Supporting Information:

A First Principles Study on the Role of an Al_2O_3 Overlayer on Fe_2O_3 for Water Splitting

Ofer Neufeld[1], Natav Yatom[2], and Maytal Caspary Toroker[2,]*

[1]The Nancy and Stephen Grand Technion Energy Program and [2]The Department of Materials Science and Engineering, Technion - Israel Institute of Technology, Haifa 32000, Israel

*Corresponding author: maytalc@tx.technion.ac.il

We provide additional information on the zero point energy (ZPE) calculations performed and the calculated energies: All ZPE calculations were performed using finite difference Hessians (using the central difference approximation, NFREE = 2, IBRION = 5 tags in VASP). The central difference approximation was converged up to an error of 0.006 eV. We calculate ZPE contributions for the adsorbed species for all slabs, as well as for the free molecules, and the information is provided in the tables below:

molecule	ZPE contribution [eV]
H_2	0.27
O_2	0.10
H_2O	0.57

ZPE contribution per adsorbed species [eV]	(1x1) pure Fe_2O_3	(2x2) pure Fe_2O_3	(1x1) pure Al_2O_3	(1x1) Al_2O_3 monolayer covered Fe_2O_3	(1x1) Al_2O_3 bilayer covered Fe_2O_3	(2x2) 75% partially covered Fe_2O_3
*vac	0	0	0	0	0	0
*OH_2	0.68	0.68	0.66	0.65	0.69	0.67
*OH	0.38	0.38	0.40	0.39	0.39	0.37
*O	0.07	0.08	0.08	0.07	0.07	0.07
*OOH	0.46	0.47	0.49	0.47	0.48	0.46

Additionally, the relaxed geometries of the following unit cells are given below: pure bulk Al_2O_3, pure Al_2O_3 reaction intermediate slabs, Al_2O_3 monolayer covered Fe_2O_3 reaction intermediate slabs, Al_2O_3 bi-layer covered Fe_2O_3 reaction intermediate slabs, Al_2O_3 partial 75% coverage of Fe_2O_3 reaction intermediate 2x2 slabs, pure

Fe_2O_3 1x1 reaction intermediate slabs, and pure Fe_2O_3 2x2 reaction intermediate slabs. Geometries are given according to the following order: title, lattice vectors in Cartesian coordinates, atom types and numbers, respectively. Atom locations are in fractional coordinates. The atomic coordinates are ordered according to the ordering given in the atom type row (format of VASP). To each structure the total energy of one repeat unit cell in eV is added.

1. Relaxed geometry of the pure 30 atom hexagonal Al_2O_3 cell (bulk):

```
Al2O3 in hexagonal basis relaxed geometry – total energy: -164.99567 eV
   4.8049983487517469  -0.0000000441023696  -0.0000001212283194
  -2.4024992125640701   4.1612506803441081   0.0000001851383875
  -0.0000003310352968   0.0000003926011077  13.1086862296789661
 O   Al
 18   12
0.3062736417253760 0.9999999738806125 0.2500000355870284
0.6937263701391672 0.0000000621514289 0.7499999687240191
0.0000000037833203 0.3062736816776663 0.2500000377052629
0.0000000281757480 0.6937263475083029 0.7499999839059512
0.6937263385006247 0.6937263120046495 0.2500000225290080
0.3062736095858511 0.3062736051363686 0.7499999854620683
0.9729403280694555 0.3333333334089303 0.5833332933969828
0.3603930519328742 0.3333333124918170 0.0833333454987297
0.6666666654195197 0.6396069468223047 0.5833332966886360
0.6666667517621931 0.0270597315086505 0.0833333636577933
0.3603930537148941 0.0270597396941596 0.5833333133456051
0.9729403071198774 0.6396069745744981 0.0833333571355439
0.6396069440286283 0.6666666773430094 0.9166666662066731
0.0270596863867780 0.6666666904205769 0.4166666684330309
0.3333332871094541 0.9729402921065926 0.9166666620064419
0.3333333721095215 0.3603930424233752 0.4166666559172825
0.0270596983821605 0.3603930347316009 0.9166666624719610
0.6396069250947178 0.9729403104458214 0.4166666676746758
0.9999999920397613 0.0000000171750472 0.3520432188977480
0.0000000205962323 0.0000000108240670 0.6479567851472936
0.9999999792287184 0.9999999943077711 0.1479567272866120
0.0000000303452623 0.0000000220754899 0.8520432594823220
0.6666666720165964 0.3333333185061207 0.6853765912477172
0.6666666884080783 0.3333333401480729 0.9812900813562493
0.6666666637376721 0.3333333330495307 0.4812900929123245
0.6666666721162997 0.3333333339872553 0.1853765363567916
0.3333333621342263 0.6666666779504453 0.0187099076986144
0.3333333326185013 0.6666666895389426 0.3146233999386183
0.3333333481900880 0.6666666881877958 0.8146234635999861
0.3333333375284013 0.6666666679190953 0.5187099227290588
```

2. Relaxed geometry of Al_2O_3(0001) pure surface slabs at different reaction steps:

1) *Vacancy:

```
Al2O3 *vac (1x1) (0001) surface – total energy: -164.99568 eV
   4.8049983487517469   0.0000000000000000   0.0000000000000000
   2.4024992125640701   4.1612506803441081   0.0000000000000000
   0.0000000000000000   0.0000000000000000  24.2761898040999995
 O   Al  H
 13   8   4
0.6745275580041579 0.9517731584800515 0.6531165339030238
0.2763508336636633 0.6157168664288335 0.6519373587975537
0.9380190125358610 0.0062446296066483 0.5633155654005577
0.6264353328546832 0.6222187540346482 0.5623640090357043
0.3193171611792209 0.3149612521760261 0.5628656277193542
0.9885812782877608 0.2878016813029802 0.4725430910210306
0.2937750949687867 0.6766599978976728 0.4723328176584545
```

0.6013340161570113 0.9827815893150458 0.4724756313553513
0.2712684942465629 0.3392494168483182 0.3819360125847808
0.9659718709455873 0.9561458119885415 0.3814110594037530
0.6563536050660446 0.6470361423106397 0.3828413352087736
0.3248265502207914 0.6155989975414755 0.2935658563018322
0.6695019024034963 0.0036943107398955 0.2911428637418112
0.6358480391300034 0.3083546126200574 0.6167353315202675
0.9585434386359424 0.6496549543772190 0.6002146085499760
0.9610065208788896 0.6485484172631004 0.4380940668095690
0.2944893416125467 0.9824827026637308 0.4171243549042885
0.2930254975976538 0.9844940809489984 0.5279601804445733
0.6262840056597909 0.3171070451880311 0.5071219519826258
0.6286400443727089 0.3149825663014099 0.3449611261634828
0.9636925577260698 0.6481056783087666 0.3284985007121008
0.4705330872522779 0.9556995155784662 0.6594387140991671
0.4669979217044826 0.0067526748815681 0.2831630355068100
0.2197675276428299 0.6024914353612445 0.6898258877016019
0.3735693072531703 0.5273870078366230 0.2565234794735431

2) *OH2:

