Structural Analysis of Dehydrated Gibbsite-based Layered Double Hydroxides Li-Al-X (X = F^-, Cl^-, Br^-, I^-, OH^-, NO_3^-, CO_3^{2-} and SO_4^{2-}) by DFT calculations

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- ***Cell parameters and atomic positions for all Li-Al-X LDHs.***

Li-Al-F

Cell Parameters

5.159078081	*-0.000043007*	*0.000828018*
-2.579576701	*4.467965121*	*-0.000012860*
-0.001482005	*-0.000710558*	*12.207592192*

Atomic Positions

Al	*-0.002952402*	*2.983939060*	*0.000225723*
Al	*2.578696738*	*1.488765603*	*6.104351531*
O	*-1.622342654*	*2.809855831*	*0.986370493*
O	*-0.965096237*	*1.668368238*	*11.220277553*
Al	*-0.000569532*	*2.978269418*	*6.104062311*
F	*-0.002492318*	*0.001932779*	*3.052007551*
O	*1.921920668*	*-0.000512230*	*7.092353244*
O	*3.234156630*	*0.005640055*	*0.988883149*
H	*1.849522889*	*3.206489703*	*7.960528844*
Al	*2.576658113*	*1.494018001*	*0.000519138*
O	*1.613544115*	*2.808704311*	*11.221027478*
H	*1.451771195*	*-0.000564151*	*7.958293867*
H	*-1.850775483*	*3.206478435*	*4.247984528*
H	*3.705879391*	*-0.000505525*	*4.250179540*
O	*0.957389103*	*1.669737119*	*0.987710224*
H	*0.724085279*	*1.265954407*	*1.855492153*
H	*-0.733229247*	*1.267060089*	*10.351134764*
O	*-1.619645412*	*2.804223077*	*5.116942316*
Li	*-0.000775776*	*-0.000299841*	*6.103788650*
O	*3.235648406*	*-0.000533837*	*5.116153820*
Li	*-0.003037463*	*0.005246451*	*0.000043761*
O	*-0.961431241*	*1.663068853*	*7.090480285*
H	*1.846320758*	*3.213955920*	*10.353668086*
F	*-0.000998944*	*0.000801385*	*9.155665793*
H	*3.700797160*	*0.005700651*	*1.856599765*
O	*1.917183838*	*0.005330311*	*11.219949445*
H	*1.449786476*	*0.006531846*	*10.352558584*
H	*-1.854890529*	*3.212318364*	*1.855057834*
H	*0.728745894*	*1.260507601*	*4.247940423*

O	*0.960034858*	*1.662940515*	*5.116946508*
O	*1.618255401*	*2.804154377*	*7.091548287*
H	*-0.730226479*	*1.260700540*	*7.959492468*

Li-Al-OH

Cell Parameters

5.167655284	*-0.000021700*	*0.000996617*
-2.583869495	*4.475512082*	*-0.000776010*
0.000340846	*-0.002821191*	*12.532821981*

