

Single site Fe on the (110) surface of γ -Al₂O₃: Insights from DFT including periodic boundary approach

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Supporting Information

1. Coordinates of the optimized structures in the manuscript.
XYZ of (110) surface of the supercell of γ -Al₂O₃

Center Number	Atomic Number	Coordinates (Angstroms)			
			X	Y	Z
1	13	O	0.486512	2.055687	7.127500
2	13	O	1.911411	2.058079	4.127108
3	13	O	2.023780	6.236890	1.055552
4	13	O	0.463449	6.236277	6.123542
5	13	O	0.636744	7.685736	3.193700
6	13	O	0.636094	4.787070	3.193256
7	13	O	2.073630	3.494362	1.177724
8	13	O	2.073990	0.622722	1.177538
9	8	O	1.934837	6.235271	7.164877
10	8	O	0.448019	2.057183	5.239442
11	8	O	0.733219	2.057986	0.938033
12	8	O	1.918280	6.236444	3.034772
13	8	O	1.956981	3.353950	7.326534
14	8	O	1.957358	0.758857	7.326142
15	8	O	0.412482	7.626004	5.016363
16	8	O	0.412610	4.846570	5.016352
17	8	O	0.734224	4.936762	1.243490
18	8	O	0.734003	7.537042	1.243169
19	8	O	1.904155	0.673308	2.994856
20	8	O	1.902939	3.443041	2.995055
21	13	O	4.807972	6.237449	1.062842

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22	13	0	6.038096	2.055113	7.126702
23	13	0	7.463348	2.057217	4.126535
24	13	0	3.383376	6.235294	4.063513
25	13	0	8.934691	6.235269	4.063139
26	13	0	7.574899	6.236174	1.054920
27	13	0	3.271047	2.056631	7.134944
28	13	0	8.822557	2.056268	7.134700
29	13	0	6.014855	6.235469	6.122564
30	13	0	4.831218	2.056794	2.066981
31	13	0	4.658233	0.607576	4.996580
32	13	0	6.187727	7.684883	3.192983
33	13	0	6.187256	4.786203	3.192317
34	13	0	4.658685	3.506159	4.997262
35	13	0	3.221323	4.799088	7.012995
36	13	0	8.772605	4.798814	7.012835
37	13	0	7.624356	3.493658	1.176731
38	13	0	7.625109	0.622090	1.176875
39	13	0	3.221019	7.670829	7.013107
40	13	0	8.772059	7.670441	7.012773
41	8	0	7.486023	6.234783	7.164235
42	8	0	3.360057	2.058248	1.025579
43	8	0	8.911422	2.057831	1.025551
44	8	0	5.999575	2.056540	5.238502
45	8	0	4.846521	6.235835	2.951016
46	8	0	4.561614	6.235394	7.252437
47	8	0	6.284564	2.057101	0.937234
48	8	0	3.376474	2.056913	5.155994
49	8	0	8.928200	2.056923	5.155809
50	8	0	7.469598	6.235606	3.033971
51	8	0	7.508220	3.353369	7.325975
52	8	0	3.337898	4.939598	0.864060
53	8	0	8.889150	4.939123	0.863763
54	8	0	3.337624	7.534606	0.864462
55	8	0	8.888629	7.534085	0.864174
56	8	0	7.508803	0.758454	7.325512
57	8	0	5.963801	7.625311	5.015599
58	8	0	4.882298	0.667034	3.173950
59	8	0	4.881420	3.446450	3.174146
60	8	0	5.964502	4.845853	5.015341
61	8	0	4.560808	3.356640	6.946902
62	8	0	6.285173	4.935965	1.242701
63	8	0	6.285061	7.536356	1.242525
64	8	0	4.560866	0.756299	6.947132
65	8	0	3.391119	7.619957	5.195790

66	8	0	8.942697	7.620140	5.195412
67	8	0	7.455154	0.672405	2.994224
68	8	0	7.453851	3.441899	2.994047
69	8	0	3.392133	4.850521	5.195709
70	8	0	8.943346	4.850389	5.195494
71	13	0	10.359841	6.237601	1.063095
72	13	0	10.382867	2.057595	2.067102
73	13	0	10.210270	0.607734	4.997024
74	13	0	10.210544	3.506575	4.997598
75	8	0	10.398558	6.236475	2.951380
76	8	0	10.113094	6.235329	7.252543
77	8	0	10.434970	0.667986	3.174429
78	8	0	10.434041	3.447138	3.174522
79	8	0	10.112009	3.356493	6.947062
80	8	0	10.112395	0.756167	6.947293
81	Tv	0	-0.002394	8.357155	-0.003789
82	Tv	0	-0.161456	0.001762	8.090064

XYZ of (110) surface of the supercell of FeI- γ -Al₂O₃ Doublet

Center	Atomic	Coordinates (Angstroms)			
Number	Number		X	Y	Z

1	13	0	0.744641	2.057385	6.986800
2	13	0	1.955828	2.052854	4.213536
3	13	0	1.770699	6.232033	1.002074
4	13	0	0.543466	6.236053	5.854364
5	13	0	0.812045	7.781915	3.266057
6	13	0	0.818443	4.682611	3.272927
7	13	0	2.013752	3.446101	1.172463
8	13	0	2.011578	0.662498	1.171887
9	8	0	1.787683	6.234953	7.129676
10	8	0	0.576060	2.055873	5.277964
11	8	0	0.832937	2.054554	0.710360
12	8	0	1.886358	6.234424	3.160093
13	8	0	2.073052	3.375776	7.276691
14	8	0	2.072603	0.736704	7.277148
15	8	0	0.154588	7.582042	4.859495
16	8	0	0.155102	4.886676	4.863738
17	8	0	0.733398	4.807921	1.436318
18	8	0	0.729028	7.655315	1.430071
19	8	0	1.927911	0.759619	3.018246
20	8	0	1.931318	3.347552	3.019209
21	13	0	4.678806	6.235107	1.087361
22	13	0	6.174986	2.057595	7.107408
23	13	0	7.429996	2.057171	4.083831
24	13	0	3.422587	6.236711	4.083366
25	13	0	8.897467	6.239327	3.973953
26	13	0	7.448956	6.236566	0.996297
27	13	0	3.400962	2.056320	7.191954
28	13	0	9.073380	2.061126	7.213490
29	13	0	6.007379	6.237530	6.126034
30	13	0	4.836276	2.054797	2.066787
31	13	0	4.682552	0.611306	5.019934
32	13	0	6.166951	7.680208	3.171632
33	13	0	6.169180	4.791269	3.173884
34	13	0	4.681157	3.502744	5.017671
35	13	0	3.238183	4.795253	7.037415
36	13	0	8.835742	4.845499	7.017335
37	13	0	7.629256	3.488409	1.172182
38	13	0	7.631594	0.627795	1.173079
39	13	0	3.235730	7.674333	7.037084
40	13	0	8.837130	7.632028	7.017257

