Supporting Information

First Principles Calculation of Surface Dependent Electronic Structures; A Study on β-FeOOH and γ-FeOOH

Yuki Sakamoto [a,b], Yusuke Noda [a,c], Kaoru Ohno [a,d], Kayo Koike [e], Katsushi Fujii [e], Tomiko M. Suzuki [f], Takeshi Morikawa [f], Shinichiro Nakamura [a]*

[a] Cluster for Science, Technology and Innovation, Nakamura Laboratory, RIKEN, 2-1, Hirosawa, Wako, Saitama 351-0198, Japan

[b] Department of Biological Information, Tokyo Institute of Technology, 4259 Nagatsuta, Midori-ku, Yokohama 226-8501, Japan

[c] Department of Materials Physics, Nagoya University, Furo, Chikusa, Nagoya, Aichi 464-8603, Japan

[d] Department of Physics, Graduate School of Engineering, Yokohama National University, 79-5, Tokiwadai, Hodogaya, Yokohama 240-8501, Japan

[e] Photonics Control Technology Team, RIKEN Center for Advanced Photonics, 2-1 Hirosawa, Wako, Saitama 351-0198, Japan

[f] Toyota Central R&D Labs., Inc., 41-1 Yokomichi, Nagakute 480-1192, Japan

* email: snakamura@riken.jp TEL: +81-(0)48-467-9477.

2019/5/5

Supporting Information

S1. The crystal structures of FeOOH polymorphs electrodes

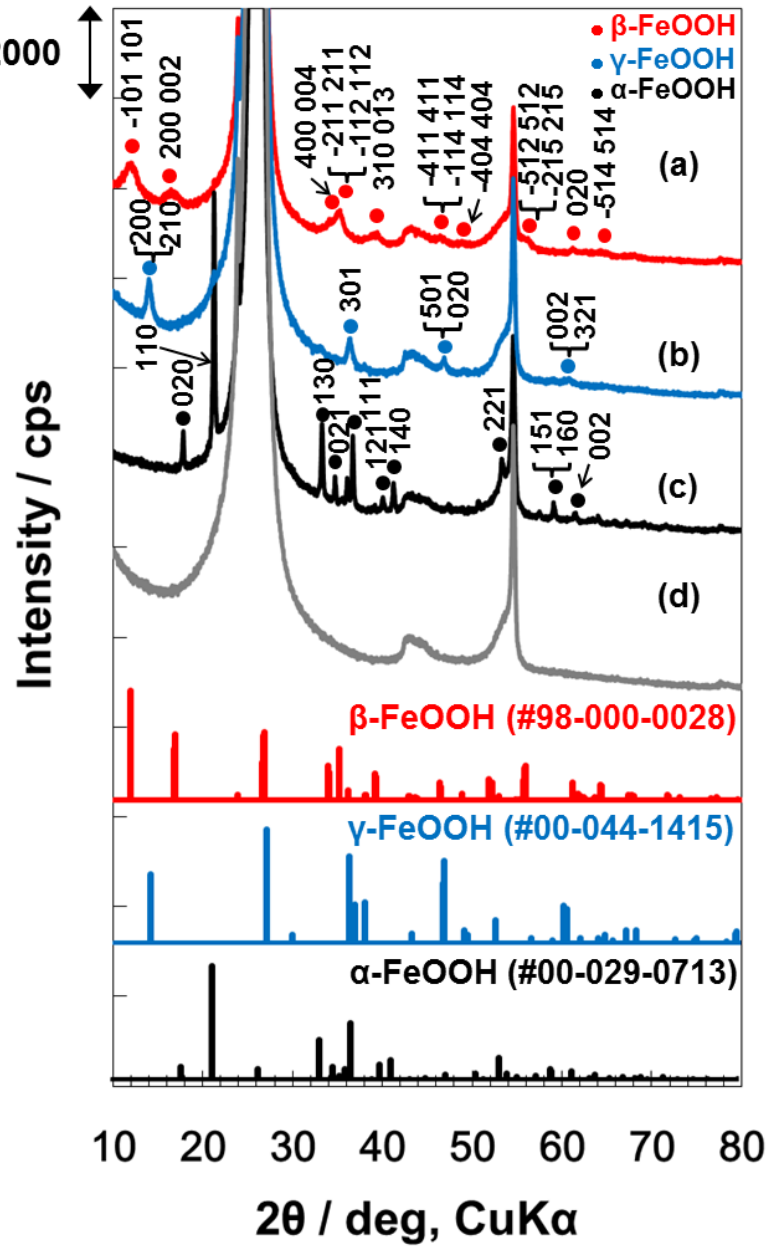

Fig S1. XRD patterns of (a) β-FeOOH (on carbon paper (CP)), (b) γ-FeOOH/CP, and (c) α-FeOOH/CP, and (d) CP support.