Al2O3 *OH2 (1x1) (0001) surface – total energy: -196.51017 eV
4.8049983487517469 0.0000000000000000 0.0000000000000000
2.4024992125640701 4.1612506803441081 0.0000000000000000
0.0000000000000000 0.0000000000000000 24.2761898040999995
O Al H
15 8 8
0.7432137179452738 0.8902914802892994 0.6524221137564936
0.0079273951676555 0.2327412233401702 0.6735905146440189
0.3916039000516136 0.5855972591917507 0.6751974855429808
0.9371962684873836 0.0259044395468209 0.5684701317294483
0.6038501630812618 0.6198187295801389 0.5696836472372553
0.2988548105255262 0.3112327132466604 0.5765384452090387
0.9891348033714067 0.3151224627158768 0.4800702793936935
0.2802363523911353 0.6883918153042501 0.4800146595835599
0.6109342336195738 0.9839035738120927 0.4833655694344046
0.2719725580564543 0.3592796824890527 0.3889860717332851
0.9353431832901151 0.9843908197644993 0.3896161048868336
0.6568121116496783 0.6544618762234862 0.3888053557834326
0.3046983286066052 0.6612114892312562 0.2999421335341594
0.6310440357783378 0.0063243017849999 0.2998390446669461
0.9495364740898538 0.3206403612749043 0.2984531210432806
0.6237379190214085 0.2980543268677565 0.6198189920143236
0.9324875118778877 0.6723999012587427 0.5862101912242252
0.9561359022793283 0.6655720408811163 0.4374730333201740
0.2859751182020318 0.9958875917829531 0.4075501664580656
0.2856731791208063 0.9962694307244391 0.5268367123753777
0.6299159418241373 0.3327806681458512 0.5031797252954533
0.6134384664905852 0.3482325250474716 0.3396816437529750
0.9761701972572041 0.6524442390638825 0.3260668505858817
0.5853994725855003 0.8406649355022111 0.6678693646454121
0.6010528478192398 0.0458550990505628 0.2605741156092023
0.2302462015581526 0.5440892674439439 0.6913663528867389

3) *OH:

Al2O3 *OH (1x1) (0001) surface – total energy: -192.293604 eV
4.8049983487517469 0.0000000000000000 0.0000000000000000
2.4024992125640701 4.1612506803441081 0.0000000000000000
0.0000000000000000 0.0000000000000000 24.2761898040999995
O Al H
15 8 6
0.6703526340046935 0.9717305335779969 0.6528803013482403
0.9622427775941276 0.3456239707782913 0.6523203036132443
0.2996753909646586 0.6454038660351316 0.6504799437252160
0.9493749700329985 0.0122441949434631 0.5629489461296302
0.6416710471521299 0.6277701023404205 0.5625829583573179
0.3302420152713950 0.3225627529050428 0.5627593814036445
0.0012894455984451 0.2940422905851818 0.4724612689373799
0.3067779100849322 0.6830955849917473 0.4725019037282152
0.6135521134879554 0.9885610524638437 0.4724828205557472

0.2812313453825013 0.3493371573486428 0.3823844905179925
0.9733680396575508 0.9648565473876616 0.3820157044310548
0.6645593456133341 0.6545851906530658 0.3821956165648359
0.3198659185644601 0.6314858401842969 0.2926430985109008
0.6541016428521189 0.0053503669275230 0.2920583406825585
0.9571927819461692 0.3315059004464231 0.2945224760561516
0.6447017495074832 0.3139723352343466 0.6147557364724108
0.9733227446805088 0.6551162246258997 0.6014841718771038
0.9742599797180560 0.6545396182658578 0.4383393602570891
0.3069942528026104 0.9894247509526508 0.4170090966350202
0.3076208393436772 0.9877067001963553 0.5279433172233894
0.6401436060696923 0.3225862768504086 0.5066122193136948
0.6403070257802881 0.3219748835081617 0.3434824439382567
0.9706174858859526 0.6631116251447793 0.3301992872406672
0.4624264599395644 0.9786889285227645 0.6541405777438598
0.4531675591575066 0.9983473020907070 0.2908058291249986
0.2508563679412745 0.6168245263839509 0.6879896700168473
0.3537231519117086 0.5084012472014692 0.2590990928105938
0.8726701827927528 0.4687869455898195 0.6858472312624571
0.8807481462614817 0.3590314538641124 0.2569644115214729

4) *O:

Al2O3 *O (1x1) (0001) surface – total energy: -180.14159 eV
4.8049983487517469 0.0000000000000000 0.0000000000000000
2.4024992125640701 4.1612506803441081 0.0000000000000000
0.0000000000000000 0.0000000000000000 24.2761898040999995
O Al H
15 8 4
0.6588212158570954 0.9542386252992827 0.6523448499934190
0.9568095175718625 0.3334166027481587 0.6483353273637036
0.2859559422655238 0.6370877368370031 0.6515461486336349
0.9421974137907299 0.0024762711903747 0.5633167900482192
0.6286320592168622 0.6230620714977135 0.5613920570007949
0.3242801835981268 0.3160155700396530 0.5624848890187764
0.9903268519445945 0.2879003304326631 0.4725193863824657
0.2914922706391820 0.6775066782912305 0.4722485053571006
0.6016301708784724 0.9861153830887517 0.4728128200527664
0.2757586830871546 0.3380719776790642 0.3819939691048759
0.9640188026547278 0.9545285948972264 0.3820585943873667
0.6537128807867916 0.6493811178823066 0.3838470125656386
0.3203733256713193 0.6281880604697676 0.2936632593366113
0.6460276948721457 0.9994519088308067 0.2916422738701101
0.9530550192960945 0.3249714005694599 0.2973984523913629
0.6320296866532615 0.3067027502276360 0.6166024918629205
0.9637215976554927 0.6392184421016864 0.6021164169925370
0.9573404158825483 0.6508623021545787 0.4377815594514587
0.2941325266709853 0.9814253586221682 0.4168781854543511
0.2971971257973109 0.9841005119781840 0.5279824419659178
0.6267977825865856 0.3214540560715520 0.5070839393634898
0.6422271008945373 0.3143274025853628 0.3416332466821004
0.9618407434983354 0.6583781451705661 0.3285664387620457
0.4589724775961272 0.9473612983846920 0.6570874462926142
0.4422968296567547 0.9991555092334181 0.2874211094532910
0.2293095056315977 0.6084217392082891 0.6886859143823969
0.3581041753458010 0.5428478075084016 0.2563914738300568

5) *OOH:

Al2O3 *OOH (1x1) (0001) surface – total energy: -200.83106 eV
4.8049983487517469 0.0000000000000000 0.0000000000000000
2.4024992125640701 4.1612506803441081 0.0000000000000000
0.0000000000000000 0.0000000000000000 24.2761898040999995
O Al H
17 8 6
0.6665367772982336 0.9566344328933738 0.6512016707013046
0.9718644044109936 0.3121711706352173 0.6483226275361744
0.2908819547556405 0.6256483735559257 0.6523852432956474
0.9415828083785698 0.0033810617033794 0.5624451362658291
0.6333113276722315 0.6177589062171407 0.5629624159128781