41	8	0	7.453455	6.237941	7.173467
42	8	0	3.401882	2.055389	1.010706
43	8	0	9.025003	2.058532	1.073114
44	8	0	6.039642	2.056331	5.236450
45	8	0	4.818092	6.236090	2.953290
46	8	0	4.515695	6.235832	7.237879
47	8	0	6.331342	2.057065	0.961112
48	8	0	3.463414	2.056087	5.188527
49	8	0	8.937046	2.059683	5.041956
50	8	0	7.393187	6.236979	3.001930
51	8	0	7.619624	3.321131	7.344293
52	8	0	3.234315	4.975085	0.852930
53	8	0	8.784740	4.919163	0.916564
54	8	0	3.231660	7.492295	0.852014
55	8	0	8.785021	7.554141	0.917296
56	8	0	7.622109	0.797027	7.345404
57	8	0	5.947152	7.610715	5.000672
58	8	0	4.901988	0.678861	3.191996
59	8	0	4.906015	3.431632	3.190623
60	8	0	5.945807	4.862871	5.002373
61	8	0	4.656906	3.378579	6.963330
62	8	0	6.197071	4.915161	1.227235
63	8	0	6.195724	7.556494	1.224396
64	8	0	4.657987	0.735499	6.966230
65	8	0	3.355260	7.631527	5.204203
66	8	0	8.936035	7.536133	5.162908
67	8	0	7.493252	0.642762	2.999667
68	8	0	7.496388	3.473329	3.000372
69	8	0	3.354331	4.839561	5.203060
70	8	0	8.933479	4.942897	5.163462
71	13	0	10.102760	6.235752	1.196750
72	26	0	10.494110	2.058693	2.215963
73	13	0	10.000107	0.548299	4.927229
74	13	0	9.995374	3.574251	4.921142
75	8	0	10.290815	6.233479	2.911286
76	8	0	10.019553	6.239095	7.474710
77	8	0	10.735597	0.772471	3.335682
78	8	0	10.738674	3.346281	3.333118
79	8	0	10.113883	3.477845	6.754973
80	8	0	10.117144	0.644988	6.760118
81	Tv	0	-0.002394	8.357155	-0.003789
82	Tv	0	-0.161456	0.001762	8.090064

XYZ of (110) surface of the supercell of FeI- γ -Al₂O₃ Quartet

Center	Atomic	Coordinates (Angstroms)			
Number	Number		X	Y	Z

1	13	0	0.743311	2.057272	6.983495
2	13	0	1.956195	2.056360	4.209977
3	13	0	1.770456	6.233624	0.998888
4	13	0	0.540836	6.236486	5.851722
5	13	0	0.815783	7.783711	3.265522
6	13	0	0.817281	4.684969	3.269072
7	13	0	2.011644	3.447241	1.168391
8	13	0	2.010260	0.663837	1.168646
9	8	0	1.785767	6.235598	7.125815
10	8	0	0.576633	2.057237	5.274404
11	8	0	0.830647	2.055150	0.707187
12	8	0	1.887219	6.235346	3.156602
13	8	0	2.071349	3.376102	7.272518
14	8	0	2.071420	0.737685	7.273158
15	8	0	0.154127	7.583077	4.857074
16	8	0	0.153640	4.887924	4.859820
17	8	0	0.732312	4.810070	1.432576
18	8	0	0.729931	7.657069	1.429324
19	8	0	1.930137	0.762120	3.015555
20	8	0	1.930078	3.350032	3.015170
21	13	0	4.677582	6.235351	1.083947
22	13	0	6.172997	2.058016	7.093923
23	13	0	7.450390	2.056931	4.088284
24	13	0	3.423843	6.236354	4.078360
25	13	0	8.898266	6.236142	3.973770
26	13	0	7.449093	6.236143	0.998236
27	13	0	3.400625	2.057050	7.188237
28	13	0	9.079592	2.059694	7.247370
29	13	0	6.001668	6.237105	6.122871
30	13	0	4.831979	2.055824	2.064610
31	13	0	4.683250	0.611242	5.013027
32	13	0	6.171048	7.681505	3.169425
33	13	0	6.171576	4.789940	3.171048
34	13	0	4.682599	3.503181	5.011342
35	13	0	3.235924	4.795472	7.032148
36	13	0	8.821952	4.843485	7.015993
37	13	0	7.609505	3.489061	1.155175
38	13	0	7.610537	0.626815	1.155329
39	13	0	3.234228	7.675241	7.032088
40	13	0	8.821727	7.631958	7.015975

41	8	0	7.445053	6.237292	7.171219
42	8	0	3.398459	2.056175	1.007082
43	8	0	8.987787	2.057151	1.045974
44	8	0	6.045992	2.056594	5.224480
45	8	0	4.819655	6.236321	2.949608
46	8	0	4.512237	6.235839	7.234073
47	8	0	6.316505	2.057666	0.947886
48	8	0	3.465878	2.057190	5.181015
49	8	0	8.983056	2.057770	5.014634
50	8	0	7.393052	6.235784	3.001164
51	8	0	7.606512	3.325366	7.326074
52	8	0	3.233276	4.975517	0.848106
53	8	0	8.778312	4.916805	0.912264
54	8	0	3.231162	7.493515	0.847693
55	8	0	8.778029	7.555900	0.912676
56	8	0	7.607623	0.791794	7.326113
57	8	0	5.948171	7.610514	4.997185
58	8	0	4.904172	0.677473	3.185514
59	8	0	4.904750	3.435120	3.184241
60	8	0	5.948086	4.862340	4.998763
61	8	0	4.655702	3.378740	6.955177
62	8	0	6.194366	4.916143	1.223824
63	8	0	6.193916	7.555757	1.221476
64	8	0	4.656064	0.736085	6.957677
65	8	0	3.355454	7.631256	5.199046
66	8	0	8.941889	7.536925	5.160241
67	8	0	7.500188	0.647052	2.989915
68	8	0	7.500801	3.468103	2.990512
69	8	0	3.354834	4.839932	5.198228
70	8	0	8.943007	4.936738	5.161013
71	13	0	10.104780	6.235738	1.182627
72	26	0	10.360272	2.054146	2.351119
73	13	0	10.036481	0.533169	4.966932
74	13	0	10.035265	3.583597	4.961814
75	8	0	10.282114	6.233360	2.899313
76	8	0	10.006884	6.238627	7.462570
77	8	0	10.831844	0.770412	3.402537
78	8	0	10.827695	3.345487	3.394814
79	8	0	10.106257	3.479187	6.780373
80	8	0	10.107356	0.639387	6.784553
81	Tv	0	-0.002394	8.357155	-0.003789
82	Tv	0	-0.161456	0.001762	8.090064

XYZ of (110) surface of the supercell of Fe₁-γ-Al₂O₃ Sextet

Center	Atomic	Coordinates (Angstroms)			
Number	Number		X	Y	Z

1	13	0	0.741147	2.056404	6.982781
2	13	0	1.955121	2.056200	4.209196
3	13	0	1.768415	6.234038	0.998004
4	13	0	0.539612	6.236045	5.850684
5	13	0	0.814260	7.783864	3.265125
6	13	0	0.817070	4.685538	3.267404
7	13	0	2.010504	3.447603	1.167540
8	13	0	2.011258	0.663975	1.168801
9	8	0	1.783795	6.235429	7.125924
10	8	0	0.575386	2.055439	5.273591
11	8	0	0.830785	2.055472	0.706301
12	8	0	1.886612	6.235210	3.156413
13	8	0	2.069427	3.376548	7.271827
14	8	0	2.069657	0.737117	7.273256
15	8	0	0.152867	7.583621	4.857154
16	8	0	0.152758	4.888199	4.857660
17	8	0	0.730248	4.810034	1.431086
18	8	0	0.728752	7.657650	1.428874
19	8	0	1.929689	0.761618	3.015307
20	8	0	1.929352	3.350062	3.014439
21	13	0	4.676188	6.236237	1.085326
22	13	0	6.166631	2.057053	7.099963
23	13	0	7.448171	2.057956	4.093413
24	13	0	3.423250	6.234994	4.079070
25	13	0	8.899413	6.237127	3.977069
26	13	0	7.445341	6.235630	1.000550
27	13	0	3.396915	2.057214	7.186723
28	13	0	9.064114	2.059202	7.226695
29	13	0	6.001831	6.237519	6.123071
30	13	0	4.834040	2.055663	2.064552
31	13	0	4.681702	0.611205	5.013991
32	13	0	6.171253	7.682417	3.170736
33	13	0	6.171384	4.789081	3.171367
34	13	0	4.681756	3.503499	5.013177
35	13	0	3.235151	4.795795	7.033783
36	13	0	8.818838	4.844379	7.020021
37	13	0	7.619238	3.485336	1.159586
38	13	0	7.621196	0.629503	1.161375
39	13	0	3.232362	7.674967	7.031572
40	13	0	8.818044	7.629993	7.018968