Atomic Positions

Al	*-0.002959591*	*2.944654939*	*0.000467665*
Al	*2.583705864*	*1.422208206*	*6.266978549*
O	*-1.629478670*	*2.761194010*	*1.006485878*
O	*-0.974372697*	*1.628720344*	*11.559032612*
Al	*-0.000233809*	*2.937899252*	*6.266320669*
O	*-0.226883198*	*0.410874055*	*3.132583829*
H	*-0.740624526*	*1.244034375*	*3.134652975*
O	*1.925658757*	*-0.060177496*	*7.256233980*
O	*3.238613914*	*-0.053558124*	*0.989896007*
H	*1.874728283*	*3.173762159*	*8.117456313*
Al	*2.580566318*	*1.429745576*	*-0.000045000*
O	*1.624335288*	*2.758959985*	*11.526055322*
H	*1.436418043*	*-0.030937151*	*8.126516479*
H	*-1.874689744*	*3.173683675*	*4.414437888*
H	*3.730449379*	*-0.030548452*	*4.407070847*
O	*0.969253955*	*1.631821479*	*0.973851856*
H	*0.703689621*	*1.230465386*	*1.853112019*
H	*-0.708493838*	*1.228426975*	*10.679580183*
O	*-1.627368245*	*2.755376692*	*5.259464192*
Li	*-0.000142336*	*-0.016700205*	*6.266161552*
O	*3.241726859*	*-0.060280552*	*5.277725338*
Li	*-0.002518704*	*-0.010463376*	*-0.000164798*
O	*-0.972619622*	*1.625781581*	*7.240148900*
H	*1.873647874*	*3.178633088*	*10.682462403*
O	*0.223988010*	*0.409063585*	*9.399598274*
H	*0.737657242*	*1.242308976*	*9.399220137*
H	*3.728169293*	*-0.025689670*	*1.860028849*
O	*1.924629614*	*-0.056807656*	*11.543764832*
H	*1.435110625*	*-0.027990944*	*10.673696419*
H	*-1.878876352*	*3.181576419*	*1.849834496*
H	*0.706613830*	*1.225828161*	*4.412925753*
O	*0.972327437*	*1.625995526*	*5.292582449*
O	*1.626780815*	*2.755025324*	*7.272999867*
H	*-0.707365024*	*1.224571618*	*8.119668760*

Li-Al-CO_3

Cell Parameters

10.319822664	*-0.054906558*	*-0.014000126*
-2.603871402	*4.510215617*	*-0.003776678*
-0.017892190	*-0.020303947*	*13.855390582*

Atomic Positions

O	*-1.633211336*	*2.877399201*	*1.011173159*
O	*-0.995336999*	*1.697660064*	*12.866349403*
O	*1.915047999*	*0.014462729*	*7.970027283*
H	*1.378352613*	*2.516032005*	*8.941463802*
O	*0.953696578*	*1.720543187*	*1.005514124*
H	*1.674050674*	*0.100254873*	*8.933402381*
O	*3.248238590*	*0.029886577*	*1.001420951*
H	*-1.744026273*	*2.860642259*	*4.958086712*
H	*3.056546081*	*-0.008781907*	*5.028620449*
O	*1.568005479*	*2.815271562*	*12.807439611*
Al	*-0.049583883*	*3.019434337*	*0.002946715*
H	*0.885510774*	*1.474398912*	*1.976244774*
H	*-1.074102271*	*1.610041728*	*11.870803364*
Al	*2.524064052*	*1.493052609*	*6.974121211*
Li	*-0.011789505*	*0.021205817*	*6.944167569*
O	*-1.638229105*	*2.858960150*	*5.960923388*
Al	*-0.053040996*	*3.004525464*	*6.966651173*
O	*1.902973714*	*0.006029910*	*12.857468056*
Al	*2.527682111*	*1.506108314*	*-0.005458034*
Li	*-0.010600772*	*0.037100658*	*0.025287071*
O	*-0.976272090*	*1.704537418*	*7.959659364*
H	*1.375187963*	*2.531901090*	*11.888872806*
O	*0.951792390*	*1.710359239*	*5.963390440*
O	*1.581511721*	*2.814342511*	*8.029354799*
H	*3.023824505*	*0.012676512*	*1.950902588*
H	*1.667338386*	*0.092180605*	*11.892571539*
O	*3.252402910*	*0.012087750*	*5.983691414*
H	*-1.737643411*	*2.876060030*	*2.014688812*
H	*0.887368269*	*1.469295601*	*4.991386790*
H	*-1.053204081*	*1.609299784*	*8.956009245*
O	*3.501309809*	*2.886223704*	*0.912618266*
O	*4.187156445*	*1.644560535*	*12.881074141*
O	*7.101025935*	*-0.003274468*	*8.036570165*
H	*6.949717873*	*2.935156664*	*8.925644646*
O	*6.096275006*	*1.678146328*	*1.012038762*
H	*7.448195723*	*0.088249462*	*8.951344389*
O	*8.377835034*	*0.007200019*	*0.983290184*
H	*3.353558521*	*3.120800844*	*5.132976736*
H	*8.550194528*	*0.042616910*	*4.973320626*
O	*6.751819821*	*2.791479533*	*12.860496813*
Al	*5.186119411*	*3.043154296*	*-0.019345657*
H	*6.258357816*	*1.845525318*	*1.961192830*
H	*4.216439815*	*1.605432636*	*11.912730464*
Al	*7.745177782*	*1.498982202*	*6.948201513*
Li	*5.164947575*	*-0.014587203*	*7.196088656*
O	*3.491850067*	*2.874507966*	*6.060025187*
Al	*5.182409399*	*3.031179494*	*6.971249784*
O	*7.070677847*	*-0.012510265*	*12.793381961*
Al	*7.748407858*	*1.513505728*	*0.002781091*
Li	*5.164378568*	*0.005935250*	*-0.137210342*
O	*4.203785738*	*1.656660948*	*7.947557649*
H	*6.937298448*	*2.930766087*	*11.878067394*
O	*6.086064854*	*1.656570578*	*5.952632906*
O	*6.772254623*	*2.804720908*	*7.941535629*
H	*8.561527053*	*0.061330048*	*1.977224917*