0.3208087056141622 0.3157057069597258 0.5617930747502342
0.9939355248008397 0.2832805320768372 0.4722206942089784
0.2993535705866393 0.6728475572044985 0.4719229033292507
0.6060630230169295 0.9779119862130017 0.4722235651415048
0.2733836293304890 0.3383298079157058 0.3818074155523234
0.9647361971723640 0.9588292317567593 0.3812577405152737
0.6599074607291300 0.6422897525588951 0.3820991776458555
0.3135755842771317 0.6222858054749238 0.2939140982057680
0.6462187349151591 0.9883775047638466 0.2918733356856222
0.9540543796296461 0.3224018565598215 0.2929632611554851
0.9450819156826000 0.3755713849478326 0.7080133728100080
0.8691069923586525 0.3981501496210811 0.2343358845682886
0.6268028604160492 0.3059691557977899 0.6145416307262082
0.9660027486768072 0.6497929417955177 0.6015102819502331
0.9656366809302597 0.6434745387432770 0.4382903810483327
0.2998694054565831 0.9781502987835395 0.4165669071592220
0.2998103423329113 0.9781841027964617 0.5277220180725948
0.6327246016420389 0.3125292125694585 0.5063023965669515
0.6297456559126928 0.3129729367685101 0.3417833222489435
0.9657361094484500 0.6554074378487371 0.3306694485472264
0.4696849336722480 0.9442581555795826 0.6541879238953570
0.4376396082911640 0.9954581689473656 0.2913762574172409
0.2411376095394786 0.5599324427167005 0.6873922203729208
0.3612242069096965 0.5336049966920555 0.2568093899626120
0.0511619727144179 0.1523070000135363 0.7209717825256021
0.7762821734278162 0.6344951998894857 0.2346204222261292

3. Relaxed geometry of Al_2O_3(0001) monolayer covered Fe_2O_3(0001) surface slabs at different reaction steps:

1) *Vacancy:

Fe2O3 *vac (1x1) (0001) surface, monolayer covered Al2O3(0001) – total energy: -163.84775 eV
4.4147882200000002 2.5488791700000002 0.0000000000000000
0.0000000000000000 5.0977583400000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 24.2761897900000001
O Fe H Al
13 4 4 4
0.7756295793089194 0.0185778675833888 0.6964621402163687
0.2681231382807781 0.5305962088667684 0.6914189104727981
0.9300916672527535 0.0179648819258915 0.5998678822611794
0.6793544923825579 0.6204818449525860 0.6256319028505075
0.3272448239219017 0.3585513952712489 0.5966890484313723
0.9692782500874202 0.2931301151447485 0.5001612070387225
0.3068832484168311 0.6527684881217795 0.4972920166201362
0.6092953286651976 0.9561681158091417 0.5030136482291638
0.2403143912756107 0.3341272523241585 0.4002610187393643
0.9029370564154320 0.9327835580490245 0.4037097179011440
0.6346132326743259 0.5847445910639593 0.3749634948269929
0.2234167634439999 0.4804758236078399 0.3013579302510720
0.7219575844481696 0.9996590404171002 0.3095987386095942
0.9674326657849406 0.6342349703240373 0.4689734110188439
0.2913663645035669 0.9544674869871130 0.4377909342910939
0.3078271732219946 0.9701143722395997 0.5624053931502573
0.6279707286712650 0.2952129243994364 0.5314745023345822
0.6206598455844556 0.0336377890917987 0.7215750624494461
0.5532651600698060 0.0620857838573272 0.2842108857702925
0.2112311140161367 0.6931855760424597 0.7178408710352926
0.2009167545988007 0.6312672930488077 0.2745373093425201
0.6178957917604464 0.3206493687330649 0.6459936979306349
0.9898014865454314 0.6768054417343805 0.6342883468748468
0.5857892666047420 0.2696751939885615 0.3673694277631085
0.9353634803604649 0.6445795958536849 0.3536959676662050

2) *OH2:

Fe2O3 *OH2 (1x1) (0001) surface, monolayer covered Al2O3(0001) – total energy: -193.0443 eV
4.4147882200000002 2.5488791700000002 0.0000000000000000
0.0000000000000000 5.0977583400000004 0.0000000000000000

0.0000000000000000 0.0000000000000000 24.2761897900000001
O Fe H Al
15 4 8 4
0.7122039938150522 0.0726658460481318 0.6920515527906659
0.2160005828366067 0.1144352797993307 0.7496509863245109
0.2474237428009260 0.6289631991492186 0.6928605677542237
0.8967006180515824 0.0922726257042399 0.5996836107514625
0.6487750474359615 0.6837168176991284 0.6232179027373022
0.2850249254482975 0.4400126737656436 0.5964766897916718
0.9265276159718283 0.3830406576538365 0.5001931385554741
0.2631999185170386 0.7434009385277562 0.4968725629642421
0.5659868933337222 0.0477080832217851 0.5024039424930393
0.1956149302266894 0.4295723559690003 0.4005812511629259
0.8603873915250091 0.0319313833549231 0.4027379286035000
0.6007992199525347 0.6698030059699249 0.3761526583312786
0.2029397228365539 0.6212956551616031 0.3042432277051077
0.6529298189063368 0.0805475824315138 0.3098878709714441
0.1995524277311134 0.0768932261232607 0.2478933922329247
0.9232350347888385 0.7247782858692204 0.4688175774215750
0.2460975045170244 0.0485809725592503 0.4377911069920231
0.2656547169472603 0.0556156400937695 0.5615977147542424
0.5840803116140165 0.3875624381579073 0.5313167709206041
0.5637442984945622 0.0634795273598456 0.7161982971377228
0.4960573061446851 0.0830998956515856 0.2859269754116909
0.2180489341544956 0.5020743741253781 0.7196300510006139
0.2049252001055848 0.4861594820459842 0.2756260253717926
0.0396192424384196 0.2033960095376202 0.7735281658288713
0.9886159444689966 0.2072440976789309 0.2376574846301907
0.1986414181220653 0.9560458212527223 0.7281921775488627
0.1953667251025024 0.9110093789531675 0.2698386582227812
0.5814518423131432 0.3889800991520715 0.6447303050007633
0.9479190275961642 0.7578247559441635 0.6349346094778241
0.5366504931045313 0.3650795627572592 0.3658264123831358
0.8928851306985024 0.7428103082817472 0.3549022947275517

3) *OH:

Fe2O3 *OH (1x1) (0001) surface, monolayer covered Al2O3(0001) – total energy: -186.77084 eV
4.4147882200000002 2.5488791700000002 0.0000000000000000
0.0000000000000000 5.0977583400000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 24.2761897900000001
O Fe H Al
15 4 6 4
0.6826393948762401 0.9746616595709483 0.6833910277075148
0.9414662773270166 0.3598952852193449 0.6828512930233046
0.3003488183997689 0.6226860236298606 0.6816530479278597
0.9407039014961711 0.0066605462604841 0.5963485645090145
0.6538288540439652 0.6190820811199629 0.5957885553815885
0.3236194634237890 0.3357586319896555 0.5959805498295765
0.0029186348936463 0.2904189048956809 0.4999400406024321
0.3046859007713891 0.6870267920008573 0.5000854010372535
0.6073703048409129 0.9888325663659074 0.5000355674545460
0.2834342449538312 0.3585651371379015 0.4043332387782002
0.9578968506003207 0.9706771066890738 0.4038261821956297
0.6699822252773799 0.6419486116798439 0.4040714245268546
0.3112370333268544 0.6186035624641448 0.3173053280835134
0.6675061696269253 0.0032310154331867 0.3166726736796761
0.9331789916453772 0.3542973676434968 0.3186778013125888
0.9719373587124025 0.6551448054909699 0.4666729122062065
0.3041967374530756 0.9902198734453194 0.4385751550826313
0.3061959093586424 0.9873989989231973 0.5614606410361986
0.6383236409409179 0.3225199328113888 0.5334482801462883
0.4896656382922160 0.9773588525793642 0.6858618837918158
0.4778553554311600 0.9992228693443437 0.3142613820810567
0.2637135912642421 0.6061230868699070 0.7202618750182523
0.3362249365053742 0.5333898994411044 0.2806790443834899
0.8775418693809200 0.4482798807190633 0.7191997102118819
0.8904887850615566 0.3593658673485081 0.2797526289814272
0.6426568253730807 0.3147107694543649 0.6453653661813661
0.9725222913586933 0.6547977423436038 0.6345268084694524