41	8	0	7.442415	6.236601	7.175589
42	8	0	3.399519	2.056559	1.006768
43	8	0	8.990423	2.058504	1.049393
44	8	0	6.045358	2.057830	5.229662
45	8	0	4.818720	6.235398	2.950410
46	8	0	4.511245	6.236651	7.234827
47	8	0	6.321461	2.056241	0.950694
48	8	0	3.464091	2.056789	5.181989
49	8	0	8.991573	2.057416	5.007088
50	8	0	7.393566	6.236367	3.002669
51	8	0	7.605604	3.324143	7.323241
52	8	0	3.231208	4.975979	0.849460
53	8	0	8.776656	4.916678	0.912301
54	8	0	3.230039	7.493678	0.847662
55	8	0	8.776573	7.555669	0.911491
56	8	0	7.606856	0.792230	7.325543
57	8	0	5.945987	7.611302	4.998480
58	8	0	4.905267	0.678873	3.187408
59	8	0	4.905541	3.432781	3.186905
60	8	0	5.945594	4.863557	4.998762
61	8	0	4.652995	3.378684	6.957453
62	8	0	6.194245	4.913584	1.225886
63	8	0	6.193267	7.556407	1.224763
64	8	0	4.653860	0.736952	6.958589
65	8	0	3.353217	7.631285	5.198485
66	8	0	8.934604	7.534985	5.169224
67	8	0	7.501287	0.649079	2.993887
68	8	0	7.500605	3.466314	2.992830
69	8	0	3.353922	4.839525	5.199971
70	8	0	8.934133	4.939936	5.170062
71	13	0	10.096647	6.236056	1.189380
72	26	0	10.452129	2.054550	2.273715
73	13	0	10.043459	0.519909	4.963690
74	13	0	10.039237	3.597054	4.959499
75	8	0	10.280935	6.237118	2.901364
76	8	0	10.009566	6.237568	7.468555
77	8	0	10.815489	0.723580	3.402897
78	8	0	10.810714	3.390207	3.398775
79	8	0	10.108638	3.477547	6.785095
80	8	0	10.110166	0.640963	6.788764
81	Tv	0	-0.002394	8.357155	-0.003789
82	Tv	0	-0.161456	0.001762	8.090064

XYZ of (110) surface of the supercell of Fe_{II}- γ -Al₂O₃ Doublet

Center	Atomic	Coordinates (Angstroms)			
Number	Number		X	Y	Z

1	13	0	0.911547	2.055272	-1.103028
2	13	0	1.959963	2.058363	4.212881
3	13	0	1.785771	6.234963	1.004111
4	13	0	0.549214	6.235781	5.853806
5	13	0	0.826543	7.783549	3.267161
6	13	0	0.825464	4.687707	3.267230
7	13	0	2.021866	3.448459	1.170583
8	13	0	2.022346	0.664602	1.171942
9	8	0	1.955294	6.234206	-0.960957
10	8	0	0.580498	2.057546	5.278030
11	8	0	0.842166	2.056007	0.710840
12	8	0	1.897901	6.235354	3.156700
13	8	0	2.239638	3.375179	-0.815061
14	8	0	2.240234	0.736206	-0.813996
15	8	0	0.163418	7.581890	4.857721
16	8	0	0.162757	4.889741	4.857878
17	8	0	0.742857	4.811803	1.431076
18	8	0	0.742434	7.657836	1.430895
19	8	0	1.939271	0.763734	3.018594
20	8	0	1.937883	3.351547	3.017255
21	13	0	4.700887	6.235481	1.078486
22	13	0	6.343451	2.055768	-0.978399
23	13	0	7.436523	2.058132	4.111767
24	13	0	3.433649	6.234772	4.081390
25	13	0	8.855196	6.234684	3.998649
26	13	0	7.496547	6.235265	1.015810
27	13	0	3.567766	2.056027	-0.900037
28	13	0	9.259484	2.056319	-0.886108
29	13	0	6.011774	6.236794	6.128934
30	13	0	4.847539	2.056223	2.065214
31	13	0	4.686203	0.610971	5.019208
32	13	0	6.174940	7.684539	3.169824
33	13	0	6.174970	4.786930	3.170487
34	13	0	4.686201	3.503528	5.018494
35	13	0	3.402833	4.795739	-1.053788
36	13	0	9.002048	4.846802	-1.069340
37	13	0	7.630439	3.495689	1.161842
38	13	0	7.631162	0.617840	1.163057
39	13	0	3.402091	7.673267	-1.055058
40	13	0	9.001567	7.622667	-1.070673

41	8	0	7.597189	6.234605	-0.900475
42	8	0	3.412525	2.056566	1.008885
43	8	0	9.078662	2.056990	1.072852
44	8	0	6.042819	2.057631	5.243761
45	8	0	4.823762	6.235286	2.944868
46	8	0	4.677067	6.234854	-0.856656
47	8	0	6.347770	2.056386	0.961319
48	8	0	3.468797	2.057158	5.187192
49	8	0	8.971535	2.057506	5.033488
50	8	0	7.385211	6.235923	3.001727
51	8	0	7.792561	3.315579	-0.736622
52	8	0	3.246340	4.975137	0.851538
53	8	0	8.811834	4.930663	0.907035
54	8	0	3.245696	7.495367	0.850509
55	8	0	8.811166	7.540583	0.905776
56	8	0	7.793037	0.796448	-0.735627
57	8	0	5.948313	7.609563	4.997309
58	8	0	4.915989	0.683675	3.191796
59	8	0	4.914992	3.429547	3.190878
60	8	0	5.949187	4.863289	4.998152
61	8	0	4.824884	3.377533	-1.124777
62	8	0	6.221547	4.913925	1.228842
63	8	0	6.220847	7.556148	1.227800
64	8	0	4.825372	0.734752	-1.123763
65	8	0	3.359403	7.632195	5.200994
66	8	0	8.903859	7.542249	5.167262
67	8	0	7.511316	0.659243	2.992959
68	8	0	7.510319	3.456021	2.991706
69	8	0	3.360269	4.838459	5.202336
70	8	0	8.905265	4.928501	5.168544
71	26	0	10.175798	6.235940	1.198317
72	13	0	10.325186	2.057067	2.348467
73	13	0	10.036277	0.508204	4.930380
74	13	0	10.037049	3.606407	4.930253
75	8	0	10.261399	6.235346	2.932124
76	8	0	10.166303	6.235098	-0.685778
77	8	0	10.704204	0.702362	3.339279
78	8	0	10.704295	3.411886	3.339015
79	8	0	10.286630	3.481673	-1.330518
80	8	0	10.287007	0.631196	-1.330249
81	Tv	0	-0.002390	8.357160	-0.003790
82	Tv	0	-0.161460	0.001760	8.090060

