SUPPORTING INFORMATION

How Density Functional Theory Surface Energies May Explain the Morphology of Particles, Nanosheets and Conversion Films based on Layered Double Hydroxides

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The supporting information includes AFM images and DFT results.

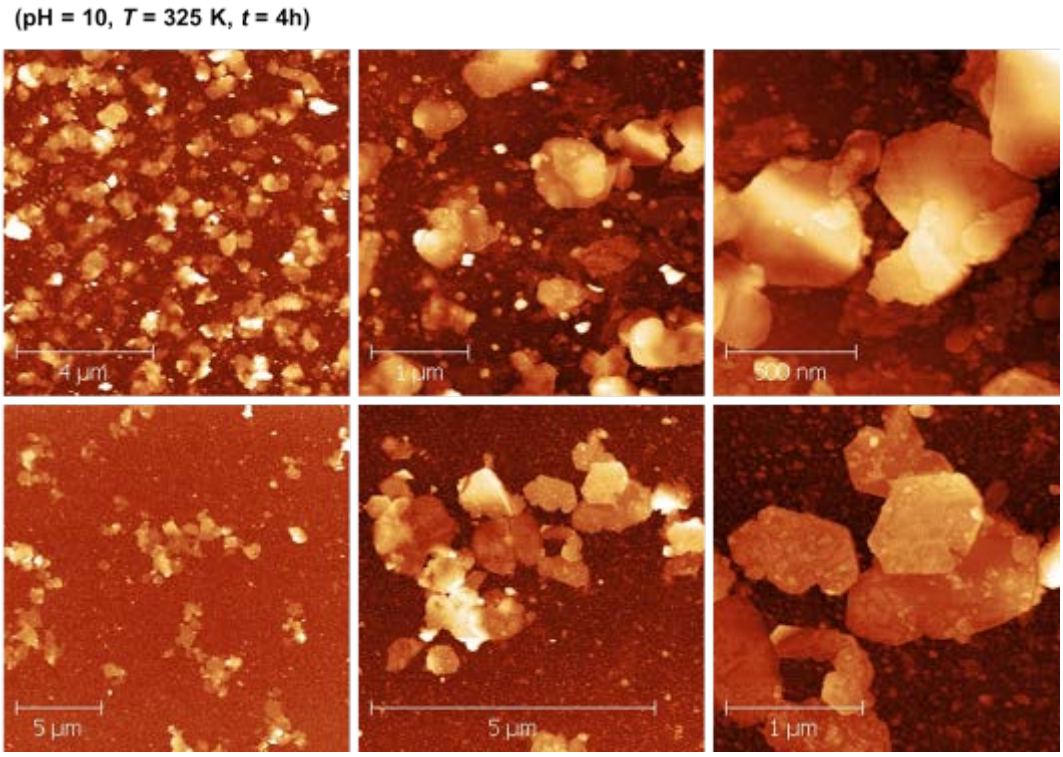

Figure S1. AFM images used to obtain the particle height for the sample (pH = 10, *T* = 325 K, *t* = 4h).

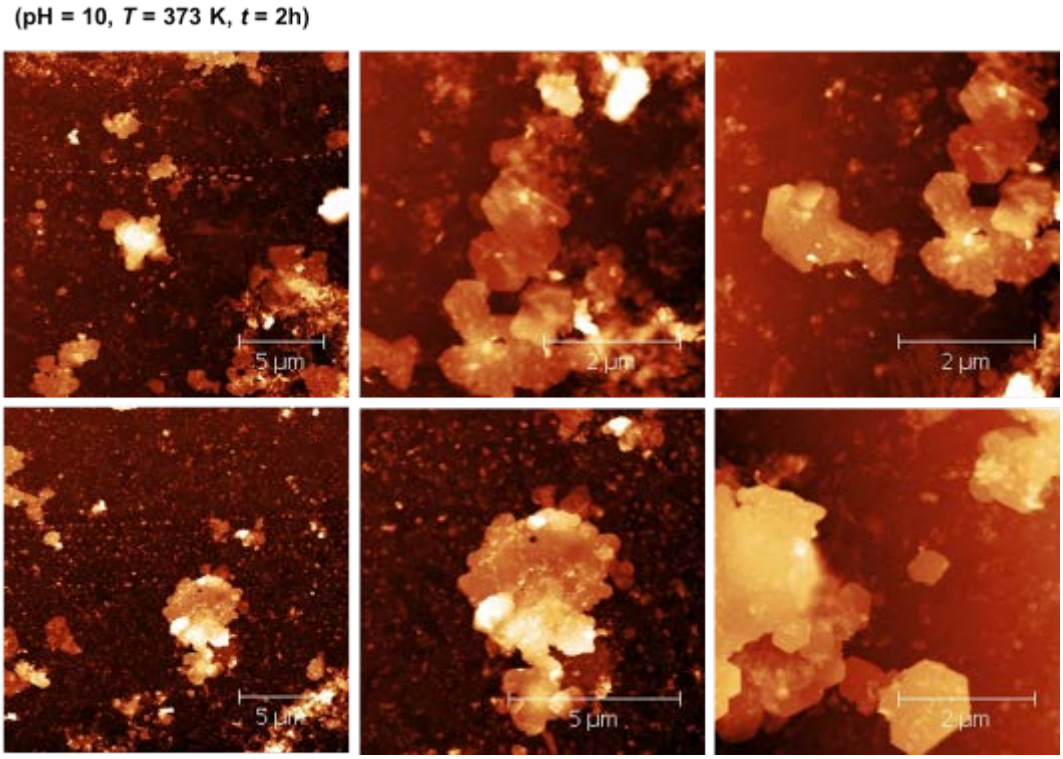

Figure S2. AFM images used to obtain the particle height for the sample (pH = 10, *T* = 373

K, *t* = 2h).

