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An ab initio investigation of the adsorption properties of water on binary AlSi clusters

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Supporting information

Summary:

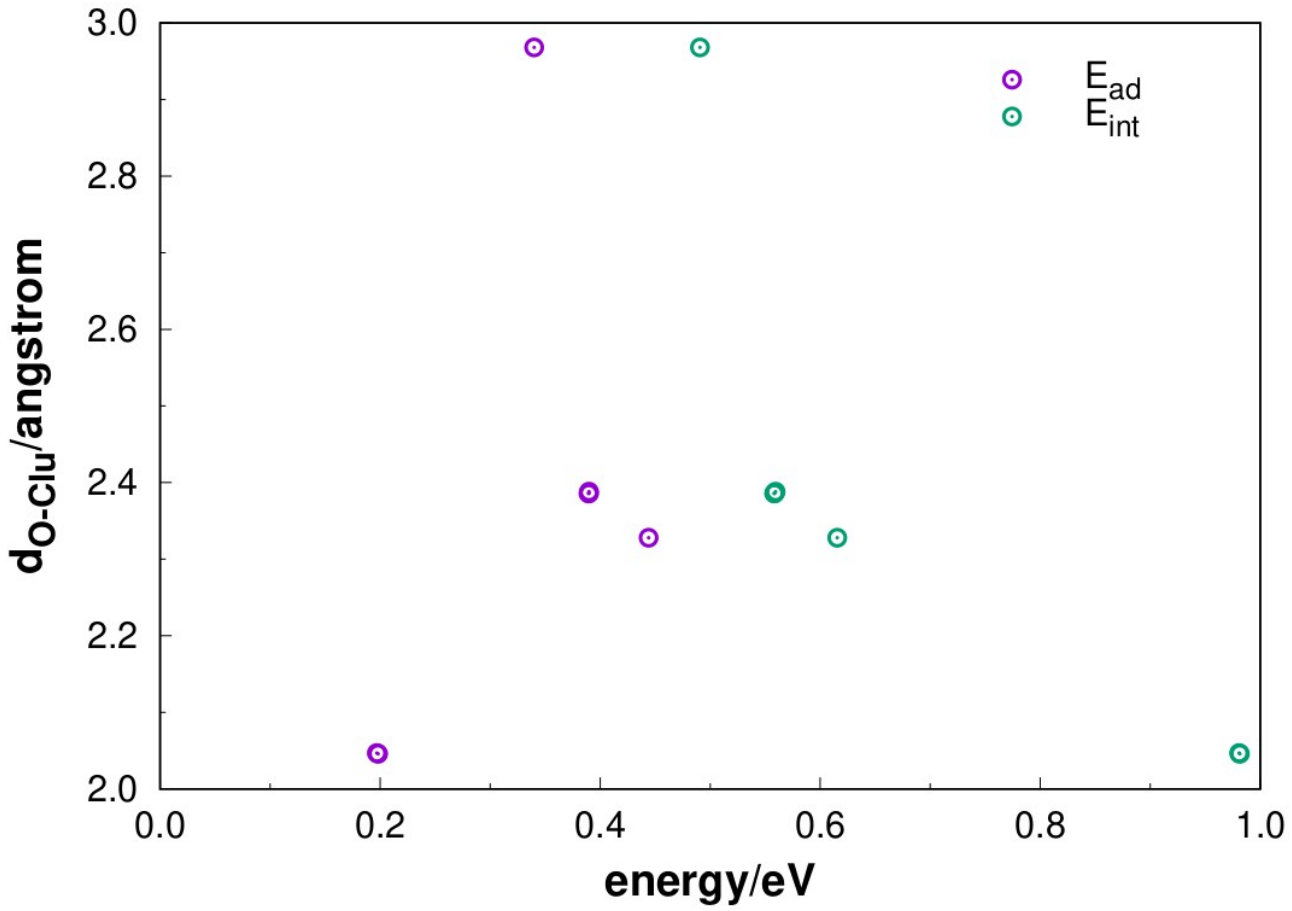

Figure S1: Cluster-oxygen distance as a function of adsorption and interaction energies for different water adsorption sites on the Al_{13} cluster. It is seen that the interaction energy follows a monotonic decrease, with the structure with shorter cluster-water length displaying the highest energy, as expected. This structure shows an anomalous behavior for the adsorption energy.

Cartesian coordinates for the lowest energy configurations

Al_8·H2O

O	2.4162785453	-1.3623710034	1.2228934445
H	3.0059027884	-2.0278273528	0.8277383317
H	2.9477188894	-0.5497017945	1.2996754080
AL	-1.1318944939	-2.3732384467	-1.1124838139
AL	-0.8592929019	0.8428480013	1.3804423961
AL	0.5085072755	1.3095598093	-0.8915798713
AL	0.5696569334	-1.0721424645	0.2669112217
AL	-1.3530954468	0.1256956417	-2.2862479231
AL	-2.7099267118	-0.3525139019	-0.0307423462
AL	-2.5960525009	2.0839600736	-1.0317060663
AL	-0.7978023868	3.3757314279	0.3550992387

Al_2Si_6·H2O

O	0.8329877269	-1.7848992919	1.3587347163
H	0.7984646394	-1.4930821284	2.2904209370
H	0.3136763200	-2.6096895148	1.3245067377
AL	0.1253423129	-0.2638771126	0.1273005144
AL	1.9881493674	0.5116843772	-1.8766293250
SI	0.9868466369	2.0915411027	-0.1887106182
SI	-0.2213399933	-0.7006333263	-2.4489669123
SI	-0.7248170662	1.6225422276	-1.8517003396
SI	-2.1445701933	-0.5350278966	-0.9342579708
SI	-1.8572308638	1.4886354117	0.2975583683
SI	-0.0975088869	1.6728061513	1.9016438921