XYZ of (110) surface of the supercell of Fe_{II}- γ -Al₂O₃ Quartet

Center	Atomic	Coordinates (Angstroms)			
Number	Number		X	Y	Z

1	13	0	0.909388	2.055290	-1.103693
2	13	0	1.957165	2.058303	4.212242
3	13	0	1.792606	6.234951	1.005555
4	13	0	0.551659	6.235751	5.854001
5	13	0	0.826300	7.783019	3.266169
6	13	0	0.825408	4.688156	3.266272
7	13	0	2.020757	3.448663	1.168883
8	13	0	2.021179	0.664370	1.170246
9	8	0	1.958677	6.234170	-0.961207
10	8	0	0.578006	2.057533	5.277472
11	8	0	0.839886	2.056014	0.709775
12	8	0	1.899026	6.235370	3.155932
13	8	0	2.238153	3.376464	-0.816095
14	8	0	2.238741	0.734998	-0.815039
15	8	0	0.164471	7.581818	4.857647
16	8	0	0.163840	4.889793	4.857745
17	8	0	0.745524	4.813150	1.429832
18	8	0	0.744978	7.656403	1.429612
19	8	0	1.938157	0.763947	3.017604
20	8	0	1.937011	3.351285	3.016287
21	13	0	4.716346	6.235565	1.076274
22	13	0	6.334266	2.056360	-0.990317
23	13	0	7.426225	2.058432	4.109796
24	13	0	3.435085	6.234887	4.078710
25	13	0	8.868733	6.235351	3.998296
26	13	0	7.538187	6.236204	1.035664
27	13	0	3.564374	2.056115	-0.901941
28	13	0	9.245360	2.056610	-0.875917
29	13	0	6.021356	6.237129	6.134346
30	13	0	4.838192	2.056380	2.067980
31	13	0	4.683911	0.609184	5.017266
32	13	0	6.175636	7.682815	3.169752
33	13	0	6.176101	4.789272	3.170677
34	13	0	4.683844	3.505693	5.016325
35	13	0	3.405202	4.796703	-1.053945
36	13	0	8.989278	4.831848	-1.054639
37	13	0	7.607048	3.492188	1.153271
38	13	0	7.606949	0.621917	1.153872
39	13	0	3.404364	7.672374	-1.055178
40	13	0	8.990076	7.637740	-1.053536

41	8	0	7.622785	6.234416	-0.905351
42	8	0	3.407782	2.056618	1.007831
43	8	0	9.056849	2.057500	1.069521
44	8	0	6.032123	2.058058	5.235557
45	8	0	4.830164	6.235363	2.949014
46	8	0	4.684457	6.234923	-0.858386
47	8	0	6.332006	2.056822	0.954798
48	8	0	3.466059	2.057327	5.185478
49	8	0	8.965142	2.057662	5.027310
50	8	0	7.397375	6.236376	3.009901
51	8	0	7.775738	3.307681	-0.759443
52	8	0	3.251760	4.975165	0.850809
53	8	0	8.796829	4.877018	0.893419
54	8	0	3.250938	7.495319	0.849740
55	8	0	8.794226	7.595831	0.891425
56	8	0	7.775958	0.806037	-0.759365
57	8	0	5.956213	7.611318	5.000587
58	8	0	4.911630	0.679537	3.189453
59	8	0	4.911192	3.434107	3.188348
60	8	0	5.957034	4.861979	5.001634
61	8	0	4.821707	3.377448	-1.127540
62	8	0	6.225740	4.924579	1.230690
63	8	0	6.223616	7.545957	1.229635
64	8	0	4.822229	0.735212	-1.126514
65	8	0	3.361078	7.630338	5.200104
66	8	0	8.935909	7.530050	5.178899
67	8	0	7.504000	0.661871	2.992231
68	8	0	7.503738	3.454308	2.991253
69	8	0	3.361877	4.840481	5.201358
70	8	0	8.936181	4.940436	5.178666
71	26	0	10.265714	6.229543	1.176125
72	13	0	10.294031	2.055424	2.352501
73	13	0	10.034062	0.520339	4.938261
74	13	0	10.034820	3.594794	4.936459
75	8	0	10.249434	6.232598	2.882531
76	8	0	10.179618	6.234196	-0.640155
77	8	0	10.702629	0.703996	3.345388
78	8	0	10.703112	3.407872	3.343837
79	8	0	10.282976	3.476668	-1.324086
80	8	0	10.283826	0.636764	-1.322609
81	Tv	0	-0.002394	8.357155	-0.003789
82	Tv	0	-0.161456	0.001762	8.090064

XYZ of (110) surface of the supercell of Fe_{II}- γ -Al₂O₃ Sextet

Center	Atomic	Coordinates (Angstroms)			
Number	Number		X	Y	Z

1	13	0	0.915591	2.055203	-1.104161
2	13	0	1.963135	2.058307	4.211890
3	13	0	1.797288	6.234908	1.004709
4	13	0	0.558692	6.235705	5.853125
5	13	0	0.833294	7.782948	3.265791
6	13	0	0.832209	4.688180	3.265830
7	13	0	2.026544	3.448529	1.168364
8	13	0	2.027032	0.664430	1.169722
9	8	0	1.964307	6.234135	-0.961135
10	8	0	0.584077	2.057432	5.277101
11	8	0	0.845836	2.055955	0.709194
12	8	0	1.905766	6.235288	3.154925
13	8	0	2.244482	3.376104	-0.816255
14	8	0	2.245075	0.735172	-0.815176
15	8	0	0.171571	7.581896	4.857171
16	8	0	0.170948	4.889594	4.857308
17	8	0	0.750947	4.812919	1.429516
18	8	0	0.750540	7.656606	1.429350
19	8	0	1.944631	0.764193	3.016939
20	8	0	1.943242	3.350966	3.015597
21	13	0	4.719561	6.235380	1.077052
22	13	0	6.342020	2.055792	-0.990005
23	13	0	7.432956	2.058124	4.110790
24	13	0	3.441203	6.234716	4.079380
25	13	0	8.865537	6.234723	4.013645
26	13	0	7.538425	6.235258	1.034344
27	13	0	3.571038	2.056001	-0.901801
28	13	0	9.254695	2.056343	-0.877510
29	13	0	6.026342	6.236800	6.134918
30	13	0	4.844278	2.056199	2.068081
31	13	0	4.688922	0.608868	5.017260
32	13	0	6.181660	7.682994	3.170526
33	13	0	6.181678	4.788462	3.171278
34	13	0	4.688930	3.505573	5.016525
35	13	0	3.410725	4.796633	-1.053865
36	13	0	9.001362	4.837991	-1.054639
37	13	0	7.611008	3.493094	1.152302
38	13	0	7.611777	0.620446	1.153518
39	13	0	3.409899	7.672228	-1.055152
40	13	0	9.000847	7.631544	-1.056039