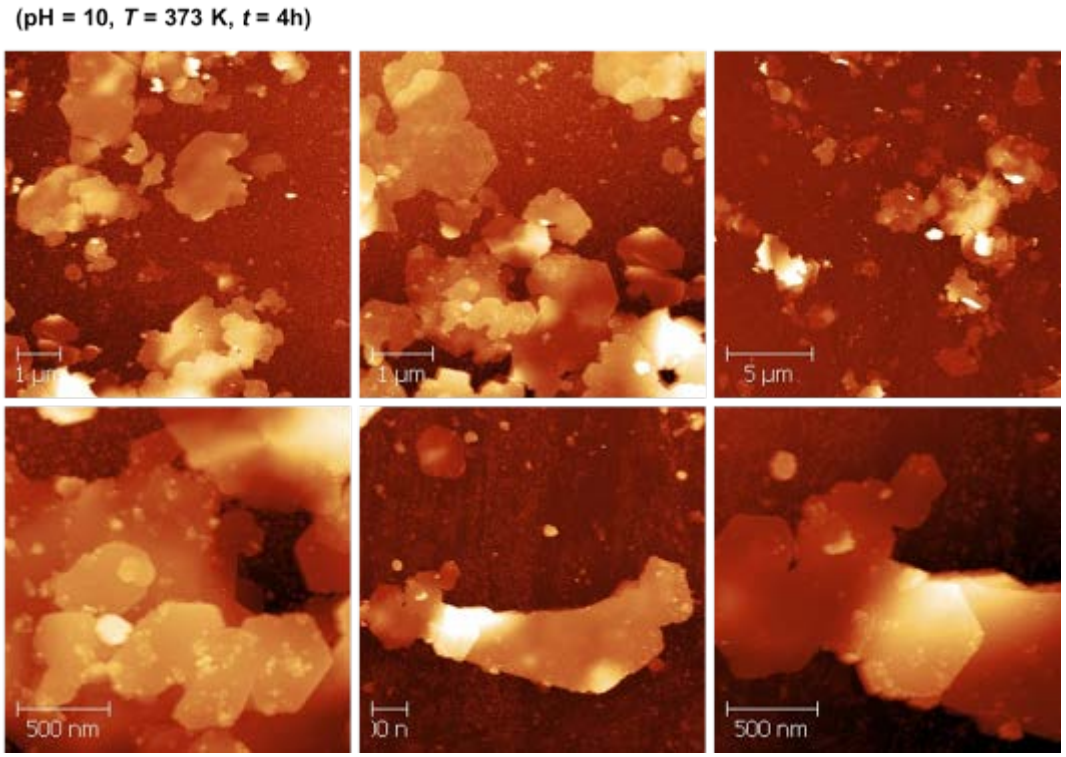

Figure S3. AFM images used to obtain the particle height for the sample (pH = 10, *T* = 373 K, *t* = 4h).

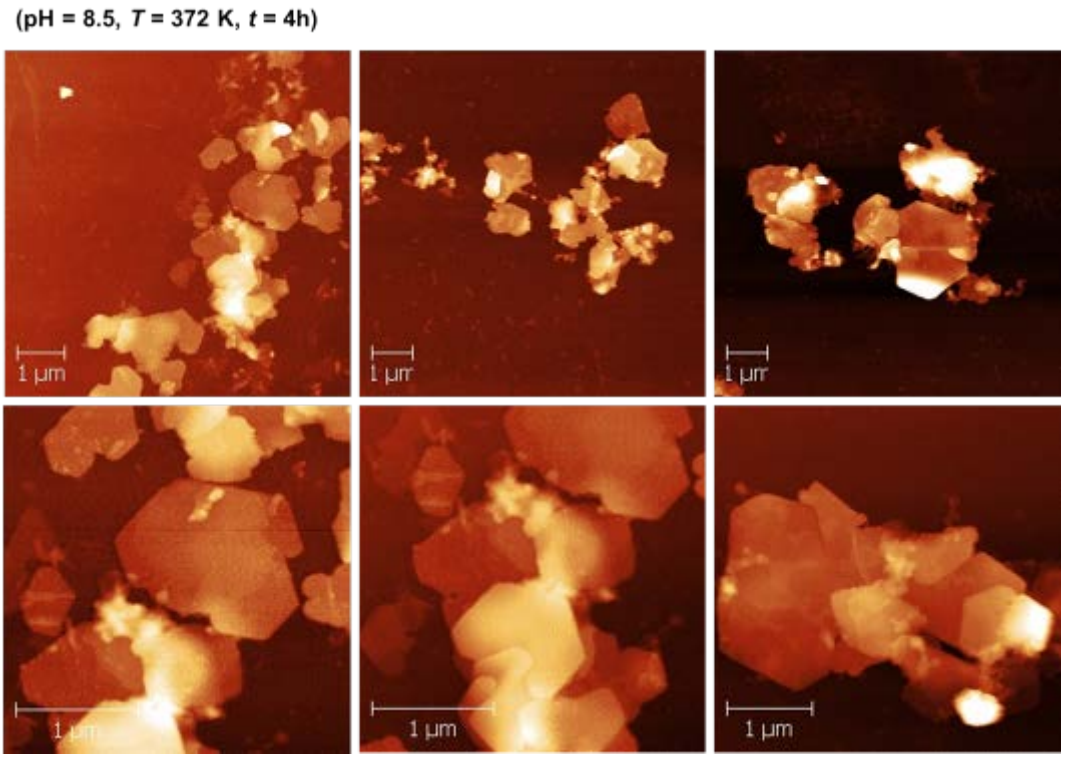

Figure S4. AFM images used to obtain the particle height for the sample (pH = 8.5, *T* = 372 K, *t* = 4h).