S2. Geometrical data of the relaxed unit cells of bulk structures (POSCAR format)

(a) β-FeOOH (bulk)

Relaxed structure of bulk beta-FeOOH. First 4 iron atoms have up-spin and others have down-spin.

```
1.0
   10.654255299     0.000000000     0.002205595
    0.000000000     3.091137789     0.000000000
   -0.000749658     0.000000000    10.667674352
     Fe      O      H
      8     16      8
Direct
    0.854235188     0.019273959     0.351492171
    0.145764812     0.019273959     0.648507829
    0.351225342     0.019027459     0.145474584
    0.648774658     0.019027459     0.854525431
    0.354288320     0.519452681     0.851578067
    0.645711680     0.519452681     0.148421933
    0.851358157     0.518920093     0.645453288
    0.148641843     0.518920093     0.354546712
    0.659283300     0.019797918     0.288798398
    0.340716700     0.019797918     0.711201573
    0.159402161     0.519230349     0.788849967
    0.840597839     0.519230349     0.211150062
    0.669076615     0.019208583     0.034485032
    0.330923385     0.019208583     0.965514942
    0.168758803     0.519074849     0.534515354
    0.831241197     0.519074849     0.465484676
    0.289135667     0.018598400     0.340422454
    0.710864333     0.018598400     0.659577546
    0.789200434     0.518657109     0.840402336
    0.210799566     0.518657109     0.159597664
    0.034479827     0.018826150     0.331741837
    0.965520166     0.018826150     0.668258163
    0.534559054     0.518974127     0.831914629
    0.465440946     0.518974127     0.168085371
    0.415469946     0.020802780     0.658585611
    0.584530084     0.020802780     0.341414389
    0.915290063     0.520604432     0.158449665
    0.084709907     0.520604432     0.841550335
    0.342096464     0.018798655     0.414866644
    0.657903536     0.018798655     0.585133386
    0.842100671     0.518752437     0.914892334
    0.157899329     0.518752437     0.085107636
```

(b) γ-FeOOH

Relaxed structure of bulk gamma-FeOOH. First iron atom has up-spin and second iron atom has down-spin.

```
1.0
        3.9676699638          0.0000000000          0.0000000000
        0.0000000000          3.1183743477          0.0000000000
        0.0000060549          1.5613000636          6.3055390657
    Fe      O      H
     2      4      2
Direct
      0.741659582           0.325934947           0.348409891
      0.241659895           0.674065530           0.651589811
```

0.742468238	0.713725865	0.572466791
0.242468163	0.286273092	0.427534759
0.747900128	0.932466209	0.135694608
0.247903764	0.067534141	0.864305198
0.549966455	0.983794093	0.032769665
0.049973752	0.016206134	0.967229307

S3. Band structures of β- and γ-FeOOH with another parameter

In order to check the influence of Hubbard-*U* parameter for the results described in the section 3.2, we calculated the band structures of β- and γ-FeOOH with 3.0 eV for Hubbard-*U* parameter of Fe. The methods and parameters except Hubbard-*U* parameters are the same described in the section 2.2.

The calculated DOS and band structures of β- and γ-FeOOH are shown in Figs. S1 and S2, respectively. According to the results, the overall electronic structures are similar to that with U = 5.0 eV, although the band gaps became narrower slightly (0.24 eV in β-FeOOH and 0.39 eV in γ-FeOOH),.