H	*7.376662417*	*0.073870698*	*11.865544618*
O	*8.363835904*	*-0.009401707*	*5.967152461*
H	*3.415090402*	*3.057780660*	*1.862701338*
H	*6.240366708*	*1.809716774*	*5.000458160*
H	*4.198994763*	*1.692134029*	*8.916729191*
C	*-0.022119491*	*-0.166901676*	*3.488879207*
O	*0.195874358*	*-1.452937668*	*3.489091517*
O	*0.989771014*	*0.666247942*	*3.482785250*
O	*-1.244303437*	*0.276968689*	*3.492674650*
C	*-0.191608234*	*0.150929940*	*10.416657033*
O	*-0.222915745*	*-1.143876345*	*10.426541249*
O	*0.959567421*	*0.783284400*	*10.415795696*
O	*-1.307387025*	*0.830551837*	*10.404609759*

Li-Al-Cl

Cell Parameters

5.191000580	*0.000000055*	*-0.000000247*
-2.595500243	*4.495330996*	*0.000529160*
-0.000000740	*0.001792682*	*14.109121125*

Atomic Positions

O	*-1.625757981*	*2.815620497*	*0.983177423*
O	*-0.970719223*	*1.683105707*	*13.126180962*
O	*1.941821135*	*0.005105381*	*8.037213658*
H	*1.787254794*	*3.096912766*	*8.964616713*
O	*0.967350663*	*1.683981642*	*0.982875933*
H	*1.621389737*	*0.004527098*	*8.965870693*
O	*3.249301757*	*0.004207558*	*0.982803624*
H	*-1.783924227*	*3.096107836*	*5.144681305*
H	*3.572895013*	*0.003393898*	*5.144416972*
O	*1.620899150*	*2.818450728*	*13.126878299*
Al	*-0.001775766*	*3.000666781*	*0.000353342*
H	*0.808133583*	*1.406377908*	*1.911884434*
H	*-0.811715760*	*1.407143975*	*12.196964119*
Al	*2.597885517*	*1.502713726*	*7.054733140*
Li	*0.001179229*	*0.002984607*	*7.054565746*
O	*-1.620840626*	*2.817447609*	*6.072467820*
Al	*0.001772062*	*3.001562006*	*7.054915000*
O	*1.940852635*	*0.006474543*	*13.126498735*
Al	*2.593111263*	*1.501818349*	*0.000171392*
Li	*-0.001179878*	*0.002083179*	*0.000004268*
O	*-0.967413276*	*1.684982680*	*8.037288000*
H	*1.783724247*	*3.096656268*	*12.198902371*
O	*0.970774499*	*1.682313723*	*6.071767030*
O	*1.625693551*	*2.816411968*	*8.037592682*
Cl	*0.000196948*	*0.002633258*	*3.528584013*
H	*3.569206574*	*0.003630346*	*1.911649983*
H	*1.618502373*	*0.004288781*	*12.198642500*
O	*3.250022392*	*0.005579748*	*6.072083041*
H	*-1.787056151*	*3.095670772*	*1.910392269*
H	*0.811513414*	*1.405898512*	*5.142739947*
H	*-0.807934892*	*1.406929597*	*8.966108484*
Cl	-0.000170113	0.003529565	10.580532123