0.6373693228049646 0.3229226917441324 0.3655909584250026
0.9675506525591757 0.6628660773844075 0.3546510279353043

4) *O:

Fe2O3 *O (1x1) (0001) surface, monolayer covered Al2O3(0001) – total energy: -174.59019 eV
4.4147882200000002 2.5488791700000002 0.0000000000000000
0.0000000000000000 5.0977583400000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 24.2761897900000001
O Fe H Al
15 4 4 4
0.6739880569887191 0.9534539365959915 0.6827255734830473
0.9404886420804317 0.3343274659696434 0.6781818106318980
0.2911208964545224 0.6081684404348024 0.6826044440175920
0.9318768024180812 0.0002744907515932 0.5976954591164372
0.6367466317923700 0.6171932407539060 0.5940786542238001
0.3129047601080899 0.3313677680299918 0.5958663850364161
0.9901564767318121 0.2887949108366428 0.4999710559899313
0.2860196607110694 0.6864264196051906 0.4997375224220590
0.5951398283564870 0.9895452878924615 0.5002852862512128
0.2717337549914305 0.3506440258157610 0.4029995929310104
0.9491706994500717 0.9648201890626495 0.4033976813250320
0.6549795431427015 0.6417979222584478 0.4060642875542655
0.3152748165835746 0.6092424069817355 0.3177858181839639
0.6652655558984719 0.9907121154163363 0.3165153513988699
0.9412495810514798 0.3371344630470077 0.3225450714400040
0.9526364546053188 0.6543542552332156 0.4658809324177255
0.2920784075550102 0.9849522565825737 0.4390110359854731
0.2944620696693292 0.9853230013214898 0.5615248930244832
0.6225972770302803 0.3277295222127563 0.5335469014363809
0.4880024866993224 0.9487799300216579 0.6902033312865115
0.4753596132818245 0.9919802267085061 0.3099979512149886
0.2524361239286392 0.5971508439819289 0.7213823367149104
0.3378531246135381 0.5569435387915860 0.2789793615474849
0.6256067016886036 0.3032114741438363 0.6467654000295866
0.9616785072215635 0.6403638816251984 0.6355386003770249
0.6346964864900997 0.3147551934487396 0.3634306873793420
0.9635370104572232 0.6572194424763893 0.3532852745805499

5) *OOH:

Fe2O3 *OOH (1x1) (0001) surface, monolayer covered Al2O3(0001) – total energy: -194.71736 eV
4.4147882200000002 2.5488791700000002 0.0000000000000000
0.0000000000000000 5.0977583400000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 24.2761897900000001
O Fe H Al
17 4 6 4
0.6817398173871609 0.9618123217067875 0.6823104461609617
0.9439270956498902 0.3351403759209504 0.6791642371969928
0.2907501948882327 0.6037370108511055 0.6832637697372519
0.9336883152240318 0.9951912297123471 0.5955365521056848
0.6467835417326810 0.6068334088668408 0.5964014321365383
0.3158176311512761 0.3267272111005823 0.5947451842396347
0.9984015656901590 0.2783613423488873 0.4998427504230847
0.3004005022795653 0.6752658523363095 0.4995432285072070
0.6031739204080822 0.9761217416912586 0.4996777537123833
0.2799291074262626 0.3463112851616970 0.4037428729679959
0.9537929170513451 0.9640164794195059 0.4029014144257701
0.6704888271860696 0.6281640885305748 0.4039628797003516
0.3121179911566898 0.6051375835657922 0.3181413523989605
0.6650229562002536 0.9845560154073283 0.3163140485102645
0.9346686484195672 0.3452698317776211 0.3171533938964402
0.9366823198297993 0.3713658223791114 0.7395232781926495
0.8590887476020228 0.4115319611194366 0.2581045664965487
0.9669959711187772 0.6416364988206382 0.4666108461002452
0.3018191205260337 0.9768534649626872 0.4382098009839481
0.3000878650266401 0.9754031329167674 0.5612714798005172
0.6333354164571290 0.3101370876062504 0.5329316576818357
0.5024265077471810 0.9464274114674467 0.6902482804897332
0.4681987352901658 0.9945260205761670 0.3144742406404930
0.2518052505583483 0.5439914459612396 0.7191417346328777

0.3491511934099520 0.5485185901408869 0.2794918768025099
0.0053370745854409 0.1613719637519822 0.7503035919859542
0.7764287637346783 0.6329978342310767 0.2575802309969148
0.6243871771154872 0.3059223506930451 0.6449452566750224
0.9663984643391146 0.6483999650086787 0.6343722127396063
0.6317776228496044 0.3120948793644374 0.3638594901926311
0.9692378713667011 0.6542857837267775 0.3550653073178154

4. Relaxed geometry of Al_2O_3(0001) bilayer covered Fe_2O_3(0001) surface slabs at different reaction steps:

1) *Vacancy:

Fe2O3 *vac (1x1) (0001) surface, bi-layer covered Al2O3(0001) – total energy: -237.38433 eV
5.0980000496000004 0.0000000000000000 0.0000000000000000
-2.5490000248000002 4.4149975513999999 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.6149997710999990
O Fe H Al
19 4 4 8
0.2753008156427725 0.9694888372245316 0.4926082377864205
0.1389737878441650 0.5119883129670555 0.6911545186163011
0.6478393828473017 0.5841940725525490 0.3021010386558700
0.9540926356999719 0.2834459481252765 0.4964730957863637
0.9233618026195174 0.8888819987535683 0.7257244234397007
0.3087054559646631 0.8682114550048468 0.3164254220957829
0.6369558508216500 0.6467018015905097 0.4939554717552426
0.5271451767448525 0.2967013699109771 0.6850152389729658
0.9838041364823553 0.2760118019938673 0.3146621835523788
0.3403923817220118 0.7482780528618065 0.2135336419666629
0.0178814394718572 0.3942908471889197 0.7815709450503832
0.3565616542080861 0.3134054439450509 0.3933191332617838
0.9316075475563466 0.6261554682178172 0.5949842118539905
0.6207346959340683 0.9727104749954734 0.3994468848239734
0.2887179387163670 0.3687836736403867 0.5894235377398189
0.1703014152435216 0.1432123104233654 0.2382546178105827
0.5048253169395238 0.3650271413240915 0.7797916094898270
0.9388983715786097 0.5682309834049306 0.3986059128848325
0.5452826014531524 0.9619448461836697 0.5960970647392969
0.9263605337422831 0.9682455664538168 0.5534131938386437
0.2963688765492307 0.6412282069143842 0.5244289287597965
0.9644020520972063 0.9570362635446159 0.4387901821015916
0.6329670557977352 0.3063833127298565 0.4610644238054036
0.2804580833045733 0.0538682191178808 0.2201362389789594
0.3078860932950178 0.6475630837226305 0.1801159195993307
0.8676189062850881 0.2456657251245389 0.8049372507366854
0.4893989487128962 0.4960539983703569 0.8054724965214959
0.8388256706050896 0.5220214536615160 0.7327574356111057
0.2970260847333179 0.6275952739907282 0.3778293751581145
0.2070661175736959 0.2545773072892743 0.7308422300353428
0.6506718890107663 0.2741417265171577 0.3524991250081868
0.5819114097947136 0.3129264454517227 0.6176642386192981
0.3013547733528057 0.5294755773714286 0.2692269943872319
0.9996316461651560 0.9337561117411326 0.2982183643788545
0.2466696744896808 0.6417967566902192 0.6294570821778009