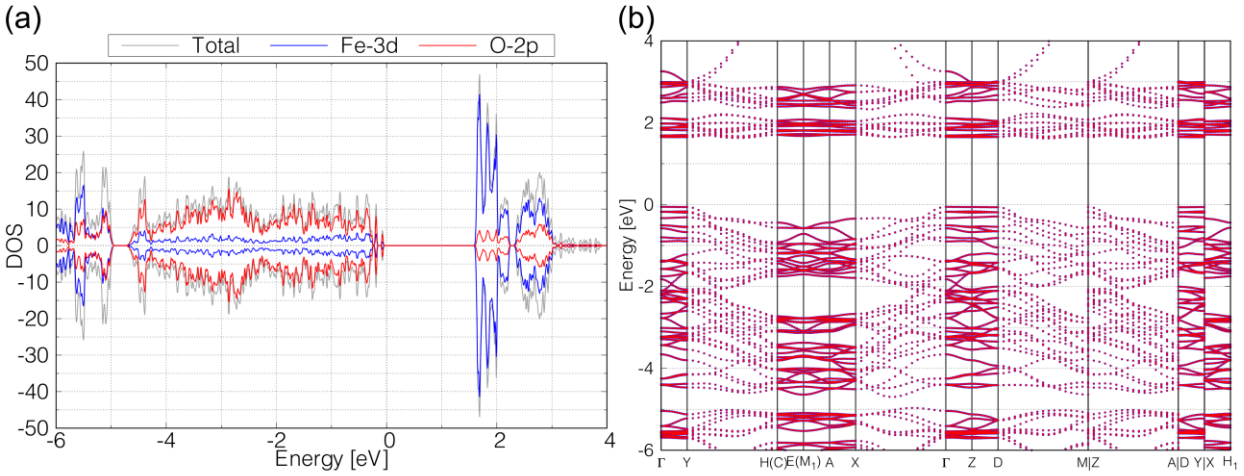

Fig. S2. The calculated (a) total DOS (gray) and Fe-3d (blue) and O-2p (red) partial DOS, (b) band structure of β-FeOOH. In (b), all up- and down- spin bands are degenerated on the calculated reciprocal points.

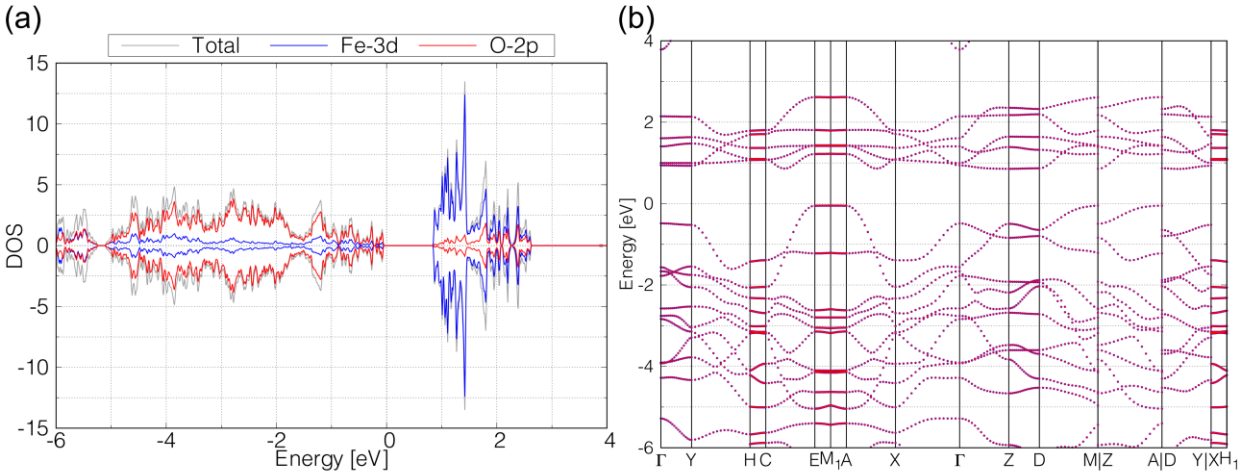

Fig. S3. The calculated (a) total DOS (gray) and Fe-3d (blue) and O-2p (red) partial DOS, (b) band structure of γ-FeOOH. In (b), all up- and down- spin bands are degenerated on the calculated reciprocal points.