41	8	0	7.623478	6.234691	-0.897850
42	8	0	3.414164	2.056547	1.007622
43	8	0	9.064849	2.057021	1.069062
44	8	0	6.039307	2.057623	5.236436
45	8	0	4.835429	6.235342	2.948530
46	8	0	4.689043	6.234798	-0.857841
47	8	0	6.337867	2.056388	0.954051
48	8	0	3.472068	2.057149	5.185523
49	8	0	8.976830	2.057626	5.021837
50	8	0	7.403103	6.235827	3.009692
51	8	0	7.785420	3.308057	-0.757049
52	8	0	3.256690	4.975096	0.850588
53	8	0	8.806122	4.881749	0.902119
54	8	0	3.256101	7.495289	0.849522
55	8	0	8.805449	7.589450	0.900894
56	8	0	7.785960	0.803985	-0.756068
57	8	0	5.958038	7.609661	4.999977
58	8	0	4.917779	0.679610	3.189526
59	8	0	4.916749	3.433623	3.188580
60	8	0	5.958938	4.863127	5.000910
61	8	0	4.828307	3.377474	-1.127611
62	8	0	6.230107	4.923717	1.230866
63	8	0	6.229551	7.546392	1.229852
64	8	0	4.828790	0.734822	-1.126611
65	8	0	3.364940	7.630606	5.200213
66	8	0	8.916783	7.541997	5.177549
67	8	0	7.509882	0.663083	2.990928
68	8	0	7.508858	3.452162	2.989676
69	8	0	3.365844	4.839943	5.201550
70	8	0	8.917948	4.928908	5.178936
71	26	0	10.328834	6.236152	1.189399
72	13	0	10.292899	2.057164	2.358185
73	13	0	10.037835	0.513615	4.935457
74	13	0	10.038532	3.601279	4.935195
75	8	0	10.272881	6.235633	2.941029
76	8	0	10.188863	6.235232	-0.678662
77	8	0	10.710786	0.700383	3.340951
78	8	0	10.710704	3.414329	3.340432
79	8	0	10.292882	3.477303	-1.324929
80	8	0	10.293332	0.635651	-1.324568
81	Tv	0	-0.002394	8.357155	-0.003789
82	Tv	0	-0.161456	0.001762	8.090064

XYZ of (110) surface of the supercell of Fe_{III}- γ -Al₂O₃ Doublet

Center	Atomic	Coordinates (Angstroms)			
Number	Number	X	Y	Z	
1	13	0	0.742547	2.071339	6.982870
2	13	0	1.954935	2.071245	4.208643
3	13	0	1.777077	6.249450	0.997914
4	13	0	0.551157	6.247914	5.849785
5	13	0	0.829457	7.797933	3.265502
6	13	0	0.818121	4.702857	3.263757
7	13	0	2.016281	3.462533	1.169199
8	13	0	2.015591	0.679210	1.165579
9	8	0	1.793310	6.250346	7.126911
10	8	0	0.575597	2.062718	5.273582
11	8	0	0.835122	2.071294	0.706691
12	8	0	1.897746	6.247135	3.154042
13	8	0	2.072709	3.390738	7.272053
14	8	0	2.069722	0.747282	7.273954
15	8	0	0.161075	7.592021	4.852640
16	8	0	0.163470	4.898535	4.859042
17	8	0	0.734578	4.827940	1.427982
18	8	0	0.738559	7.673534	1.429962
19	8	0	1.947058	0.775047	3.014088
20	8	0	1.923186	3.362909	3.013986
21	13	0	4.686141	6.257778	1.091561
22	13	0	6.158798	2.038285	7.103311
23	13	0	7.430311	2.090523	4.118396
24	13	0	3.433760	6.242130	4.078546
25	13	0	8.974873	6.082745	3.946637
26	13	0	7.458033	6.214867	0.994367
27	13	0	3.395699	2.066823	7.186219
28	13	0	9.047465	1.996054	7.173677
29	13	0	6.016289	6.224861	6.123210
30	13	0	4.837473	2.050455	2.071452
31	13	0	4.686645	0.610981	5.011738
32	13	0	6.233729	7.675045	3.199850
33	13	0	6.153979	4.785695	3.161451
34	13	0	4.676801	3.506540	5.017850
35	13	0	3.244909	4.808288	7.040417
36	13	0	8.859567	4.778956	7.034748
37	13	0	7.583825	3.481877	1.142180
38	13	0	7.616965	0.600708	1.151563
39	13	0	3.239144	7.685972	7.030315
40	13	0	8.832911	7.567850	7.000716

41	8	0	7.458883	6.188826	7.167213
42	8	0	3.404392	2.064550	1.007883
43	8	0	9.021065	2.021539	1.050380
44	8	0	6.027855	2.059160	5.237794
45	8	0	4.836668	6.240029	2.958435
46	8	0	4.523473	6.249200	7.237568
47	8	0	6.321564	2.035766	0.951079
48	8	0	3.462402	2.059520	5.182203
49	8	0	8.943553	2.032385	5.091277
50	8	0	7.427476	6.198408	3.011828
51	8	0	7.598266	3.294771	7.341495
52	8	0	3.236925	4.992245	0.852281
53	8	0	8.778565	4.897159	0.936964
54	8	0	3.241017	7.509413	0.848962
55	8	0	8.773185	7.533301	0.878899
56	8	0	7.589655	0.761556	7.322739
57	8	0	5.958930	7.613530	5.016140
58	8	0	4.954367	0.675614	3.191210
59	8	0	4.875509	3.437259	3.188219
60	8	0	5.955564	4.854088	4.993483
61	8	0	4.653529	3.384660	6.962236
62	8	0	6.184518	4.913336	1.218621
63	8	0	6.219208	7.546440	1.246783
64	8	0	4.648829	0.741974	6.961140
65	8	0	3.357156	7.639122	5.195744
66	8	0	8.950164	7.411776	5.146004
67	8	0	7.563906	0.665232	3.007032
68	8	0	7.445100	3.440198	2.967313
69	8	0	3.362732	4.852413	5.206444
70	8	0	9.000266	4.810984	5.192780
71	13	0	10.112843	6.233191	1.190903
72	13	0	10.221235	2.173364	2.343437
73	13	0	10.015303	0.440612	4.906555
74	26	0	10.161659	3.468388	4.970689
75	8	0	10.324340	6.452310	2.886174
76	8	0	10.025238	6.185693	7.475503
77	8	0	10.811077	1.031186	3.489521
78	8	0	10.381416	3.679493	3.191461
79	8	0	10.115771	3.412184	6.854302
80	8	0	10.091643	0.570106	6.740519
81	Tv	0	-0.002394	8.357155	-0.003789
82	Tv	0	-0.161456	0.001762	8.090064