2) *OH2:

Fe2O3 *OH2 (1x1) (0001) surface, bi-layer covered Al2O3(0001) – total energy: -266.13937 eV
5.0980000496000004 0.0000000000000000 0.0000000000000000
-2.5490000248000002 4.4149975513999999 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.6149997710999990
O Fe H Al
21 4 8 8
0.3157823077856889 0.9965701689029842 0.5017528506083337
0.9583751363164481 0.3184417991980766 0.6803307336009610
0.6473417318433405 0.6685956383570471 0.3199650421617974
0.9908384625595872 0.3070700956724579 0.5003802531810848
0.6426456883430092 0.5857836967500276 0.6819167469244078
0.3063536860014153 0.9440943015011811 0.3098442032330624

0.6689923241044511 0.6747346151780036 0.4991891335047072
0.3028050697709261 0.9748470699853513 0.6890152323422143
0.0013787405098498 0.3543570897298594 0.3162245901493037
0.7019526128463838 0.8920094427768888 0.2332417117103844
0.7540923179278849 0.9926496938037630 0.7570368182574470
0.3927686224762397 0.3700363337371115 0.4021813766664692
0.9938654013013632 0.6468352749673087 0.5962668646040825
0.6564044942000393 0.0479199105918156 0.4021975248580532
0.3264045038187788 0.3767786175880943 0.5966434406357308
0.2736452968371808 0.2950768970379372 0.2388585098342304
0.4272771201253107 0.3304829267752041 0.7806889101984424
0.0027882462537079 0.6478272132448382 0.4037489113282646
0.5903945770012626 0.9719357893018739 0.6020472781008124
0.0211608331857462 0.6157075921832558 0.2115114641768443
0.0131844657355558 0.5802204040209915 0.7798722991372244
0.0151049226417470 0.0102755382175488 0.4435621086685302
0.6532746605485968 0.3260483348516345 0.4678675839279052
0.9698736498348453 0.9901244182247595 0.5562751474740253
0.3287055555452483 0.6635385332745543 0.5331790005246830
0.4554715427429699 0.2791792767257704 0.2412777327760622
0.7605249234593430 0.0802717490652967 0.2146409689959796
0.6048340244821091 0.7951762967681120 0.7709951338450267
0.2734357606463789 0.1387600044054835 0.7954783060189285
0.1321784626806561 0.6625458619227445 0.1787739378442481
0.9045882511891676 0.7286931177046725 0.2119053973006189
0.8721358746798984 0.4985571325795561 0.8093005564724223
0.1435874145054825 0.4858750436116495 0.7808488406071774
0.6410943511112706 0.3405552604767408 0.6189042548642760
0.3361208269634730 0.6440163254793063 0.2746907942669239
0.9943386632917424 0.0135769742260834 0.2945861380698389
0.2854690230942012 0.6502487800244197 0.6414423047708553
0.6396595989926297 0.2763706858783976 0.7269253573538634
0.3559172740875525 0.6882111547188146 0.3818708222375946
0.9461836184084191 0.9660213505779467 0.6960472207010611
0.6997270881501052 0.3706550229624170 0.3603329430661333

3) *OH:

Fe2O3 *OH (1x1) (0001) surface, bi-layer covered Al2O3(0001) – total energy: -260.57261 eV
5.0980000496000004 0.0000000000000000 0.0000000000000000
-2.5490000248000002 4.4149975513999999 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.6149997710999990
O Fe H Al
21 4 6 8
0.3033118312663419 0.0095574347879932 0.5003005626452364
0.9744337828379557 0.3445386810803868 0.6750034839132653
0.6436104305312043 0.6755427737631905 0.3259438229363738
0.0009252264367561 0.3112591231925350 0.5003371959637732
0.6651455291843362 0.6461746472213790 0.6744336749025521
0.3366806333569201 0.9819649170333875 0.3262431350368686
0.6985314109069165 0.7071651162100920 0.5003732689107494
0.3583548631153448 0.0329418846737681 0.6747016137967137
0.0278221947637505 0.3712100952961563 0.3257144272025343
0.6780261682425959 0.9770159273170336 0.2448220991157868
0.7141070630499442 0.0399686296096249 0.7578760703299920
0.3725244154341212 0.3585393643428958 0.4094708027474852
0.0218970905278084 0.6601464219782613 0.5909933460080410
0.0353203785172411 0.7184842555704236 0.2430595330960585
0.9665584291630793 0.6846100171635854 0.7576550265245174
0.6544285974280939 0.0325328948680834 0.4095796681761996
0.3474233918631313 0.3791132007310267 0.5910801107622987
0.2877969833543119 0.3266891907687040 0.2427812335066974
0.3245092070972007 0.3004014288628412 0.7559925688951452
0.9799241397256822 0.6391464928970407 0.4096849477602333
0.6293997640086317 0.9870393452772674 0.5912072032958022
0.9996559167604531 0.0087233830455915 0.5581964196076825
0.3336874114978059 0.6758902161558851 0.5332587598628109
0.0021775085096181 0.0099289552426143 0.4424787341348164
0.6681759995209120 0.3431498729217637 0.4674208017147450
0.0984943980836590 0.8154677883300749 0.2091827540884452
0.4820035620044294 0.3319077343878334 0.2405479986967762

0.7246133231016643 0.9810060221825765 0.2081318610057536
0.9011326590206750 0.7176985798189079 0.7913832849257005
0.5200291858056971 0.8508109646121085 0.7601451193607787
0.2788307018329093 0.2516785367475265 0.7925674763226738
0.6702658912191666 0.3390657450245627 0.7233662846407469
0.3358131026727520 0.6777186659974390 0.3789927348275270
0.9999602121632662 0.0083204613593466 0.7102658904438783
0.6691305838200705 0.3429798401121928 0.3580628594495678
0.6659384169073519 0.3428862631852283 0.6216681702155498
0.3319404013976524 0.6697860128941571 0.2772824540925214
0.0022400861452496 0.0092249578439194 0.2904302411010278
0.3328310747253198 0.6749197804926084 0.6426048299827158