S3. Geometrical data of the relaxed unit cells of surface exposed structures (POSCAR format)
(a) The (100) surface exposed structure of β-FeOOH

Relaxed structures of the 100 surface of beta-FeOOH. First 8 iron atoms have up-spin.

```
1.0
        3.0911378860        0.0000000000        0.0000000000
        0.0000000000       10.6676740646        0.0000000000
        0.0000000000        0.0053666414       39.2432247307
 Fe      O      H
 16     34     20
Direct
 0.019273959  0.351492167  0.269310117
 0.021634524  0.644217977  0.078899707
 0.017819168  0.143538691  0.132497933
 0.019027459  0.854525447  0.213529050
 0.022521022  0.357453417  0.538534628
 0.019273959  0.648507833  0.348458320
 0.019027459  0.145474583  0.404239386
 0.018269336  0.858109241  0.485219483
 0.519414717  0.853295551  0.133134870
 0.519452691  0.148421928  0.212697461
 0.518920064  0.645453274  0.268529028
 0.515549076  0.358458049  0.080991388
 0.519452691  0.851578057  0.405070961
 0.519452691  0.148421928  0.484190315
 0.516367615  0.643268147  0.536731720
 0.519412574  0.354573753  0.349294504
 0.010035327  0.607355174  0.030251834
 0.018902075  0.288783290  0.216082939
 0.019805607  0.716610673  0.130330236
 0.519254792  0.783940781  0.078789939
 0.518963942  0.211736162  0.265531180
 0.019138962  0.034584817  0.219614592
 0.018954640  0.965696427  0.125890813
 0.520664241  0.534681460  0.090589405
 0.519124103  0.465487130  0.263009053
 0.016342511  0.337901564  0.118684427
 0.018568337  0.659326483  0.230277638
 0.518617010  0.839818730  0.251628382
 0.516505934  0.165196841  0.093636882
 0.014662958  0.357235551  0.048216890
 0.018922885  0.668105078  0.299527554
 0.518986072  0.834583023  0.182345955
 0.517984201  0.162442184  0.163616494
 0.020048827  0.285247897  0.487018511
 0.019601574  0.711305169  0.401724255
 0.519051446  0.788288002  0.352255093
 0.519816429  0.217873825  0.538582681
 0.019250818  0.036084992  0.491589898
 0.019213281  0.965482394  0.398204375
 0.519219568  0.534598747  0.354868153
 0.521784925  0.467112002  0.526928741
 0.019389935  0.340728476  0.387509843
 0.017101243  0.663922612  0.499083653
```

0.516986894 0.836690054 0.524092692
0.518895246 0.160232377 0.366077802
0.019304998 0.332062222 0.318262246
0.015496085 0.644214142 0.569516794
0.518476587 0.838518430 0.454140993
0.519102838 0.166098894 0.435175836
0.011376983 0.394312413 0.587206062
0.020095695 0.663209131 0.150459843
0.019682855 0.341642894 0.195836689
0.519245642 0.158451872 0.285694585
0.522887836 0.838466706 0.058850793
0.014661623 0.411941205 0.133212460
0.018696785 0.584476739 0.216051133
0.518762292 0.914484634 0.265923460
0.515729348 0.100018275 0.076241110
0.020198044 0.658421674 0.421965232
0.020297907 0.339150787 0.466989685
0.522928042 0.163224362 0.558497177
0.519718784 0.841644757 0.332106444
0.019505336 0.415647114 0.401710134
0.014908277 0.589897096 0.484552691
0.516319277 0.901762911 0.541516929
0.519331576 0.085715245 0.351728395
0.011472252 0.560344905 0.581409131
0.300725370 0.383718060 0.597244640
0.299344044 0.617821840 0.020197293
0.010407981 0.440893254 0.036239497

(b) The (010) surface exposed structure of β-FeOOH

Relaxed structures of the 010 surface of beta-FeOOH. First 16 iron atoms have up-spin.
1.0
10.6676740646 0.0000000000 0.0000000000
0.0014570049 10.6542557674 0.0000000000
0.0000000000 0.0000000000 31.5468273163
Fe O H
32 80 48
Direct
0.351492167 0.854235172 0.099874273
0.648507833 0.145764813 0.099874273
0.145474583 0.351225346 0.099850118
0.854525447 0.648774683 0.099850118
0.351492167 0.854235172 0.197859973
0.648507833 0.145764813 0.197859973
0.145474583 0.351225346 0.197835818
0.854525447 0.648774683 0.197835818
0.351492167 0.854235172 0.295845658
0.648507833 0.145764813 0.295845658
0.145474583 0.351225346 0.295821518
0.854525447 0.648774683 0.295821518
0.350369655 0.854345244 0.395902635
0.649630345 0.145654741 0.395902635
0.145480067 0.350245918 0.395891706
0.854519963 0.649754111 0.395891706
0.850456173 0.354462773 0.146807150
0.149543812 0.645537197 0.146807150