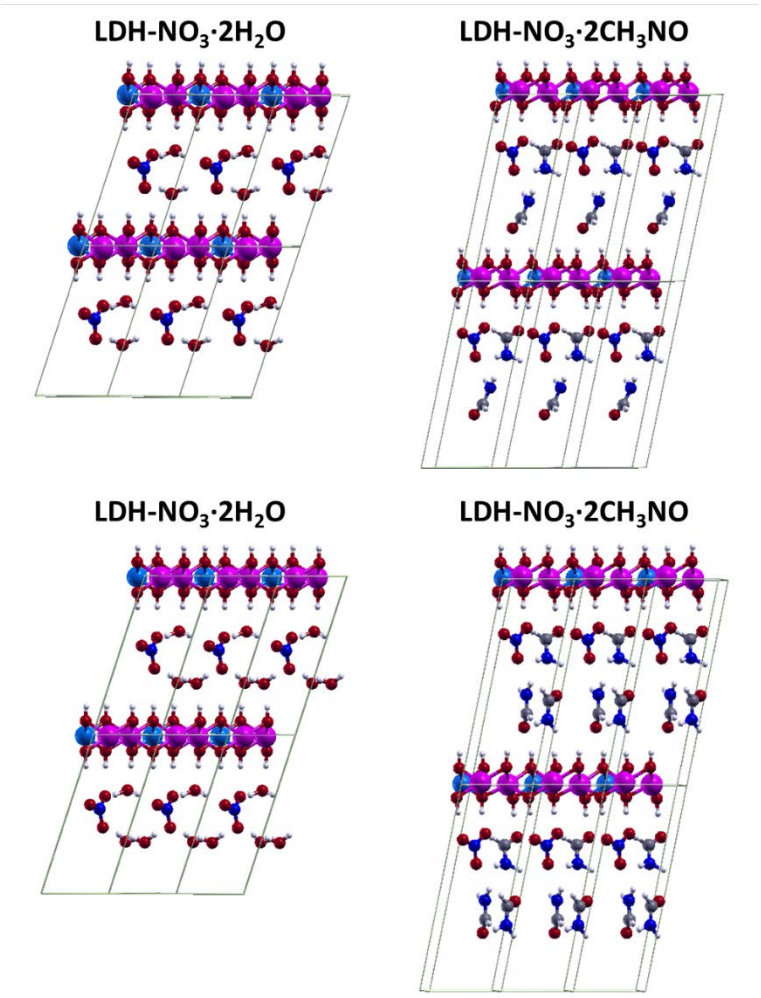

Figure S5. LDH-NO_3 structures with 2 and 3 molecules of water and formamide per anion (spheres color code: Zn - pink; Al - light blue; O - red; N - blue; H - white; C - grey).

Table S1

Electronic energies obtained from the optimization of the geometries at PBE level of theory with ultrasoft pseudopotentials.

Supercell	$\frac{E_{el}}{Ry}$
$[Zn_2Al(OH)_6](NO_3)\cdot H_2O$	−616.125567
$\{[Zn_2Al(OH)_6](NO_3)\cdot H_2O\}_x$	−615.945868
$\{[Zn_2Al(OH)_6](NO_3)\cdot H_2O\}_y$	−615.942978
$\{[Zn_2Al(OH)_6](NO_3)\cdot H_2O\}_z$	−616.046378
$[Zn_2Al(OH)_6](NO_3)\cdot 2H_2O$	−650.597549
$\{[Zn_2Al(OH)_6](NO_3)\cdot 2H_2O\}_z$	−650.510594
$[Zn_2Al(OH)_6](NO_3)\cdot 3H_2O$	−685.084072
$\{[Zn_2Al(OH)_6](NO_3)\cdot 3H_2O\}_z$	−684.972840
$[Zn_2Al(OH)_6](NO_3)\cdot CH_3NO$	−648.523510
$\{[Zn_2Al(OH)_6](NO_3)\cdot CH_3NO\}_z$	−648.485588
$[Zn_2Al(OH)_6](NO_3)\cdot 2CH_3NO$	−715.454229
$\{[Zn_2Al(OH)_6](NO_3)\cdot 2CH_3NO\}_z$	−715.418241
$[Zn_2Al(OH)_6](NO_3)\cdot 3CH_3NO$	−782.328883
$\{[Zn_2Al(OH)_6](NO_3)\cdot 3CH_3NO\}_z$	−782.292455
$[Zn_2Al(OH)_6](NO_3)\cdot H_2O\cdot$(4 × 4) Al(111)–4L (═ layer)	−1412.688792
$[Zn_2Al(OH)_6](NO_3)\cdot H_2O\cdot$(4 × 4) Al(111)–4L (═ anion)	−1412.668724
$[Zn_2Al(OH)_6](NO_3)\cdot H_2O\cdot$(4 × 4) Al(111)–4L (⊥ normal)	−1412.819459
$[Zn_2Al(OH)_6](NO_3)\cdot H_2O\cdot$(4 × 4) Al(111)–2L (═ layer)	−1413.840314
$[Zn_2Al(OH)_6](NO_3)\cdot H_2O\cdot$(4 × 4) Al(111)–2L (═ anion)	−1413.707288
$[Zn_2Al(OH)_6](NO_3)\cdot H_2O\cdot$(4 × 4) Al(111)–2L (⊥ normal)	−1413.680623
$[Zn_8Al_4(OH)_{24}](NO_3)_4\cdot 4\ H_2O\cdot$(8 × 4) Al(111)–2L (═ layer)	−3259.424485
$[Zn_8Al_4(OH)_{24}](NO_3)_4\cdot 4\ H_2O\cdot$(8 × 4) Al(111)–2L (═ anion)	−3259.480066
$[Zn_8Al_4(OH)_{24}](NO_3)_4\cdot 4\ H_2O\cdot$(8 × 4) Al(111)–2L (⊥ normal)	−3259.674500
$[Zn_2Al(OH)_6](NO_3)\cdot H_2O\cdot$(2 × 2) α-$Al_2O_3$(0001)–9L (═ layer)	−2179.453486
$[Zn_2Al(OH)_6](NO_3)\cdot H_2O\cdot$(2 × 2) α-$Al_2O_3$(0001)–9L (═ anion)	−2179.494553
$[Zn_2Al(OH)_6](NO_3)\cdot H_2O\cdot$(2 × 2) α-$Al_2O_3$(0001)–9L (⊥ normal)	−2179.595401