4) *O:

Fe2O3 *O (1x1) (0001) surface, bi-layer covered Al2O3(0001) – total energy: -248.50978 eV
5.0980000496000004 0.0000000000000000 0.0000000000000000
-2.5490000248000002 4.4149975513999999 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.6149997710999990
O Fe H Al
21 4 4 8
0.3032675137828917 0.0133510481474204 0.4998415568025294
0.9826786690346481 0.3518846062140781 0.6757456529171577
0.6361449991149470 0.6671251309941013 0.3259897832655270
0.0011188996512459 0.3157842394702612 0.5001050584123021
0.6624532493252246 0.6469310091329703 0.6725734211833299
0.3377269576841400 0.9786624906784951 0.3275767116312593
0.6984238435700689 0.7110225258969578 0.5002676851856478
0.3641114269538193 0.0375810912262367 0.6739907992420342
0.0163268477133656 0.3622781301990514 0.3239389313262535
0.6747009012161911 0.9524645005953118 0.2430396058504272
0.7165123641348998 0.0227730797441552 0.7563996302912557
0.3676838421780957 0.3616328564997673 0.4090345182286157
0.0243003591328304 0.6662083475579408 0.5908005635901858
0.0173883376495922 0.6759102838933870 0.2486937477647615
0.9831139716885886 0.6687923118360786 0.7515444379388114
0.6554669288761019 0.0356611766979640 0.4096233797920590
0.3458754376138913 0.3840672137460288 0.5904096608092146
0.2838536382584707 0.2964406426167230 0.2435683090274736
0.3253161661487525 0.2878481890010960 0.7566738044027161
0.9769841580091310 0.6389355121141946 0.4092930766481899
0.6336467069484897 0.9975251545629860 0.5910688137049505
0.9996495318876057 0.0138038383343471 0.5579428878753632
0.3330888188707064 0.6804092420245951 0.5329876340025805
0.0021185393485865 0.0128041179258744 0.4421514479867668
0.6690589976762809 0.3476836174427191 0.4672033106269353
0.4716366001449614 0.2931406572628461 0.2375875453488447
0.7204033080358059 0.9497312469422639 0.2063968012343764
0.5283237412460693 0.8324918713552805 0.7625575559910018
0.2790662158966128 0.2416200855533219 0.7933641117054933
0.6642428044804802 0.3233501913415893 0.7245304606855640
0.3363079526377888 0.6857310104547665 0.3783475829968381
0.0012680823057423 0.9931803954265135 0.7114710104877560
0.6616115090840609 0.3383149876181477 0.3577699143089319
0.6651241654904183 0.3537337510649223 0.6218302111965386
0.3366698116839544 0.6493194800565192 0.2754401332076455
0.9988008276796165 0.9830742890879236 0.2885427363196129
0.3387756528458894 0.6825209052831696 0.6423897590110172

5) *OOH:

Fe2O3 *OOH (1x1) (0001) surface, bi-layer covered Al2O3(0001)- total energy: -268.63671 eV
5.0980000496000004 0.0000000000000000 0.0000000000000000
-2.5490000248000002 4.4149975513999999 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.6149997710999990
O Fe H Al
23 4 6 8
0.2941413050515322 0.9668804796665000 0.5003142808940950
0.9620995180685199 0.3009710338347134 0.6743148291361081
0.6384941381055427 0.6368612634110846 0.3272430763847893
0.9918203390592808 0.2682580747889531 0.5002851839050280

0.6543359291134720 0.6019862978035917 0.6738566949321410
0.3318722355987234 0.9406649610095883 0.3259256091944280
0.6896387546323055 0.6645909176348894 0.5002969158229078
0.3476030191997168 0.9918184453240713 0.6737632497674326
0.0219780460359473 0.3295577307197490 0.3265784269557130
0.6761723449826960 0.9302120143178243 0.2431685804688399
0.6988825601701336 0.9920126460146719 0.7540254197752176
0.3647130726125170 0.3160557220516935 0.4098193169588669
0.0118260929857641 0.6175976899928557 0.5906490132822171
0.0198494347213369 0.6624163222749644 0.2470694973338325
0.6458813700549797 0.9911122485631978 0.4099729346830969
0.3374270961303623 0.3371665014080563 0.5906056320759987
0.2793524208112999 0.2847451570341732 0.2442463507157484
0.3066091744319195 0.2382597919695613 0.7582660564817800
0.9730177684573320 0.5976460599285787 0.4100125001305130
0.6195738211419837 0.9444689553862915 0.5908926776137449
0.0258622972775058 0.7026308846548162 0.1899193108222192
0.9665789085533021 0.6419130205781656 0.7541799957321018
0.9573334964901008 0.7070772730479362 0.8102135146232854
0.9938120644059225 0.9675692551304351 0.4425201981736890
0.6590418536198470 0.3002294105601067 0.4675501838204852
0.9897972558983739 0.9660233964431058 0.5579162938807514
0.3244436420341117 0.6330403045257427 0.5329740577669924
0.4592808385141254 0.2697038922160786 0.2371804869706295
0.7236836832914193 0.8732415138676615 0.2095971164030672
0.7194054548881397 0.9585005196902046 0.7907225499492299
0.2982170803222886 0.4219391716926424 0.7655264009536396
0.9477992407956464 0.4915041625196466 0.1793412131044434
0.1295401238470006 0.9184109526965116 0.8093533113954834
0.6555651352195540 0.3007716995375560 0.6212465025811014
0.3400605589756864 0.6324762364649743 0.2779286730655599
0.9973212562719880 0.9754357930821200 0.2907337606436968
0.3217164136368567 0.6329266885779319 0.6421043057411637
0.6470671312130847 0.2889987965188894 0.7232645980683046
0.3283928850552726 0.6357724946237013 0.3794639287705763
0.9862751449257701 0.9659429493303477 0.7085964126599436
0.6635180243986269 0.3026101471064564 0.3583606533611174

5. Relaxed geometry of Al_2O_3(0001) 75% coverage of Fe_2O_3(0001) surface (2x2) slabs at different reaction steps:

1) *Vacancy:

Fe2O3 *vac (2x2) (0001) surface, 75% covered Al2O3(0001) – total energy: -718.34395 eV
10.1955165863000001 0.0000000000000000 0.0000000000000000
5.0977577053000003 8.8295767077999994 0.0000000000000000
0.0000000000000000 0.0000000000000000 24.2761898040999995
Fe O H Al
20 58 22 12
0.3143664396390164 0.1528159869116905 0.6523960832987683
0.4799285792116805 0.3339306132748590 0.6274337809938615
0.4822650569317801 0.3290713222830703 0.4633815106013941
0.1483889176093598 0.4963159870600151 0.4391430245031458
0.4836703943578513 0.8288912186651913 0.4668135943664851
0.9820748962749022 0.3262161906815422 0.4673705694560155
0.9836112641208388 0.8264350710116446 0.4662170321876644
0.1482869260112807 0.9906522099681396 0.4406267798305734
0.6490840049807503 0.4958600683268699 0.4374665630747856
0.6548369999970234 0.9940916671925066 0.4390321723895525
0.1473171510451650 0.4953858733994210 0.5608673113384839
0.3151446092715773 0.1620005924740298 0.5367823976607013
0.3069359530977920 0.1616642839428906 0.3732483625365077
0.4864689700919911 0.3334718024442935 0.3482024228467822
0.1486108045520780 0.9958735357846606 0.5631010561405247
0.6535212025344848 0.4948666646780211 0.5596887160427144
0.6513063951360323 0.9884757127503008 0.5605959143462158
0.3172314869774695 0.6622688041167848 0.5326263978402679
0.8149984580814973 0.1603904120066844 0.5341036711306799
0.8175931623531554 0.6599355562566060 0.5337748409644263