Li-Al-Br

Cell Parameters

5.199044716	-0.000107066	-0.000082630
-2.599614840	4.503124330	0.000003761
-0.000272526	-0.000129201	14.765025342

Atomic Positions

Al	-0.003243973	3.007048485	-0.000015574
Al	2.599315679	1.501447347	7.382449517
O	-1.630779563	2.824875439	0.980735009
O	-0.974488676	1.687443626	13.783439335
Al	-0.000151696	3.001430024	7.382480362
Br	-0.001710184	0.002117322	3.691255358
O	1.942199868	-0.000129657	8.363772849
O	3.253595588	0.006363196	0.981524085
H	1.767322253	3.062045557	9.305857562
Al	2.596839151	1.506066478	-0.000045849
O	1.623540138	2.825929646	13.784053437
H	1.662936826	-0.000240614	9.305776352
H	-1.767649856	3.062280840	5.459119782
H	3.535842715	0.000057096	5.459191484
O	0.967098944	1.688175344	0.981256829
H	0.827448857	1.446794076	1.923604078
H	-0.835096523	1.446651350	12.841018288
O	-1.628162109	2.820284553	6.401276750
Li	-0.000150382	-0.000041336	7.382512552
O	3.256484184	-0.000152865	6.401300309
Li	-0.003264171	0.005650945	-0.000001059
O	-0.971793735	1.682827877	8.363642170
H	1.763674265	3.068283820	12.842055599
Br	-0.000833167	0.001695409	11.073772162
H	3.532300628	0.006285589	1.923735645
O	1.939719285	0.006387307	13.783781726
H	1.659943297	0.006527860	12.841913212
H	-1.771361558	3.067720299	1.922667135
H	0.831785368	1.440861952	5.459113164
O	0.971474884	1.682793461	6.401228911
O	1.627766861	2.820149752	8.363850854
H	-0.832248358	1.440731532	9.305756818

Li-Al-NO_3

Cell Parameters

5.195537566	-0.000100888	-0.000010744
-2.597856095	4.499362203	0.000035268
-0.000030043	0.000097162	14.834446828

Atomic Positions

O	1.258173409	0.181741287	11.125559128
O	1.632287664	2.836081129	13.844250595
H	1.682317603	2.894923773	12.862891745
N	-0.000311008	0.008269699	3.708879457