1 Ry = 1312.75 $kJ\cdot mol^{-1}$

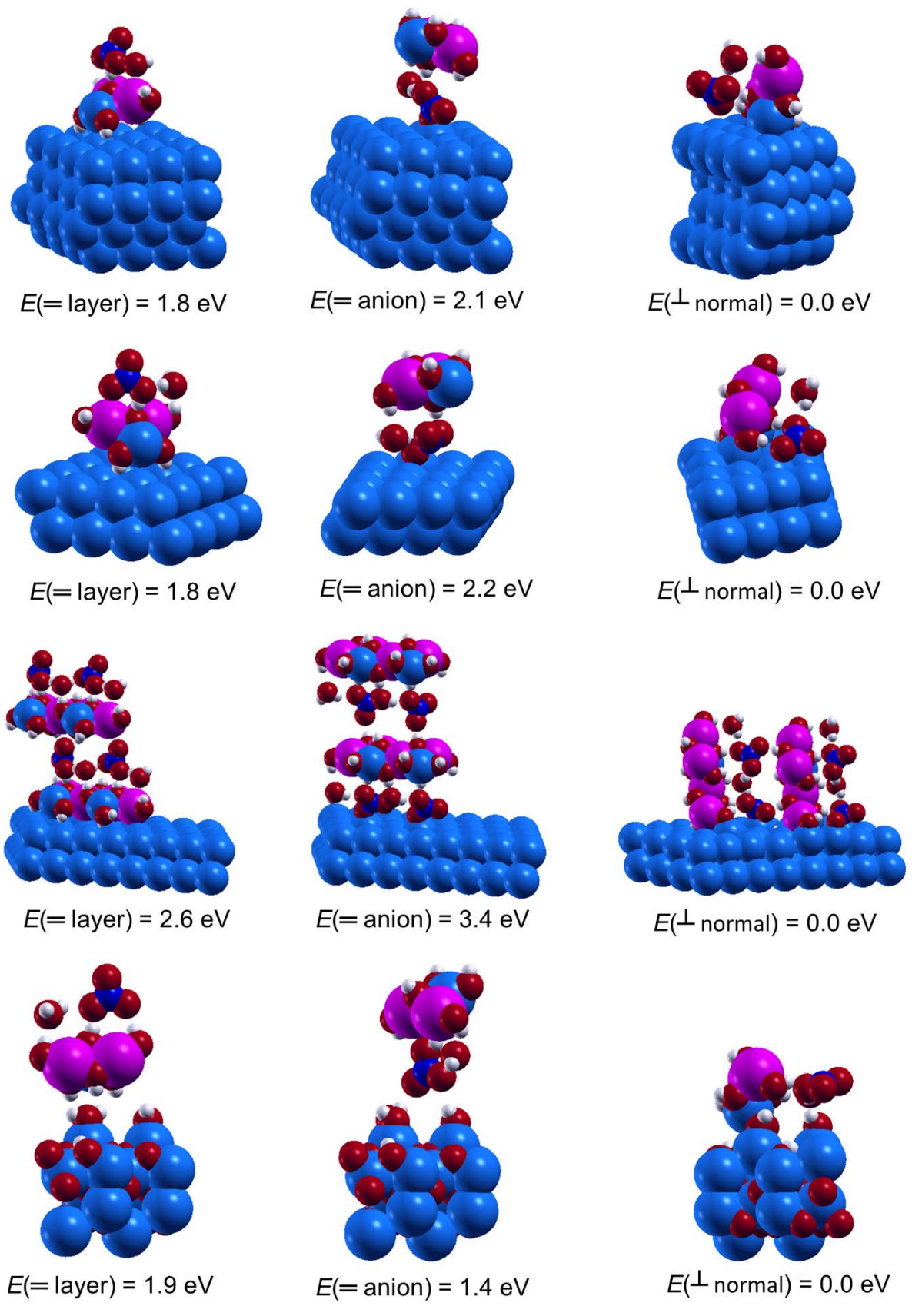

Figure S6. Representation of the atoms of the supercells and relative energies of Zn(2)Al clusters interacting with periodic models of aluminum surfaces: a $[Zn_2Al(OH)_6](NO_3)\cdot H_2O$ unit on a (4 × 4) Al(111)–4L surface, a $[Zn_2Al(OH)_6](NO_3)\cdot H_2O$ unit on a (4 × 4) Al(111)–

2L surface, a $[Zn_8Al_4(OH)_{24}](NO_3)_4 \cdot 4\ H_2O$ unit on a (8 × 4) Al(111)–2L surface, and a $[Zn_2Al(OH)_6](NO_3) \cdot H_2O$ unit on a (2 × 2) α-Al_2O_3(0001)–9L surface (spheres color code: Zn - pink; Al - light blue; O - red; N - blue; H - white; C - grey).

Table S2. Crystal lattice vectors in the Cartesian axis of the supercell of the most stable interaction (⊥ normal) between a $[Zn_2Al(OH)_6](NO_3) \cdot H_2O$ unit and a (4 × 4) Al(111)–4L surface.