XYZ of (110) surface of the supercell of Fe^{III}- γ -Al₂O₃ Quartet

Center	Atomic	Coordinates (Angstroms)			
Number	Number		X	Y	Z

1	13	0	0.742291	2.065057	6.984816
2	13	0	1.951259	2.062158	4.209589
3	13	0	1.776684	6.242156	0.995923
4	13	0	0.548601	6.238787	5.847782
5	13	0	0.820230	7.788312	3.262249
6	13	0	0.824351	4.694012	3.263808
7	13	0	2.018002	3.455256	1.168075
8	13	0	2.015839	0.672163	1.168308
9	8	0	1.791787	6.244807	7.124499
10	8	0	0.573086	2.058315	5.275887
11	8	0	0.835465	2.063710	0.708397
12	8	0	1.896731	6.242212	3.153180
13	8	0	2.071373	3.387511	7.273055
14	8	0	2.070954	0.744873	7.273224
15	8	0	0.156541	7.583238	4.851779
16	8	0	0.162257	4.889998	4.855533
17	8	0	0.737709	4.818495	1.428619
18	8	0	0.735588	7.664359	1.426651
19	8	0	1.935206	0.767093	3.015581
20	8	0	1.932339	3.355353	3.014277
21	13	0	4.686839	6.256987	1.090951
22	13	0	6.158001	2.038794	7.095869
23	13	0	7.444887	2.118822	4.134609
24	13	0	3.433881	6.246688	4.075518
25	13	0	8.957016	6.114982	3.963167
26	13	0	7.461829	6.232373	1.004692
27	13	0	3.396142	2.066223	7.185938
28	13	0	9.040623	2.024395	7.112626
29	13	0	6.010682	6.244744	6.123614
30	13	0	4.840389	2.053973	2.069557
31	13	0	4.682569	0.618742	5.007929
32	13	0	6.224775	7.697445	3.193499
33	13	0	6.169468	4.798383	3.165665
34	13	0	4.679663	3.511477	5.015122
35	13	0	3.244481	4.805936	7.037818
36	13	0	8.815515	4.805886	7.024223
37	13	0	7.581834	3.491719	1.130498
38	13	0	7.617565	0.618507	1.147347
39	13	0	3.237075	7.684335	7.029402
40	13	0	8.839608	7.594112	7.007295

41	8	0	7.451837	6.212414	7.173750
42	8	0	3.404805	2.062278	1.008518
43	8	0	9.020965	2.059793	1.039769
44	8	0	6.018544	2.068927	5.232357
45	8	0	4.838204	6.244158	2.957123
46	8	0	4.520729	6.250237	7.237133
47	8	0	6.319789	2.053062	0.941845
48	8	0	3.459251	2.064073	5.181137
49	8	0	8.903154	1.970975	5.128350
50	8	0	7.424272	6.225828	3.011892
51	8	0	7.600316	3.307004	7.322663
52	8	0	3.239320	4.988319	0.851383
53	8	0	8.775394	4.903448	0.917263
54	8	0	3.238328	7.505364	0.847930
55	8	0	8.789665	7.546201	0.903509
56	8	0	7.594162	0.767995	7.334095
57	8	0	5.959480	7.627319	5.011107
58	8	0	4.925765	0.675118	3.185751
59	8	0	4.906162	3.439316	3.186285
60	8	0	5.960530	4.865425	4.998432
61	8	0	4.651754	3.387385	6.961323
62	8	0	6.193249	4.924268	1.220822
63	8	0	6.218122	7.559240	1.241167
64	8	0	4.650009	0.743066	6.959138
65	8	0	3.358879	7.639871	5.196392
66	8	0	8.948863	7.428432	5.157953
67	8	0	7.531690	0.701977	2.993360
68	8	0	7.494449	3.466526	2.964952
69	8	0	3.363680	4.854002	5.201927
70	8	0	8.973079	4.818172	5.184077
71	13	0	10.115260	6.230469	1.179927
72	13	0	10.187377	2.107840	2.365408
73	13	0	9.982751	0.477513	4.912903
74	26	0	10.357459	3.638302	5.036763
75	8	0	10.324743	6.258505	2.885277
76	8	0	10.016731	6.195831	7.462396
77	8	0	10.702705	0.817832	3.370869
78	8	0	10.618572	3.510124	3.319398
79	8	0	10.145799	3.469737	6.846997
80	8	0	10.114879	0.590660	6.757681
81	Tv	0	-0.002394	8.357155	-0.003789
82	Tv	0	-0.161456	0.001762	8.090064

XYZ of (110) surface of the supercell of Fe^{III}- γ -Al₂O₃ Sextet

Center	Atomic	Coordinates (Angstroms)			
Number	Number		X	Y	Z

1	13	0	0.744107	2.061181	6.985301
2	13	0	1.955440	2.058024	4.210718
3	13	0	1.771338	6.236949	0.997511
4	13	0	0.543237	6.236497	5.850557
5	13	0	0.815140	7.785408	3.264761
6	13	0	0.818438	4.687817	3.267752
7	13	0	2.017042	3.451200	1.170208
8	13	0	2.014374	0.667018	1.170147
9	8	0	1.787835	6.239956	7.125649
10	8	0	0.576265	2.057604	5.276176
11	8	0	0.836162	2.058888	0.709136
12	8	0	1.889298	6.238089	3.157528
13	8	0	2.072280	3.382135	7.274266
14	8	0	2.072845	0.741465	7.274233
15	8	0	0.152770	7.582263	4.855784
16	8	0	0.155126	4.887711	4.859072
17	8	0	0.733943	4.812752	1.431606
18	8	0	0.731489	7.660204	1.428504
19	8	0	1.931057	0.763278	3.016847
20	8	0	1.930919	3.352283	3.016419
21	13	0	4.680649	6.246803	1.088302
22	13	0	6.164937	2.046738	7.100230
23	13	0	7.454132	2.104669	4.123966
24	13	0	3.427582	6.243731	4.078273
25	13	0	8.912606	6.195372	3.968389
26	13	0	7.452210	6.236219	0.998562
27	13	0	3.398923	2.061840	7.188541
28	13	0	9.059095	2.044408	7.146831
29	13	0	6.011592	6.240893	6.123291
30	13	0	4.842198	2.056336	2.068165
31	13	0	4.684395	0.615829	5.013564
32	13	0	6.195393	7.697958	3.180502
33	13	0	6.168250	4.798766	3.167912
34	13	0	4.681794	3.507932	5.014391
35	13	0	3.241269	4.800914	7.035759
36	13	0	8.821550	4.815201	7.028984
37	13	0	7.599000	3.491482	1.146121
38	13	0	7.618310	0.619335	1.151456
39	13	0	3.235750	7.678938	7.032023
40	13	0	8.844647	7.609296	7.017607

41	8	0	7.448662	6.228416	7.179571
42	8	0	3.406367	2.059064	1.009023
43	8	0	9.032347	2.041995	1.047816
44	8	0	6.034550	2.063918	5.233712
45	8	0	4.826275	6.244539	2.953309
46	8	0	4.518253	6.243261	7.236246
47	8	0	6.329287	2.055394	0.948720
48	8	0	3.464019	2.061499	5.183593
49	8	0	8.951679	2.032522	5.099584
50	8	0	7.400361	6.240279	3.004589
51	8	0	7.604320	3.312333	7.332377
52	8	0	3.235341	4.982632	0.850350
53	8	0	8.767641	4.909524	0.918048
54	8	0	3.233610	7.498872	0.848483
55	8	0	8.790321	7.547356	0.916573
56	8	0	7.609042	0.781445	7.333076
57	8	0	5.953245	7.618655	5.003571
58	8	0	4.911487	0.679322	3.188334
59	8	0	4.906388	3.438472	3.186269
60	8	0	5.954735	4.863145	4.998567
61	8	0	4.655118	3.382878	6.960981
62	8	0	6.190042	4.923397	1.224125
63	8	0	6.207624	7.564769	1.231535
64	8	0	4.655573	0.740324	6.962285
65	8	0	3.357275	7.637446	5.199837
66	8	0	8.948839	7.490089	5.168076
67	8	0	7.515482	0.690928	2.995409
68	8	0	7.495341	3.471807	2.976611
69	8	0	3.360379	4.847908	5.200914
70	8	0	8.926774	4.901585	5.185408
71	13	0	10.107498	6.209606	1.196628
72	13	0	10.277039	2.037583	2.303101
73	13	0	10.022751	0.508093	4.930541
74	26	0	10.281238	3.653580	4.966524
75	8	0	10.299916	6.211661	2.907621
76	8	0	10.016611	6.209771	7.473753
77	8	0	10.699117	0.745148	3.350915
78	8	0	10.712795	3.426608	3.247046
79	8	0	10.144641	3.476630	6.867135
80	8	0	10.124484	0.613554	6.770295
81	Tv	0	-0.002394	8.357155	-0.003789
82	Tv	0	-0.161456	0.001762	8.090064

2. d type molecular orbitals of corresponding Fe on γ -Alumina surface.