O	*0.509425361*	*-1.156156783*	*3.708920682*
O	*3.266431005*	*0.006607193*	*6.431629959*
H	*3.347920417*	*0.015966708*	*5.450424707*
N	*-0.002022049*	*0.011799534*	*11.125602132*
O	*-0.966598196*	*1.676794863*	*8.406820219*
H	*-0.940779031*	*1.605001308*	*9.387774207*
O	*0.961910900*	*1.675812225*	*6.431969772*
H	*0.929244262*	*1.600949870*	*5.450772796*
Al	*-0.001618558*	*3.006490548*	*-0.001569246*
O	*3.266456559*	*0.006528841*	*0.985692405*
H	*3.347801605*	*0.015920969*	*1.966781604*
O	*3.931476420*	*0.149314342*	*3.708871071*
O	*4.416612586*	*1.017853264*	*11.125566234*
Al	*-0.001640929*	*3.006563074*	*7.418768376*
Al	*2.596143264*	*1.506806379*	*7.417429638*
Li	*-0.001234092*	*0.006368402*	*7.428416304*
O	*-0.670191744*	*4.507470556*	*13.843795541*
H	*-0.744019484*	*4.520948371*	*12.862423477*
O	*0.961907059*	*1.675720711*	*0.985185889*
H	*0.929342632*	*1.600925725*	*1.966578169*
Al	*2.596162379*	*1.506740621*	*-0.000236245*
Li	*-0.001220813*	*0.006308364*	*-0.011066038*
O	*3.559712137*	*2.837786104*	*6.431560575*
H	*3.510569508*	*2.904213844*	*5.450397950*
O	*1.632224597*	*2.836077188*	*8.407436227*
H	*1.682266512*	*2.894792616*	*9.388738684*
O	*-0.670169037*	*4.507335620*	*8.407683204*
H	*-0.744072758*	*4.520893589*	*9.389338466*
O	*-0.484876182*	*-1.164353396*	*11.125623611*
O	*0.753602630*	*1.032444984*	*3.708910570*
O	*3.559737057*	*2.837697477*	*0.985736621*
H	*3.510648650*	*2.903998259*	*1.966872662*
O	*-0.966687690*	*1.676843343*	*13.845082598*
H	*-0.940803730*	*1.605036266*	*12.863629653*

Li-Al-I

Cell Parameters

5.207590409	*-0.000147708*	*-0.000019411*
-2.603922655	*4.510707299*	*0.000004319*
0.000095487	*0.000086639*	*15.771522868*

Atomic Positions

Al	*-0.003251663*	*3.012154902*	*-0.000015935*
Al	*2.603768562*	*1.503937959*	*7.885750162*
O	*-1.634478705*	*2.831404465*	*0.980912511*
O	*-0.975403752*	*1.689860950*	*14.789392925*
Al	*0.000029822*	*3.006648909*	*7.885754839*
I	*-0.000720918*	*0.002040852*	*3.942877400*
O	*1.944335570*	*-0.000051262*	*8.867379653*
O	*3.260139918*	*0.006140200*	*0.982084139*
H	*1.743128686*	*3.020214024*	*9.824330104*
Al	*2.601048800*	*1.508563878*	*-0.000019938*
O	*1.627410203*	*2.832240685*	*14.790359806*
H	*1.720628901*	*-0.000026111*	*9.824516872*

H	*-1.743149815*	*3.020255847*	*5.947239858*
H	*3.487086857*	*0.000011717*	*5.947023107*
O	*0.968358594*	*1.690010361*	*0.981775858*
H	*0.856188782*	*1.496276066*	*1.938708653*
H	*-0.863246200*	*1.495866056*	*13.832706980*
O	*-1.631286907*	*2.826352626*	*6.904142351*
Li	*0.000041877*	*0.000051915*	*7.885761589*
O	*3.263312831*	*-0.000119869*	*6.904257498*
Li	*-0.003311735*	*0.005720423*	*-0.000014494*
O	*-0.972584450*	*1.684515791*	*8.867126288*
H	*1.739180482*	*3.026141407*	*13.833129508*
I	*-0.001725357*	*0.002477498*	*11.828646334*
H	*3.483907817*	*0.006298690*	*1.938895003*
O	*1.941482829*	*0.006514570*	*14.790049956*
H	*1.717800829*	*0.006801692*	*13.832957420*
H	*-1.746524526*	*3.025230368*	*1.938130411*
H	*0.860578976*	*1.490431632*	*5.947214226*
O	*0.972593188*	*1.684326915*	*6.904179385*
O	*1.631283660*	*2.826299486*	*8.867472142*
H	*-0.860639504*	*1.490473680*	*9.824206148*

Li-Al-SO_4

Cell Parameters

10.345088595	*-0.042977569*	*-0.172426582*
-2.604900203	*4.511517294*	*-0.012607307*
-0.207627409	*-0.140146518*	*16.654539088*