Vector	x / Å	y / Å	z / Å
1	11.44382	0.00000	0.00000
2	−5.72191	9.91064	0.00000
3	0.00000	0.00000	25.0000

Table S3. Cartesian coordinates of the supercell of the most stable interaction (⊥ normal) between a $[Zn_2Al(OH)_6](NO_3) \cdot H_2O$ unit and a (4 × 4) Al(111)–4L surface.

Atom type	Coordinates / Å		
	x	y	z
Al	-0.221439361	-0.182695425	7.018910940
Al	-1.626874764	2.391156833	7.107191830
Al	-2.922839676	4.914083789	6.934575075
Al	1.340782027	-2.529426896	6.891554009
Al	2.577520786	0.016061328	7.700113991
Al	1.225325124	2.370383210	6.904480057
Al	-0.104874203	4.904218621	6.931581099
Al	4.141533878	-2.469051334	6.953161243
Al	5.450043966	-0.023420801	6.949108578
Al	4.092288191	2.376021958	6.928991023
Al	2.729904597	4.819017796	6.941259777
Al	6.996984788	-2.551357582	6.932078427
Al	-3.171655188	-0.061307537	6.875108160
Al	-4.446765427	2.454308927	6.915274891
Al	-5.812336295	4.882122605	6.913214489
Al	-1.620253600	-2.680082335	6.785716848
Al	-1.490253150	0.810964478	4.647947028
Al	-2.882871032	3.269162582	4.599789709
Al	1.406577924	-4.154878425	4.571064197
Al	-0.064039630	-1.674141934	4.572825008
Al	1.384390001	0.758555381	4.604448076
Al	-0.063224549	3.253334543	4.586413073
Al	4.268052304	-4.153037566	4.571339020
Al	2.816725944	-1.644074604	4.594682155
Al	4.225192328	0.814349058	4.575030194
Al	2.824297445	3.269143314	4.568467388
Al	7.114415344	-4.161069240	4.584446459
Al	5.661550218	-1.663296712	4.596197803
Al	-4.348377344	0.830869638	4.548897084
Al	-5.739490862	3.284532304	4.565195985
Al	-1.452713099	-4.194176339	4.544131982
Al	-2.935495115	-1.660020503	4.545148996
Al	1.430477020	-0.825886290	2.335959190
Al	0.000000000	1.651772580	2.335959190
Al	-1.430477020	4.129431460	2.335959190
Al	2.860954040	-3.303545170	2.335959190
Al	4.291431060	-0.825886290	2.335959190
Al	2.860954040	1.651772580	2.335959190
Al	1.430477020	4.129431460	2.335959190
Al	5.721908070	-3.303545170	2.335959190
Al	-4.291431060	-0.825886290	2.335959190
Al	-5.721908070	1.651772580	2.335959190
Al	-7.152385090	4.129431460	2.335959190

Al	-2.860954040	-3.303545170	2.335959190
Al	-1.430477020	-0.825886290	2.335959190
Al	-2.860954040	1.651772580	2.335959190
Al	-4.291431060	4.129431460	2.335959190
Al	0.000000000	-3.303545170	2.335959190
Al	0.000000000	0.000000000	0.000000000
Al	-1.430477020	2.477658870	0.000000000
Al	-2.860954040	4.955317750	0.000000000
Al	1.430477020	-2.477658870	0.000000000
Al	2.860954040	0.000000000	0.000000000
Al	1.430477020	2.477658870	0.000000000
Al	0.000000000	4.955317750	0.000000000
Al	4.291431060	-2.477658870	0.000000000
Al	5.721908070	0.000000000	0.000000000
Al	4.291431060	2.477658870	0.000000000
Al	2.860954040	4.955317750	0.000000000
Al	7.152385090	-2.477658870	0.000000000
Al	-2.860954040	0.000000000	0.000000000
Al	-4.291431060	2.477658870	0.000000000
Al	-5.721908070	4.955317750	0.000000000
Al	-1.430477020	-2.477658870	0.000000000
Al	-1.846200481	0.985369170	9.349502750
Zn	0.644249183	-0.137106552	10.566538559
Zn	-1.870358570	0.463039568	12.315622345
O	-2.978826980	0.245872415	10.492629198
O	-2.576517999	0.972285588	13.906580031
O	-0.693241540	-0.501284596	8.926360566
O	-0.715392405	1.442770843	10.677978391
O	2.222399280	0.344241031	9.541612966
O	-0.406245015	-0.892452444	11.914096476
H	-3.909865187	0.005862783	10.373985963
H	-2.357249796	1.927376853	14.017083303
H	-1.122889856	-1.388653207	8.981667925
H	-0.355952601	2.402205300	10.930072373
H	2.318017229	1.308242131	9.778835353
H	-0.431029730	-1.804598306	12.247173698
N	1.314655383	3.952089814	11.141978138
O	1.845966077	4.929262490	11.679389613
O	0.079891871	3.651595763	11.464308309
O	1.909027047	3.229686071	10.270291187
O	-1.462194804	3.790651110	13.909042892
H	-0.906505155	3.813580853	14.710809790
H	-0.829443222	3.891044610	13.161838449

Table S4. Crystal lattice vectors in the Cartesian axis of the supercell of the most stable interaction (⊥ normal) between a $[Zn_2Al(OH)_6](NO_3)\cdot H_2O$ unit and a (4 × 4) Al(111)–2L surface.

Vector	x / Å	y / Å	z / Å
1	11.44382	0.00000	0.00000
2	−5.72191	9.91064	0.00000
3	0.00000	0.00000	25.0000

Table S5. Cartesian coordinates of the supercell of the most stable interaction (⊥ normal) between a $[Zn_2Al(OH)_6](NO_3)\cdot H_2O$ unit and a (4 × 4) Al(111)–2L surface.