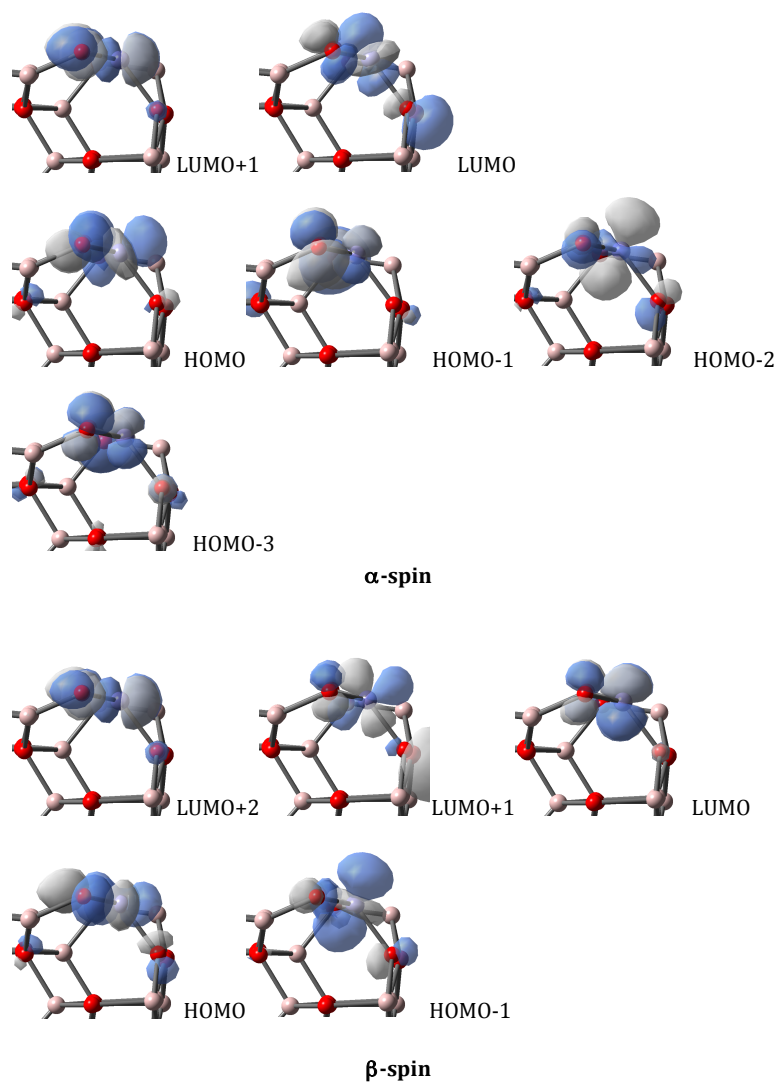


Figure S1. The d orbitals of Fe_i related frontier MO's for the doublet of the Fe_i substituted (110) surface of γ -alumina.

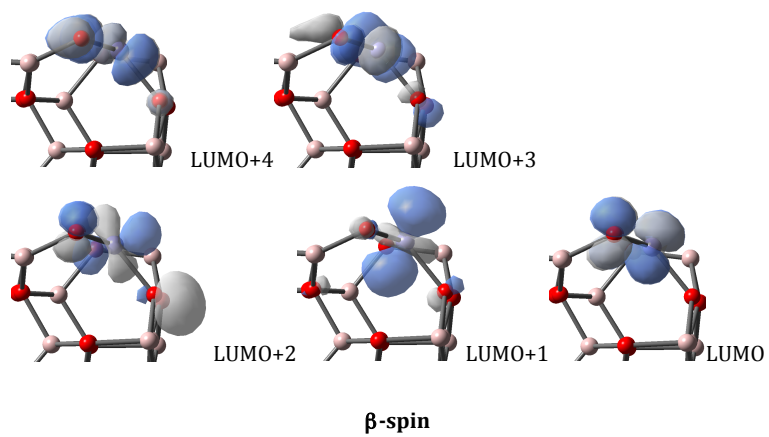
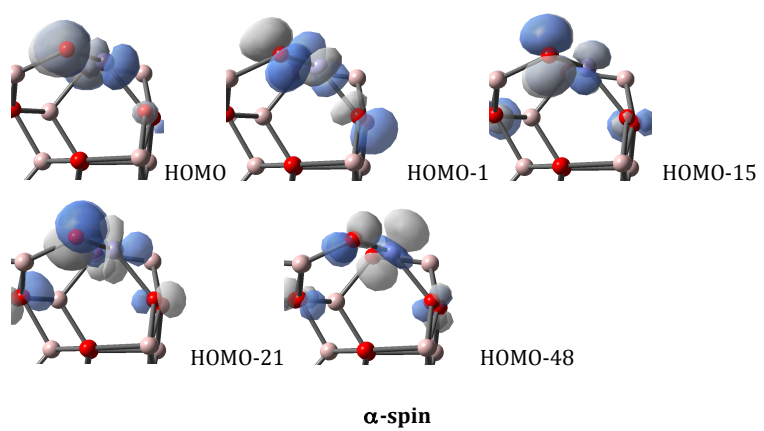


Figure S2. The d orbitals of Fe_I related frontier MO's for the sextet of the Fe_I substituted (110) surface of γ -alumina.

