668
		039 - 037	8.12737
		038 - 039	6.30410



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

Elements	Atomic %		
	ZLDH	Z1	
Zn	22.26	24.62	
Fe	8.65	8.78	
Cl	9.48	0.14	
Р	0.00	6.12	
0	60.50	56.33	

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



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.