Atom type	Coordinates / Å		
	x	y	z
Al	1.916928630	-3.036899867	5.287244101
Zn	0.090671158	-1.516757691	3.358424929
Zn	2.189975789	-3.327137120	2.239898866
O	2.124107223	-4.305798728	4.023841911

O	2.997947316	-3.453378139	0.620848814
O	0.015658665	-2.699892280	5.241661770
O	2.124449449	-1.815404076	3.927438835
O	-0.453079455	-0.205964583	4.622606662
O	0.176319569	-2.725374387	1.966664130
H	2.301493652	-5.251736076	4.157407707
H	3.764210124	-2.845535850	0.656857936
H	-0.495252080	-3.485818540	5.571873657
H	2.584346588	-0.928674349	4.053711636
H	0.157205039	0.584873599	4.589940961
H	-0.549464608	-3.378954152	1.955076046
N	2.700402408	1.665125921	4.440006792
O	3.272556088	2.762662564	4.365755358
O	3.261202015	0.588006026	4.030329416
O	1.533410365	1.589939984	5.024335323
O	4.820647077	-0.854751999	1.910846525
H	5.080363700	-0.345460514	1.121980488
H	4.503047206	-0.186296139	2.555067619
Al	0.000000000	0.000000000	10.007877570
Al	-1.430477020	2.477658870	10.007877570
Al	-2.860954040	4.955317750	10.007877570
Al	1.430477020	-2.477658870	10.007877570
Al	2.860954040	0.000000000	10.007877570
Al	1.430477020	2.477658870	10.007877570
Al	0.000000000	4.955317750	10.007877570
Al	4.291431060	-2.477658870	10.007877570
Al	5.721908070	0.000000000	10.007877570
Al	4.291431060	2.477658870	10.007877570
Al	2.860954040	4.955317750	10.007877570
Al	7.152385090	-2.477658870	10.007877570
Al	-2.860954040	0.000000000	10.007877570
Al	-4.291431060	2.477658870	10.007877570
Al	-5.721908070	4.955317750	10.007877570
Al	-1.430477020	-2.477658870	10.007877570
Al	-1.497223753	0.953685590	7.645518067
Al	-2.891489650	3.325226736	7.549676919
Al	1.433527273	-4.228588992	7.719106159
Al	-0.377290639	-1.095703966	6.283968454
Al	1.328558277	0.857293517	7.420337945
Al	-0.026335585	3.371509119	7.581472603
Al	4.318112847	-4.084380464	7.536363538
Al	2.640952266	-1.590591342	7.543474216
Al	4.226262528	0.796706485	7.601368941
Al	2.823751518	3.310586978	7.565415365
Al	7.117760729	-4.070080631	7.566828904
Al	5.682133227	-1.638917983	7.554951515
Al	-4.334361428	0.822097819	7.572778366
Al	-5.748174139	3.285979057	7.556661441
Al	-1.510030931	-4.193543029	7.713001864
Al	-2.765525085	-1.619675674	7.574390178

Table S6. Crystal lattice vectors in the Cartesian axis of the supercell of the most stable interaction (⊥ normal) between a $[Zn_8Al_4(OH)_{24}](NO_3)_4 \cdot 4\ H_2O \cdot (8 \times 4)$ Al(111)–2L surface.

Vector	x / Å	y / Å	z / Å
1	22.88763	0.00000	0.00000
2	−5.72191	9.91064	0.00000
3	0.00000	0.00000	26.0000

Table S7. Cartesian coordinates of the supercell of the most stable interaction (⊥ normal) between a $[Zn_8Al_4(OH)_{24}](NO_3)_4 \cdot 4\ H_2O \cdot (8 \times 4)$ Al(111)–2L surface.

Atom type	Coordinates / Å		
	x	y	z
Al	-0.047794860	0.211280278	-3.861179096
Al	-1.457715636	2.675881997	-3.963007667
Al	-3.085238797	5.119855120	-3.892901304
Al	1.350660175	-2.160269128	-3.888566039
Al	2.675818603	0.208039102	-2.895189345
Al	1.442796465	2.458228989	-4.099878277
Al	-0.515927952	5.429328320	-3.929138108
Al	4.047926155	-2.023308182	-3.835991874
Al	5.673410256	0.151788143	-3.935437544
Al	4.200775687	2.446167118	-4.010869554
Al	3.191674864	5.252782515	-4.128225399
Al	6.958469239	-2.516371462	-3.935070893
Al	-2.837286361	0.015463900	-3.938501265
Al	-4.177159936	2.485250814	-3.924098697
Al	-5.709206083	5.091080271	-3.924358289
Al	-1.407786857	-2.370380661	-3.903584201
Al	-1.430477020	0.825886290	-6.328081620
Al	-2.860954040	3.303545170	-6.328081620
Al	1.430477020	-4.129431460	-6.328081620
Al	0.000000000	-1.651772580	-6.328081620
Al	1.430477020	0.825886290	-6.328081620
Al	0.000000000	3.303545170	-6.328081620
Al	4.291431060	-4.129431460	-6.328081620
Al	2.860954040	-1.651772580	-6.328081620
Al	4.291431060	0.825886290	-6.328081620
Al	2.860954040	3.303545170	-6.328081620
Al	7.152385090	-4.129431460	-6.328081620
Al	5.721908070	-1.651772580	-6.328081620
Al	-4.291431060	0.825886290	-6.328081620
Al	-5.721908070	3.303545170	-6.328081620
Al	-1.430477020	-4.129431460	-6.328081620
Al	-2.860954040	-1.651772580	-6.328081620
Al	11.600840935	-0.278724472	-4.087194386
Al	9.650287306	2.491938254	-4.046121388
Al	8.645910587	4.976335873	-3.961102320
Al	13.131232058	-2.491461387	-3.328424038
Al	14.397740728	-0.061612016	-3.976882291
Al	13.474995866	2.651412192	-4.007758101
Al	11.499894798	4.839698852	-3.992927195
Al	15.826060045	-2.572458740	-3.967466745
Al	17.265237032	-0.047190686	-3.922222926
Al	16.061144253	2.467449950	-3.875580560
Al	14.459439305	5.113406971	-3.923512714
Al	18.652538277	-2.519227630	-3.920260052
Al	8.487131695	-0.336844423	-3.875938752
Al	6.844016832	2.657752301	-3.129612389
Al	5.949447208	5.089468719	-3.966372674
Al	10.290172473	-2.509748531	-3.219571632
Al	10.013339130	0.825886290	-6.328081620
Al	8.582862110	3.303545170	-6.328081620
Al	12.874293160	-4.129431460	-6.328081620
Al	11.443816150	-1.651772580	-6.328081620
Al	12.874293160	0.825886290	-6.328081620
Al	11.443816150	3.303545170	-6.328081620
Al	15.735247200	-4.129431460	-6.328081620
Al	14.304770180	-1.651772580	-6.328081620
Al	15.735247200	0.825886290	-6.328081620
Al	14.304770180	3.303545170	-6.328081620
Al	18.596201240	-4.129431460	-6.328081620
Al	17.165724220	-1.651772580	-6.328081620
Al	7.152385090	0.825886290	-6.328081620
Al	5.721908070	3.303545170	-6.328081620
Al	10.013339130	-4.129431460	-6.328081620
Al	8.582862110	-1.651772580	-6.328081620
Al	2.661419840	4.707231060	-1.773116510
Zn	0.981235870	2.292082600	-0.987591120
Zn	1.721044100	4.386601020	1.130445610
O	1.567682227	5.645394434	-0.699359415
O	3.245010497	5.686143527	1.865633815
O	1.297343455	3.548412395	-2.500807346