0.645407597	0.850348376	0.146789037
0.354592403	0.149651639	0.146789037
0.851578057	0.354288310	0.246870324
0.148421928	0.645711660	0.246870324
0.645453274	0.851358175	0.246818140
0.354546726	0.148641840	0.246818140
0.851578057	0.354288310	0.344856024
0.148421928	0.645711660	0.344856024
0.645453274	0.851358175	0.344803840
0.354546726	0.148641840	0.344803840
0.851578057	0.354288310	0.442841738
0.148421928	0.645711660	0.442841738
0.645453274	0.851358175	0.442789525
0.354546726	0.148641840	0.442789525
0.776331653	0.132910526	0.060625214
0.223668362	0.867089504	0.060625214
0.519993876	0.165777740	0.063241190
0.480006184	0.834222260	0.063241190
0.867161421	0.776820038	0.060626995
0.132838609	0.223179947	0.060626995
0.834670158	0.520117202	0.063208275
0.165329812	0.479882828	0.063208275
0.308053012	0.672968672	0.105528172
0.691946929	0.327031298	0.105528172
0.784447313	0.151919206	0.147041830
0.215552702	0.848080824	0.147041830
0.024456911	0.648768134	0.101442364
0.975543078	0.351231866	0.101442364
0.538703098	0.165558818	0.148431000
0.461296962	0.834441182	0.148431000
0.326628136	0.308092115	0.105500376
0.673371864	0.691907855	0.105500376
0.848074542	0.784847766	0.147037191
0.151925488	0.215152219	0.147037191
0.351606643	0.024374058	0.101451242
0.648393387	0.975625913	0.101451242
0.834950355	0.538825389	0.148412860
0.165049615	0.461174641	0.148412860
0.286919310	0.662255681	0.196874211
0.713080631	0.337744289	0.196874211
0.788501631	0.159249712	0.246560105
0.211498384	0.840750318	0.246560105
0.036597094	0.667769111	0.197223242
0.963402895	0.332230889	0.197223242
0.534949795	0.168058752	0.246710220
0.465050265	0.831941248	0.246710220
0.337497793	0.287177303	0.196843121
0.662502207	0.712822667	0.196843121
0.840611935	0.788847885	0.246538294
0.159388095	0.211152100	0.246538294
0.332773492	0.036557717	0.197219687
0.667226538	0.963442254	0.197219687
0.832572028	0.534996488	0.246703205
0.167427942	0.465003542	0.246703205
0.288458194	0.659140856	0.296094035
0.711541747	0.340859114	0.296094035

0.787026591	0.162306534	0.345807613
0.212973424	0.837693496	0.345807613
0.034909165	0.668419001	0.295986412
0.965090824	0.331580999	0.295986412
0.536618640	0.167651413	0.345452766
0.463381420	0.832348587	0.345452766
0.340664843	0.288765812	0.296052040
0.659335157	0.711234158	0.296052040
0.837492701	0.787290913	0.345785054
0.162507329	0.212709072	0.345785054
0.332243851	0.034917118	0.295953405
0.667756179	0.965082853	0.295953405
0.832858312	0.536629473	0.345439813
0.167141658	0.463370557	0.345439813
0.284412800	0.651905524	0.395665794
0.715587141	0.348094446	0.395665794
0.808327636	0.172989136	0.437187574
0.191672379	0.827010894	0.437187574
0.038655422	0.665268480	0.394297188
0.961344567	0.334731520	0.394297188
0.524503635	0.149002695	0.441235785
0.475496425	0.850997305	0.441235785
0.348032304	0.284728191	0.395603988
0.651967696	0.715271779	0.395603988
0.826657026	0.808452289	0.437160776
0.173343004	0.191547696	0.437160776
0.335213983	0.038723930	0.394264888
0.664786047	0.961276041	0.394264888
0.851374035	0.524483312	0.441249691
0.148625935	0.475516718	0.441249691
0.276271778	0.632923404	0.482102843
0.723728163	0.367076566	0.482102843
0.019958253	0.665387979	0.479513979
0.980041736	0.334612021	0.479513979
0.367065234	0.276766571	0.482012504
0.632934766	0.723233399	0.482012504
0.335001337	0.020073930	0.479495060
0.664998693	0.979926041	0.479495060
0.695168062	0.377005653	0.079328317
0.304831938	0.622994347	0.079328317
0.166279443	0.923600623	0.141361948
0.833720572	0.076399340	0.141361948
0.376556155	0.304992887	0.079302683
0.623443875	0.695007143	0.079302683
0.923416684	0.834298801	0.141366986
0.076583271	0.165701214	0.141366986
0.653446811	0.405598946	0.192071917
0.346553189	0.594401054	0.192071917
0.157516878	0.914524231	0.246573206
0.842483137	0.085475732	0.246573206
0.405075766	0.347054069	0.191996794
0.594924264	0.652945961	0.191996794
0.914123273	0.843110328	0.246534645
0.085876682	0.156889687	0.246534645
0.657601737	0.414669078	0.296144382
0.342398263	0.585330922	0.296144382