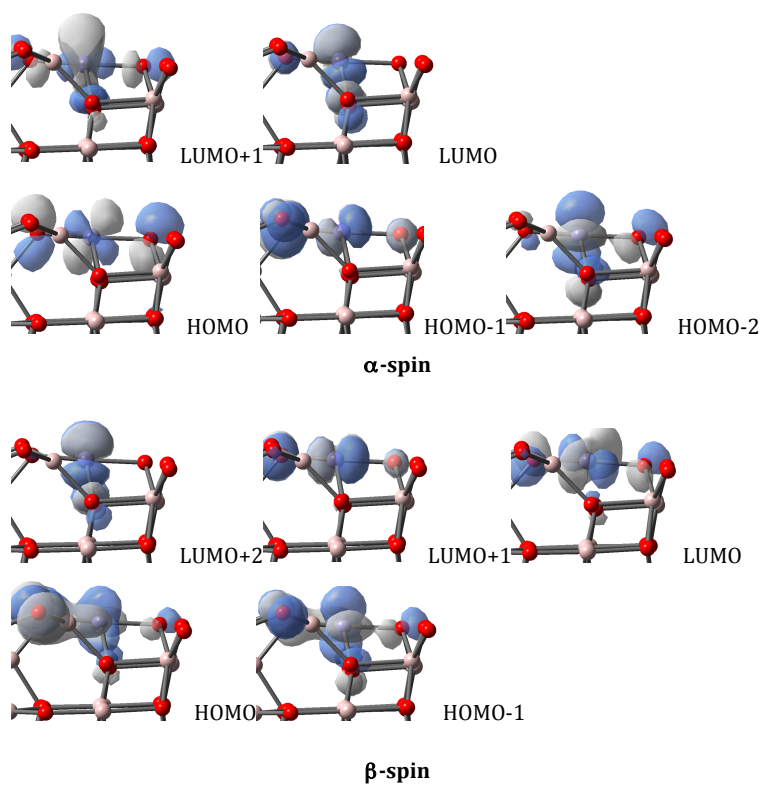
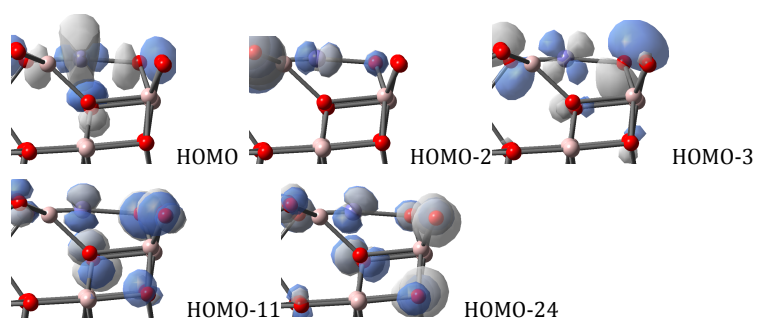
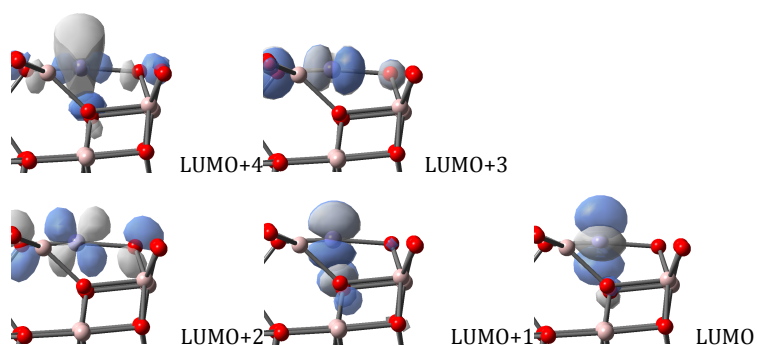


Figure S3. The d orbitals of Fe_{II} related frontier MO's for the doublet of the Fe_{II} substituted (110) surface of γ -alumina.



α -spin



β -spin

Figure S4. The d orbitals of Fe_{II} related frontier MO's for the sextet of the Fe_{II} substituted (110) surface of γ -alumina.

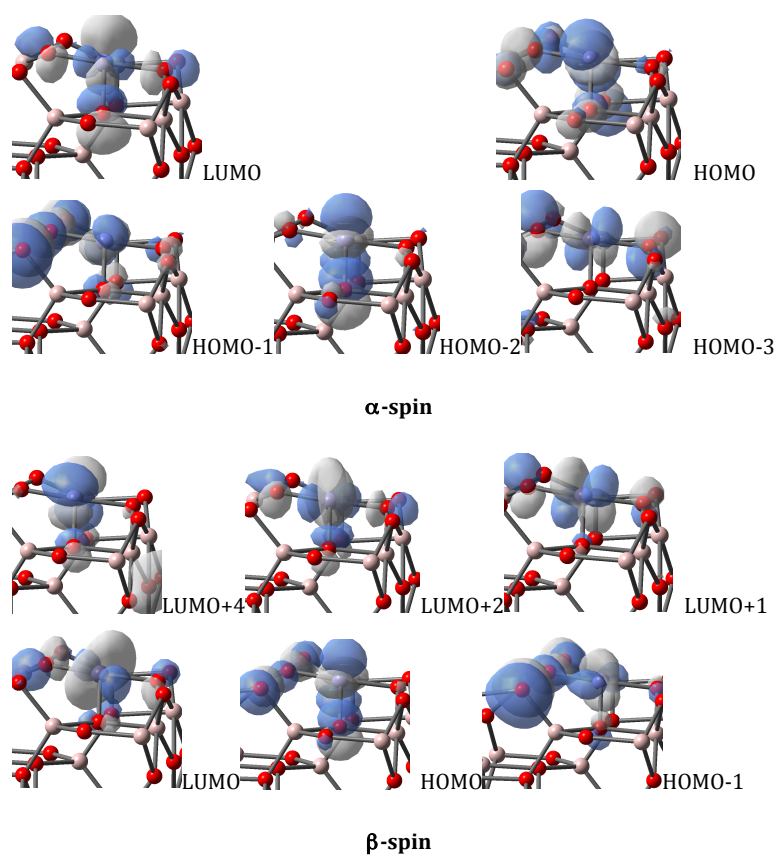


Figure S5. The d orbitals of Fe_{III} related frontier MO's for the quartet of the Fe_{III} substituted (110) surface of γ -alumina.

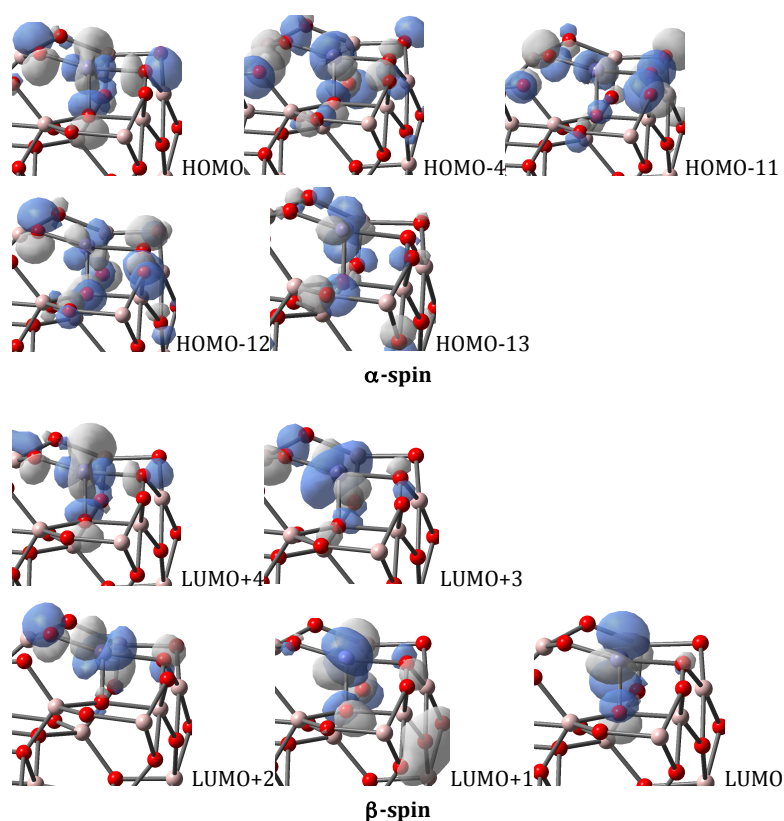


Figure S6. The d orbitals of Fe^{III} related frontier MO's for the sextet of the Fe^{III} substituted (110) surface of γ -alumina.

3. Full citation of Reference 56.

56. Gaussian 09, Revision **D.01**, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.