Atomic Positions

O	*-1.763930022*	*2.927533241*	*0.943306667*
O	*-1.505822253*	*1.599304469*	*15.478820338*
O	*1.976133742*	*-0.099356385*	*9.257227205*
H	*1.571656959*	*2.656378149*	*10.194141638*
O	*0.826397682*	*1.776395310*	*0.903097995*
H	*1.635940816*	*-0.103030537*	*10.199224865*
O	*3.127338086*	*0.081259201*	*0.888459852*
H	*-1.871849724*	*3.170534106*	*6.390672053*
H	*3.160763783*	*-0.174444042*	*6.265821148*
O	*1.088502214*	*2.735936936*	*15.413376883*
Al	*-0.191738423*	*3.059260494*	*-0.092387387*
H	*0.760003322*	*1.586695027*	*1.894005563*
H	*-1.272398463*	*1.146664935*	*14.626660969*
Al	*2.556618523*	*1.375971792*	*8.217894198*
Li	*0.021095114*	*-0.092131384*	*8.501006150*
O	*-1.615253319*	*2.717234225*	*7.238015940*
Al	*-0.030080686*	*2.883004008*	*8.242460210*
O	*1.426855989*	*-0.107457568*	*15.447963938*
Al	*2.385520273*	*1.545660582*	*-0.129402010*
Li	*-0.142835367*	*0.082455853*	*0.204833046*
O	*-0.945097451*	*1.575782733*	*9.222127844*
H	*0.996437655*	*2.696556208*	*14.446918019*
O	*0.962558491*	*1.590644639*	*7.258802639*
O	*1.654243904*	*2.745375256*	*9.229626239*
H	*2.967770264*	*0.053249376*	*1.849232181*
H	*0.860605613*	*-0.139538495*	*14.628687409*
O	*3.252254502*	*-0.119493384*	*7.231774215*

H	-1.748075964	2.951656457	1.961943079
H	0.671980134	1.139778101	6.418276824
H	-1.045805266	1.425050897	10.214286189
O	3.392806245	2.918103684	0.789270097
O	3.670189809	1.535123208	15.401972209
O	7.123653330	-0.100182596	9.046442661
H	6.803230044	2.679881598	9.978608891
O	5.977604959	1.731859927	0.780983818
H	7.445513990	0.006498403	9.972589261
O	8.258353507	0.063144743	0.715044166
H	3.337776419	2.826077862	6.226486253
H	8.890936461	-0.130875840	6.139615100
O	6.220832551	2.657386093	15.270378008
Al	5.030390192	3.073991744	-0.239002074
H	6.130523330	1.907627953	1.727847670
H	3.710318732	1.388400408	14.443904756
Al	7.759342958	1.375820739	7.952281200
Li	5.187214382	-0.111579947	8.254902471
O	3.484406913	2.711636331	7.178378991
Al	5.191473202	2.906923799	8.025298162
O	6.521544568	-0.127017557	15.296533561
Al	7.605310677	1.557723534	-0.280948604
Li	5.008662642	0.063329977	-0.107200321
O	4.259953443	1.573846535	9.103223432
H	6.497552190	3.109196131	14.427228747
O	6.071334649	1.515261948	7.012393283
O	6.805561834	2.695859332	8.964233295
H	8.483567198	0.032058891	1.702290854
H	6.542581207	-0.079156376	14.326033089
O	8.338368999	-0.143693724	6.965850232
H	3.402200645	2.983114109	1.757813027
H	6.078324781	1.479595705	6.041686948
H	4.365054781	1.613403529	10.068530414
S	0.048735466	-0.137930012	3.920722067
O	0.031332018	-0.090731501	5.447590032
O	0.756505520	1.093319398	3.432312366
O	-1.381449002	-0.209067873	3.461210063
O	0.796209767	-1.374361961	3.517242260
S	-0.545593940	-0.249180353	12.166414709
O	-1.513682598	0.757459042	11.606872545
O	-1.003071226	-1.635662635	11.824895863
O	0.853661996	0.035975460	11.702612812
O	-0.563718519	-0.114514935	13.688603611