0.153347923 0.905550504 0.350614255
0.846652092 0.094449459 0.350614255
0.414204755 0.342996442 0.296070544
0.585795275 0.657003588 0.296070544
0.905107685 0.847159654 0.350585169
0.094892270 0.152840361 0.350585169
0.666309698 0.423574938 0.401398768
0.333690302 0.576425062 0.401398768
0.195001798 0.876889299 0.463405453
0.804998217 0.123110664 0.463405453
0.423366955 0.334161204 0.401302806
0.576633075 0.665838826 0.401302806
0.876354946 0.805188460 0.463404260
0.123645009 0.194811555 0.463404260
0.827575000 0.209819905 0.060732236
0.172425015 0.790180125 0.060732236
0.456204157 0.099536807 0.071647484
0.543795903 0.900463193 0.071647484
0.790288366 0.828055030 0.060758976
0.209711664 0.171944955 0.060758976
0.900683691 0.456122975 0.071660810
0.099316279 0.543877055 0.071660810
0.327385138 0.709915797 0.482054826
0.672614803 0.290084173 0.482054826
-0.043943082 0.599310366 0.471041238
1.043943071 0.400689634 0.471041238
0.290179333 0.327988382 0.481889985
0.709820667 0.672011588 0.481889985
0.400903581 -0.044001011 0.471010157
0.599096449 1.044000982 0.471010157

(c) The (010) surface exposed structure of γ -FeOOH

Relaxed structures of the 010 surface of gamma-FeOOH. First 16 iron atoms have up-spin.
1.0
7.9362406731 0.0000000000 0.0000000000
0.0000000000 6.2380423546 0.0000000000
-0.0000396628 0.0000000000 37.2328033447
Fe O H
32 64 32
Direct
0.129235938 0.000000000 0.228456363
0.128939899 0.250002978 0.058286289
0.129098598 0.000000000 0.567940292
0.129229978 0.250000000 0.397885591
0.129235938 0.500000000 0.228456363
0.128939899 0.749997022 0.058286289
0.129107945 0.500000000 0.567933366
0.129229978 0.750000000 0.397885591
0.629235923 0.000000000 0.228456363
0.628939735 0.250003044 0.058286218
0.629098230 0.000000000 0.567940286
0.629229963 0.250000000 0.397885591
0.629235923 0.500000000 0.228456363
0.628939735 0.749996956 0.058286218
0.629106442 0.500000000 0.567933361