O	3.046558214	3.584781777	-0.432169688
O	2.225862616	0.711040889	-1.147826914
O	0.151726785	3.253118073	0.433291122
H	1.620395050	6.617491777	-0.655266950
H	4.160065248	5.301922317	1.706075327
H	0.417826795	4.073507556	-2.615276692
H	3.865962590	3.060645193	-0.263030917
H	2.977746529	0.798659154	-0.524247009
H	-0.587803033	3.794133252	0.090894571
N	6.033567299	1.525431457	-0.630405467
O	6.656788672	0.462814026	-0.795428704
O	4.960285918	1.616026534	0.016811033
O	6.489324673	2.645522321	-1.217352706
O	5.577193625	4.465890198	1.509365390
H	5.638546673	3.713568400	2.167280117
H	5.930410145	4.138859453	0.660589093
Al	11.907536420	1.974003680	-2.249374370
Zn	10.227352460	-0.441144800	-1.463848980
Zn	10.967160690	1.653373620	0.654187740
O	10.908504438	2.948063755	-1.135442565
O	12.501846815	2.949117664	1.364477131
O	10.752629063	1.216589633	-3.335028320
O	12.040790643	0.587912650	-1.047305299
O	10.254750241	-2.531670515	-1.362202367
O	9.425534535	0.575946399	-0.060469644
H	11.118802771	3.885291739	-0.983095873
H	8.326300162	1.696318602	-3.074745625
H	12.863537070	0.032184757	-0.934455341
H	11.057773255	-2.852996702	-0.898578722
H	8.544670445	0.922242654	-0.310184465
N	14.356311174	-2.028098789	-0.830169498
O	15.286943615	-2.779731921	-0.573058057
O	14.359375016	-0.786643766	-0.640658038
O	13.254903599	-2.544227537	-1.425262372
O	14.727591350	1.421315925	1.439314720
H	14.388268707	0.771255714	2.120525182
H	14.999896826	0.853837950	0.688550805
Al	2.486311290	6.429337050	3.244478060
Zn	0.806127330	4.014188580	4.030003450
Zn	1.545935560	6.108707000	6.148040170
O	2.430666252	7.979500666	3.941781479
O	2.139809930	6.951470503	7.613571919
O	0.835807380	5.787211633	2.688226430
O	2.608870271	5.272547590	4.614972723
O	1.703587761	2.982709366	2.756539579
O	0.019080609	5.059458628	5.391886312
H	1.975848447	8.777066830	3.627470919
H	3.106490727	6.739076204	7.625415035
H	0.035328588	6.337893322	2.622456280
H	3.479859709	4.802844041	4.753852482
H	2.604679234	2.782091742	3.087307837
H	-0.675208916	4.739573337	5.996025443
N	5.909344083	3.265176076	4.626896070
O	6.756896497	2.980735639	5.514126697
O	5.067095439	4.213006269	4.857623309
O	5.874130339	2.639047067	3.516466532
O	4.780277531	5.572943001	7.298973102
H	5.343698885	5.287771798	8.038955273
H	5.116763998	5.082566121	6.505887781
Al	11.732427880	3.696109650	2.768220190
Zn	10.052243920	1.280961190	3.553745580
Zn	10.792052150	3.375479600	5.671782310
O	11.894232515	5.272726926	3.374304664
O	11.510084904	4.219076707	7.092315603
O	10.075376812	3.125535229	2.224630628
O	11.879133101	2.561607937	4.137068903
O	10.932743346	0.283735311	2.251482720
O	9.351496428	2.225597039	5.012542648
H	11.509175339	6.134661496	3.152792666
H	12.489121823	4.092525676	7.032620538
H	9.288990796	3.699069276	2.187851091
H	12.765713949	2.074045417	4.339888025
H	11.824442757	0.050988366	2.624467245
H	8.381338857	2.404288916	5.144049034
N	14.225283677	0.115644071	4.395048932
O	14.960340009	-0.636904699	5.036230894
O	14.043179234	1.349826768	4.776606280

O	13.627057102	-0.268807850	3.308557724
O	14.456897884	3.127769201	6.969851197
H	14.506762852	2.628614791	7.806429142
H	14.516528296	2.429873805	6.272253314
H	13.395094026	2.492346399	1.355078716

Table S8. Crystal lattice vectors in the Cartesian axis of the supercell of the most stable interaction (⊥ normal) between a $[Zn_2Al(OH)_6](NO_3)\cdot H_2O$ unit and a (2 × 2) α-Al_2O_3(0001)–9L surface.