Al_4Si_4·H2O

O	1.3435663536	1.2032867478	2.4050057920
H	1.5298710695	0.2570873090	2.5504930646
H	0.4456686870	1.3053582277	2.7704254962
SI	-1.7305598425	-1.8393228721	-1.8230896381
AL	-0.6843565827	-0.9378521352	0.3474866553
SI	1.6479647987	-0.7018872155	-0.8023917596
AL	0.5694476972	-2.6519881623	-1.8454623327
SI	-0.2329730609	0.1151540549	-2.1588303915
AL	1.2705191601	1.5484271067	0.2241856480
SI	-1.1610279202	1.5244733142	-0.3708917698
AL	-2.9981203598	0.1772636247	-1.2967307645

Si_8·H2O

O	-0.0234116119	1.4505809815	2.4759990331
H	0.9237419220	1.6257880025	2.5678551118
H	-0.2533970902	2.0253378466	1.7293589584

SI	-0.1213616041	-3.1858121214	-0.5153360062
SI	-0.3307224279	-0.9796769598	0.5711783384
SI	1.1162735149	0.6330187404	-0.7964860762
SI	1.9024199717	-1.6818004382	-0.3375964154
SI	0.1552860611	-1.3724706145	-2.1246011944
SI	-2.0965157653	-1.7250070615	-1.0656148419
SI	-1.2410276655	0.6079138823	-1.2169519368
SI	-0.0312853046	2.6021277420	-1.2878049709

Al_{13}·H2O

O	-3.6171244518	-1.9670934576	0.7743830797
H	-4.2088902941	-1.7834479725	0.0245501027
H	-3.4410151620	-2.9207038762	0.6978368818
AL	0.7837188070	-0.7585807675	2.2754829493
AL	-1.5824215874	-0.7437895330	0.5160816289
AL	-1.3633739971	1.8646110042	-0.8479259571
AL	0.9794521072	3.1742630563	-0.1205609448
AL	2.3434638480	1.5070788449	1.8676836218
AL	0.7745886921	-2.1385771892	-0.1257936663
AL	-0.5853708803	-0.4779209629	-2.1010132881
AL	0.9885619498	1.8055078123	-2.5141125901
AL	3.2140817120	1.7176411458	-0.7157746018
AL	3.1351950244	-0.8145667047	0.6064869807
AL	-0.6544036155	1.5545834591	1.8059004544
AL	0.8445074719	0.5053445375	-0.1060751976
AL	2.3890303758	-0.5243493963	-2.0370494533

Al_2Si_{11}·H2O

O	-2.7332873651	0.7191493244	2.3334325017
H	-2.6380584100	1.5692145011	2.7967532149
H	-2.8460868508	0.0428527827	3.0236153948
SI	1.5179837704	0.6244759382	-2.5809761601
SI	1.0797369753	1.6185790490	-0.2535212632
SI	1.2289785665	0.0764552923	1.6473409032
SI	-1.1001999161	2.5515034516	-0.2352736806
SI	-0.7705188983	1.0123632703	-1.9665137436
SI	-1.0850987075	-1.2917035985	-1.6249131837
SI	1.2000326712	-1.7100327159	-2.2347780079
SI	3.1651778138	1.8100060558	-1.4161406460
SI	2.5227595691	-2.9026372654	-0.7163897862
SI	0.6064634658	-1.8475884378	0.2604355311
SI	-1.7396291870	-2.1308808654	0.4586733240
AL	2.9051731051	-0.4453158702	-0.3296542812
AL	-1.3134266025	0.3035590877	0.8384098830

$Al_{12}Si{\cdot}H2O$

O	0.1665288206	4.0518383209	-0.4145537302
H	1.0396296288	4.3727997070	-0.1291834857
H	0.1266045281	4.2870700591	-1.3579195687
AL	0.4251875978	-1.9901691900	2.5469143238
AL	-2.1481871424	-2.0223098788	1.4851345568
AL	-2.4371625848	0.2450202032	-0.1500523556
AL	-0.0430673574	1.7751068692	-0.0990265495
AL	1.7303462904	0.2990714172	1.5729792799
AL	-0.1680259138	-3.6205686439	0.3882380709
AL	-1.9288471349	-2.2823886051	-1.2782432155
AL	-0.6277526997	0.0073810818	-2.2571850773
AL	1.9413716014	0.0462762029	-1.1903970742
AL	2.2288680503	-2.2278557438	0.4406457370
AL	-0.9790639914	0.4265272673	2.2184605141
AL	0.7754711315	-2.4077457309	-1.9203799421
SI	-0.1019008246	-0.9600533059	0.1445685164

$Si_{13}{\cdot}H2O$

O	-0.9235487736	3.7571291703	-0.3665857868
H	-1.4112616051	3.4024272311	-1.1243480283
H	-1.6201659810	3.8431899438	0.3004214570
SI	0.7708006112	0.6661270094	-1.3377850358
SI	-0.5300502061	0.8677230727	0.9534396506
SI	0.5842977880	-0.9152737294	2.3147791718
SI	-2.9308809065	0.5666403541	0.6228059817
SI	-1.4959141512	-0.0959304043	-1.2396840049
SI	-0.5093570810	-2.2732440520	-1.2777785340
SI	1.7181538558	-1.5017199454	-1.6858666758
SI	1.5623360878	2.0081223393	0.4031932860
SI	3.5615503600	-2.2828915716	-0.2818416832
SI	2.2840705907	-0.3649338270	0.5574557174
SI	1.3184976294	-2.6072419866	0.6129955841
SI	-0.8840691933	-3.7005392701	0.5406411304
SI	-1.4944590250	-1.3695843341	1.0079577699