0.629229963	0.750000000	0.397885591
0.379085700	0.000000000	0.109794780
0.379230231	0.250000000	0.279818624
0.379235923	0.000000000	0.449249595
0.378951925	0.250003785	0.619449156
0.379093238	0.500000000	0.109800945
0.379230231	0.750000000	0.279818624
0.379235923	0.500000000	0.449249595
0.378951925	0.749996215	0.619449156
0.879086423	0.000000000	0.109794785
0.879230201	0.250000000	0.279818624
0.879235923	0.000000000	0.449249595
0.878951728	0.250003102	0.619449168
0.879093954	0.500000000	0.109800953
0.879230201	0.750000000	0.279818624
0.879235923	0.500000000	0.449249595
0.878951728	0.749996898	0.619449168
0.128685902	0.000000000	0.096310705
0.378828693	0.000000000	0.241864230
0.128833667	0.249910947	0.266390124
0.378990600	0.249917337	0.071764547
0.129615739	0.000000000	0.022317912
0.375885451	0.000000000	0.315843757
0.125950183	0.249914984	0.192353309
0.375918063	0.249909007	0.145867834
0.128824664	0.000000000	0.435839559
0.378698108	0.000000000	0.581426398
0.129002568	0.249919316	0.605970139
0.378832339	0.249912806	0.411314804
0.125902387	0.000000000	0.361860118
0.379624804	0.000000000	0.655417356
0.125925627	0.249907332	0.531864478
0.375954228	0.249914738	0.485358046
0.128690980	0.500000000	0.096311790
0.378835482	0.500000000	0.241865576
0.128833667	0.750089053	0.266390124
0.378990600	0.750082663	0.071764547
0.129519419	0.500000000	0.022312902
0.376257526	0.500000000	0.315852815
0.125950183	0.750085016	0.192353309
0.375918063	0.750090993	0.145867834
0.128836056	0.500000000	0.435837827
0.378702853	0.500000000	0.581424488
0.129002568	0.750080684	0.605970139
0.378832339	0.750087194	0.411314804
0.126252350	0.500000000	0.361849979
0.379513261	0.500000000	0.655421821
0.125925627	0.750092668	0.531864478
0.375954228	0.750085262	0.485358046
0.628685911	0.000000000	0.096310709
0.878828708	0.000000000	0.241864226
0.628833654	0.249910944	0.266390126
0.878990784	0.249917360	0.071764544
0.629616628	0.000000000	0.022317746
0.875885434	0.000000000	0.315843761
0.625950120	0.249914985	0.192353306

0.875918214	0.249909008	0.145867835
0.628824636	0.000000000	0.435839537
0.878698190	0.000000000	0.581426326
0.629002407	0.249919406	0.605970111
0.878832363	0.249912802	0.411314776
0.625902286	0.000000000	0.361860112
0.879626291	0.000000000	0.655417536
0.625925782	0.249907315	0.531864529
0.875954066	0.249914737	0.485358031
0.628691009	0.500000000	0.096311791
0.878835492	0.500000000	0.241865572
0.628833654	0.750089056	0.266390126
0.878990784	0.750082640	0.071764544
0.629520263	0.500000000	0.022312704
0.876257494	0.500000000	0.315852819
0.625950120	0.750085015	0.192353306
0.875918214	0.750090992	0.145867835
0.628836026	0.500000000	0.435837802
0.878702924	0.500000000	0.581424371
0.629002407	0.750080594	0.605970111
0.878832363	0.750087198	0.411314776
0.626252256	0.500000000	0.361849972
0.879511793	0.500000000	0.655421468
0.625925782	0.750092685	0.531864529
0.875954066	0.750085263	0.485358031
0.224528864	0.249904802	0.174888982
0.474514424	0.249903029	0.163328029
0.230734540	0.000000000	0.007351736
0.474790699	0.000000000	0.333285883
0.224507235	0.249898662	0.514403126
0.474519684	0.249903507	0.502823365
0.224803166	0.000000000	0.344416745
0.480727657	0.000000000	0.670388626
0.224528864	0.750095198	0.174888982
0.474514424	0.750096971	0.163328029
0.230533374	0.500000000	0.007315262
0.475240812	0.500000000	0.333276992
0.224507235	0.750101338	0.514403126
0.474519684	0.750096493	0.502823365
0.225237901	0.500000000	0.344426934
0.480510591	0.500000000	0.670424090
0.724528784	0.249904798	0.174888987
0.974514475	0.249903032	0.163328055
0.730734246	0.000000000	0.007351849
0.974790685	0.000000000	0.333285883
0.724507637	0.249898723	0.514403241
0.974519626	0.249903613	0.502823317
0.724803099	0.000000000	0.344416750
0.980725742	0.000000000	0.670388203
0.724528784	0.750095202	0.174888987
0.974514475	0.750096968	0.163328055
0.730532269	0.500000000	0.007315329
0.975240781	0.500000000	0.333276992
0.724507637	0.750101277	0.514403241
0.974519626	0.750096387	0.502823317
0.725237843	0.500000000	0.344426939