Vector	x / Å	y / Å	z / Å
1	9.52040	0.00000	0.00000
2	−4.76020	8.24491	0.00000
3	0.00000	0.00000	20.0000

Table S9. Cartesian coordinates of the supercell of the most stable interaction (⊥ normal) between a $[Zn_2Al(OH)_6](NO_3)\cdot H_2O$ unit and a (2 × 2) α-Al_2O_3(0001)–9L surface.

Atom type	Coordinates / Å		
	x	y	z
Al	0.000000000	0.000000000	8.417579470
Al	0.033584314	-0.041071054	11.047131648
Al	2.380100000	1.374151380	8.906820530
Al	2.201053699	1.381424729	12.537705378
Al	0.022720057	2.756653880	10.749647319
Al	0.000000000	2.748302750	6.741270530
O	3.302436350	0.000000000	9.744975000
O	-1.651218180	2.859993780	9.744975000
O	0.728881820	1.262460350	9.744975000
O	3.837863650	1.374151380	7.579425000
O	1.651218180	2.636611730	7.579425000
O	1.651218180	0.111691020	7.579425000
O	1.500650693	2.802544961	11.876498327
O	-0.827028894	4.034174828	11.920039322
O	-0.664439201	1.391107821	11.939639887
Al	-2.380100000	4.122454130	8.417579470
Al	-2.357808956	4.098754808	11.013671476
Al	0.000000000	5.496605510	8.906820530
Al	-0.098091545	5.459482845	12.614659196
Al	-2.369173406	6.910140833	10.654479448
Al	-2.380100000	6.870756880	6.741270530
O	0.922336350	4.122454130	9.744975000
O	-4.031318180	6.982447910	9.744975000
O	-1.651218180	5.384914480	9.744975000
O	1.457763650	5.496605510	7.579425000
O	-0.728881820	6.759065860	7.579425000
O	-0.728881820	4.234145150	7.579425000
O	-0.921720535	6.835965581	11.886284380
O	-3.147523910	8.128045771	11.911840072
O	-3.175613734	5.511376851	12.016895451
Al	4.760200000	0.000000000	8.417579470
Al	4.736551071	-0.098227854	11.028292762
Al	7.140300000	1.374151380	8.906820530
Al	7.168383495	1.333281891	11.980372551
Al	4.758891683	2.815947441	10.628819683
Al	4.760200000	2.748302750	6.741270530
O	8.062636350	0.000000000	9.744975000
O	3.108981820	2.859993780	9.744975000
O	5.489081820	1.262460350	9.744975000
O	8.598063650	1.374151380	7.579425000
O	6.411418180	2.636611730	7.579425000
O	6.411418180	0.111691020	7.579425000
O	6.216636301	2.753155190	11.898069503
O	3.962519872	4.000903494	11.870049005
O	3.979385136	1.357718046	12.062536640

Al	2.380100000	4.122454130	8.417579470
Al	2.391748266	4.077173127	10.995441294
Al	4.760200000	5.496605510	8.906820530
Al	4.583862325	5.464234515	12.595244191
Al	2.416966809	6.882319844	10.648700216
Al	2.380100000	6.870756880	6.741270530
O	5.682536350	4.122454130	9.744975000
O	0.728881820	6.982447910	9.744975000
O	3.108981820	5.384914480	9.744975000
O	6.217963650	5.496605510	7.579425000
O	4.031318180	6.759065860	7.579425000
O	4.031318180	4.234145150	7.579425000
O	3.861279843	6.864991301	11.842637799
O	1.545830585	8.115488818	11.914146691
O	1.643932337	5.524961551	11.974489632
H	4.576910303	1.766415871	12.728043875
H	2.074561684	5.815827573	12.817156646
H	-2.661594301	5.859187636	12.779482236
O	0.378335415	5.587713215	14.242368123
H	-0.083021143	5.676798393	15.092534352
O	2.175962278	1.697177666	14.300669109
H	2.800013121	1.255943549	14.942116235
O	4.536566220	5.650121353	14.282614820
H	4.388804020	4.969488799	14.964020949
Al	0.897907261	2.320287585	15.473600700
Zn	1.991008035	1.508726898	17.848324459
Zn	0.371496563	4.211592391	17.569769738
O	-0.567642281	3.239524996	15.662965122
O	0.046760991	5.988725201	17.507939177
O	0.711014717	0.806063362	16.336714630
O	1.888442469	3.411096999	16.449522148
O	3.555302780	0.998324179	17.065815560
O	0.691484680	2.624504130	18.777119707
H	-1.467450348	2.903677935	15.823153804
H	0.772885247	6.456084843	17.050028658
H	-0.113624673	0.275400179	16.430592779
H	2.820417101	3.745366543	16.471471466
H	4.318936093	1.547731269	17.327236152
H	-0.108615487	2.153903475	19.076298570
N	5.435668754	4.760200358	17.103188142
O	6.075713028	5.776123217	17.423724646
O	4.146604316	4.845311865	16.945151998
O	5.992199701	3.643222996	16.917259373
O	2.904020350	7.493690768	16.600013577
H	2.753778867	7.364436745	17.557485344
H	3.320247173	6.644428871	16.322062459