0.980513499 0.500000000 0.670423987

(d) The (001) surface exposed structure of γ -FeOOH

Relaxed structures of the 001 surface of gamma-FeOOH. First 8 iron atoms have up-spin.

```
1.0
        3.1190211773          0.0000000000          0.0000000000
        0.0000000000         12.6164026260          0.0000000000
        0.0000000000         -0.0000405935         33.8724822998
   Fe    O    H
   16   36   20
Direct
  0.000000000  0.684452397  0.119537075
  0.500000000  0.184415419  0.119535662
  0.000000000  0.674207330  0.235995933
  0.500000000  0.174217209  0.235994533
  0.000000000  0.674207330  0.353144735
  0.500000000  0.174217209  0.353143334
  0.000000000  0.671488089  0.470457232
  0.500000000  0.171483538  0.470450799
  0.000000000  0.328274480  0.177186554
  0.500000000  0.828287237  0.177194777
  0.000000000  0.325799704  0.294570327
  0.500000000  0.825784683  0.294568986
  0.000000000  0.325799704  0.411719114
  0.500000000  0.825784683  0.411717772
  0.000000000  0.314048725  0.528375841
  0.500000000  0.814067131  0.528377564
  0.000000000  0.285288575  0.121707518
  0.000000000  0.712454939  0.177437883
  0.500000000  0.785327742  0.121716422
  0.500000000  0.212438993  0.177433917
  0.000000000  0.081546595  0.121593491
  0.000000000  0.932049826  0.177474914
  0.500000000  0.581588855  0.121589524
  0.500000000  0.432047237  0.177461355
  0.000000000  0.284951313  0.236053624
  0.000000000  0.713643053  0.294597234
  0.500000000  0.784944180  0.236055885
  0.500000000  0.213664650  0.294593515
  0.000000000  0.068780475  0.235830198
  0.000000000  0.931920861  0.294019762
  0.500000000  0.568771491  0.235826155
  0.500000000  0.431934230  0.294018176
  0.000000000  0.286959204  0.353058299
  0.000000000  0.715211937  0.411314673
  0.500000000  0.786947028  0.353058024
  0.500000000  0.215228456  0.411311876
  0.000000000  0.067987113  0.352625106
  0.000000000  0.931948573  0.411043715
  0.500000000  0.567981643  0.352627956
  0.500000000  0.431962740  0.411048608
  0.000000000  0.287041618  0.469522214
  0.000000000  0.712914891  0.526116704
  0.500000000  0.787044046  0.469522998
  0.500000000  0.212897808  0.526111734
```

0.000000000	0.066636636	0.468957684
0.000000000	0.928053195	0.524212737
0.500000000	0.566638856	0.468964638
0.500000000	0.428037001	0.524216667
0.000000000	0.338152516	0.582583410
0.500000000	0.838183479	0.582584390
0.000000000	0.679362675	0.065942228
0.500000000	0.179293725	0.065941295
0.500000000	0.523609134	0.142078366
0.500000000	0.484035994	0.200274004
0.000000000	0.023585397	0.142089856
0.000000000	0.984048980	0.200284829
0.500000000	0.517068420	0.258895086
0.500000000	0.483198308	0.317260395
0.000000000	0.017078309	0.258898722
0.000000000	0.983190662	0.317260138
0.500000000	0.516454832	0.375848237
0.500000000	0.483607857	0.434466137
0.000000000	0.016454552	0.375843398
0.000000000	0.983595490	0.434460147
0.500000000	0.514955902	0.492577805
0.500000000	0.456949256	0.551127759
0.000000000	0.014953773	0.492571572
0.000000000	0.956980697	0.551121905
0.000000000	0.271617010	0.597367589
0.500000000	0.771651423	0.597371232
0.000000000	0.604318345	0.058146545
0.500000000	0.104241427	0.058155189

References.

1. T. M. Suzuki, T. Nonaka, A. Suda, N. Suzuki, Y. Matsuoka, T. Arai, S. Sato and T. Morikawa, *Sustainable Energy & Fuels*, 2017, **1**, 636-643.