0.3357456504373317 0.4918090147963241 0.6842537129906248
0.1309023061025698 0.3222663666593988 0.6852878256020531
0.4670289423901153 0.5131459307758561 0.5939559924569338
0.3193608589244405 0.3133795756465432 0.5947952989888918
0.1456162413489395 0.1722251471095149 0.5951436912882002
0.4973233094103620 0.1467093508878818 0.4999044912404713
0.1491390494865996 0.3425482821210437 0.5003517751805973
0.3015554266822136 0.4941920688570320 0.5001040139544486
0.1276517330357407 0.1793232131567493 0.4069688495818795
0.4725664729607217 0.4964303479525611 0.4064131942627256
0.3288955067525663 0.3236891919771594 0.4053468488900478
0.1533124012862928 0.3089533807734313 0.3161763753438933
0.3199252741297300 0.5158025958875783 0.3126911048585157
0.3541634163370873 0.9596850272491153 0.6907500637578821
0.8329772263742257 0.4936459119063130 0.6842175801495642
0.8467726261969446 0.9767464303190536 0.6839230076838376
0.4817858828602724 0.6625604753305510 0.6827384688761597
0.9578071788790226 0.1842761235612755 0.6838669457581616
0.9757172789251669 0.6743046939117789 0.6824810078667269
0.1515166307308462 0.8123251965257552 0.6825072183107466
0.6377366992914801 0.2756134971810766 0.6872162495679390
0.6530220988032553 0.8125918682354438 0.6825491767236329
0.4740631810271267 0.9980870476653934 0.5981022628349635
0.9657612717190602 0.5031296072112070 0.5961697194599935
0.9676131435983066 0.0022103187416391 0.5971079397659409
0.3248149094575012 0.8115620346501942 0.5974795183293438
0.8158340235406030 0.3114734412862887 0.5979826168828879
0.8277063221935776 0.8068550328444815 0.5957870475583675
0.1612553513906150 0.6678607047041325 0.5958639760364974
0.6651986299130286 0.1578932079489590 0.5954746425972459
0.6610363718060484 0.6676940887268685 0.5961077421147607
0.4995070024535124 0.6479437957574845 0.5001455881681522
0.9955018847594275 0.1451273556591701 0.5004285642161364
0.9990535126846751 0.6446054094282943 0.4999043200962987
0.1495139400715431 0.8434910597526581 0.5002328092441743
0.6489916299523628 0.3418918539783959 0.4994811833740513
0.6516303934913878 0.8418442045055272 0.5001741999077112
0.3016776064647857 0.9956156154749536 0.5009508807218097
0.8011044398500644 0.4937440236590476 0.4999501608203616
0.8024708494617130 0.9927466398361844 0.4997149054115866
0.1413748915035100 0.6792216894130192 0.4045342190222954
0.6461434692675425 0.1696733161092396 0.4011686320533627
0.6422604370103073 0.6787710120979398 0.4034612323391755
0.4845509023710690 0.9800417431075843 0.4041624489559794
0.9772552987919383 0.4827225658810264 0.4034929728178867
0.9779282620348866 0.9836079198058130 0.4034372303504057
0.3339770348672317 0.8246108598597388 0.4038106119672378
0.8286804882529637 0.3217358703806070 0.4017680158392025
0.8366279158510466 0.8180877636921764 0.4038930981780879
0.1566489526539954 0.8124533681768469 0.3177091861587442
0.6763745689444747 0.2916381482724191 0.3084093348542396
0.6576347520357189 0.8123376244963367 0.3173547033644297
0.3435297975130567 0.9974213674907375 0.3141293883031793
0.8325236712012583 0.5028875786298883 0.3153298511944200
0.8408269038852154 0.9914501720865516 0.3145365521894661
0.4689429916204162 0.6745499918269715 0.3186000825378983
0.9752445909165530 0.1711455825573296 0.3179663740796386
0.9699318673814616 0.6723816094862656 0.3192252889905163
0.2382558888231543 0.4948593015810516 0.6860163115455791
0.2242729095083718 0.5149734771112904 0.3133158999865557
0.0983782094476311 0.3530519873665128 0.7228113112904140
0.1746756929619551 0.2516635147918720 0.2821189167101537
0.2577683837945770 0.9603188057282068 0.6912164522808837
0.7307423659221328 0.5080440661052776 0.6856376294939395
0.7556034928365918 0.9699383918953970 0.6894019878049491
0.2474803749288270 0.9983045486567477 0.3096579247447551
0.7370856692511865 0.5027053916592763 0.3115051429580333
0.7512520136624445 0.9802352298563051 0.3125792860871641
0.1323238198383976 0.8016085700829834 0.7208246781403389
0.6116473793256887 0.3565701404638517 0.7134640671276671
0.6345813337524291 0.7994153921266474 0.7207592488499728

0.1728619528827622 0.7655860491119952 0.2816672123457380
0.6957602504052645 0.2335214639253991 0.2746738833684006
0.6699145657421397 0.7763747418257481 0.2796827985850356
0.4499378419431892 0.7118083313292729 0.7184535011588267
0.9469043462661304 0.2074987260686711 0.7227955666866634
0.9474988326551426 0.7156124721797141 0.7193644322534567
0.4468892408367182 0.6764311895079729 0.2797435915841078
0.9451802173033101 0.1831745967269853 0.2796196670746198
0.9583603421116891 0.6640412127249959 0.2800652716639860
0.3189630121821381 0.6601809898623614 0.6455659860890393
0.8164447450701573 0.1523655911808817 0.6474977463877281
0.8223000845776980 0.6576958983932073 0.6452874254474281
0.4883228187625477 0.8230140543995788 0.6353482090749338
0.9776469601021702 0.3285332866721191 0.6364074427468864
0.9876779431604916 0.8247783223679974 0.6342101411188921
0.3177852361337230 0.6631981149850930 0.3655370480970959
0.8215679205341928 0.1566390439879015 0.3631144319268245
0.8192827222600272 0.6602935861845296 0.3653259247875980
0.4867057747865786 0.8283631942807190 0.3540658334359961
0.9778181654569096 0.3331909487107794 0.3536825432398061
0.9879388492140961 0.8270914788966266 0.3544120902866439

2) *OH2:

Fe2O3 *OH2 (2x2) (0001) surface, 75% covered Al2O3(0001) – total energy: -747.87296 eV
10.1955165863000001 0.0000000000000000 0.0000000000000000
5.0977577053000003 8.8295767077999994 0.0000000000000000
0.0000000000000000 0.0000000000000000 24.2761898040999995
Fe O H Al
20 60 26 12
0.3220773310407452 0.1605223391042401 0.6532440728421989
0.4854258649325232 0.3374135930533342 0.6279462762844759
0.4824462770419089 0.3335070604142629 0.4622893187067660
0.1488386179152528 0.5000141957366040 0.4391408499359954
0.4840158203735996 0.8332345925123548 0.4666728665268280
0.9819943358180296 0.3304896289444414 0.4673474182074102
0.9839567568127592 0.8306729868941858 0.4655219412792775
0.1488982482092496 0.9948354268340154 0.4401353270956392
0.6482485833277991 0.4999517584380300 0.4371916338258472
0.6538618400003529 0.9991939440983870 0.4386510101093890
0.1491349116114264 0.4992421223736372 0.5606452878604884
0.3150453798850990 0.1667070634133552 0.5369852712941992
0.3073901500061567 0.1654191542519499 0.3722099121415852
0.4888152786010167 0.3259187073994241 0.3464344800119861
0.1481145012987284 0.0013005785668412 0.5621564929685761
0.6539689708900909 0.4991573952277903 0.5594644215441491
0.6506566295854626 0.9938558422361794 0.5602324568914412
0.3171468225615897 0.6670812828410675 0.5321826793183249
0.8145671711900633 0.1644733763548345 0.5332562090682416
0.8179835579387102 0.6645995331637451 0.5334476554858796
0.3367393720997711 0.4911728240344573 0.6840966599676150
0.5145802500094447 0.1012172885607825 0.7171235771095681
0.1339221849745158 0.3340176036180154 0.6839412668930365
0.4668095574307003 0.5176973800497535 0.5934623204292535
0.3234498578213092 0.3179257763331691 0.5940634616539597
0.1494992559413575 0.1759080816427456 0.5944532464982899
0.4977331319312697 0.1502675859359783 0.4993916207279199
0.1487104879974055 0.3474666559923207 0.5004355359088279
0.3014560943455606 0.4990684079845664 0.4994525554204756
0.1286198077937328 0.1843583967135558 0.4068938319457445
0.4743496116578285 0.4973063697922342 0.4056990265469196
0.3279998392022208 0.3264452351741554 0.4053461919468759
0.1528173281907357 0.3151357550888321 0.3148997125701385
0.3212960988675491 0.5146434413777712 0.3124661731861025
0.5230168981167793 0.1194295154413396 0.2881829377532412
0.3434258171216982 0.9661621463312642 0.6881662009299845
0.8337360942241006 0.4962580353624659 0.6837211353491099
0.8507628418147064 0.9882948146926296 0.6853438594904446
0.4744985683101746 0.6721785870050354 0.6821892638355394
0.9692065047284828 0.1866685497754830 0.6828023640978813
0.9685579063798428 0.6834147010595686 0.6827357069585034

0.1500174792271025 0.8140029583283734 0.6818337684406117
0.6513467333255818 0.3012749372472641 0.6849959684407096
0.6474567462413177 0.8123995626602749 0.6869361239005869
0.4766272725634622 0.9991445412459115 0.5981917366039369
0.9650152461018138 0.5094096030519424 0.5956558052056096
0.9686442553618519 0.0061433407789195 0.5968101313325249
0.3222618563352100 0.8146627352305345 0.5956192062394052
0.8193383993572922 0.3154347078619608 0.5967245831938399
0.8241797293316395 0.8138438575863916 0.5969657140933933
0.1597100487299983 0.6714967114300876 0.5960623008482600
0.6672532466306791 0.1622457548808640 0.5952273206748302
0.6590614072920573 0.6728469585385710 0.5965227107756306
0.5000963623972439 0.6519012478830959 0.4996778885453637
0.9959793619290878 0.1489341615269311 0.5000232230074602
0.9984142917969621 0.6500751523140806 0.4996706518839602
0.1492981476548536 0.8476552257733374 0.4995845654750539
0.6490053769198099 0.3465016379963259 0.4991188148917161
0.6520513382547719 0.8456297019259651 0.4997042846494111
0.3022776692943054 0.9999053872116974 0.5004215609479061
0.8009619800171563 0.4989870072673028 0.4997100118572959
0.8030133954276550 0.9960635497433046 0.4994822045672151
0.1400271109792754 0.6824229886499467 0.4038325482934511
0.6491252386280308 0.1725590926110812 0.4015637260141673
0.6412190505991617 0.6834812641003083 0.4025331890583175
0.4841409625851156 0.9828372183229348 0.4028077431959076
0.9767789711761594 0.4891167322818362 0.4031320470326349
0.9788309974806140 0.9875928185312119 0.4031506231963249
0.3335174567181696 0.8258498290394982 0.4038499481493787
0.8310995845666085 0.3267987493925020 0.4024340499800374
0.8343287522740823 0.8244484272182362 0.4026252001232038
0.1583015098698368 0.8125054901187596 0.3174447493434300
0.6806337697057643 0.3038462125942800 0.3103626847597738
0.6456934632882891 0.8218108321369257 0.3141120032392024
0.3336923643145013 0.9986665785352429 0.3140936553181390
0.8293720247041421 0.5101882573461936 0.3154358576445730
0.8502862403137215 0.0012673432944013 0.3133025752937399
0.4684296200299869 0.6749046074258018 0.3183251487699366
0.9799640956734521 0.1772446942706978 0.3181560172996498
0.9600792379303797 0.6836963152419813 0.3182410721000437
0.2412878330360471 0.4897354279817421 0.6845735157641641
0.2268569082566927 0.5117674238897081 0.3131371372164082
0.0975665001195765 0.3575358884073410 0.7214622272920508
0.1663282663562384 0.2524134874800694 0.2828105155112652
0.4599425623140334 0.1116406203073410 0.7512162982958728
0.4429463697686558 0.1415879233197259 0.2617017452597921
0.5638773090649920 0.9889880735960617 0.7076701854341678
0.5629138844272532 0.0095801526962092 0.2984102274539850
0.2446717093984674 0.9722650972628770 0.6861573113180341
0.7372246603331334 0.4973667393778598 0.6855686140666322
0.7567100653769216 0.9920031936705698 0.6951473144698141
0.2369641210867144 0.9997622742404531 0.3117537473373346
0.7367624370910164 0.5038110740613391 0.3125619377651603
0.7576901391824720 0.0056066892716871 0.3010958284461225
0.1303387117516834 0.8129053933363366 0.7207316098582695
0.6252373579385662 0.2758325083657098 0.7202709709377544
0.6380128653675996 0.7599329641826671 0.7188638755778598
0.1729319233422686 0.7686059918049821 0.2809403560521844
0.6953842704881978 0.2509902407443150 0.2756115678138258
0.6654820379599116 0.7659356571333262 0.2797469937221493
0.4347406967821641 0.7273029373858080 0.7165274738124268
0.9403469810362424 0.2266245137509131 0.7197932147595125
0.9442652831015295 0.7196404642507446 0.7203017227162718
0.4448407793238331 0.6773071747009993 0.2796075115415348
0.9449699160089153 0.1892029090495768 0.2804043750907255
0.9628084946328102 0.6597295194849764 0.2796222906043511
0.3173237832951870 0.6612388843390775 0.6453966147434187
0.8231569153277150 0.1592825212856894 0.6462194282125466
0.8190407433382489 0.6627080542937023 0.6448026948455805
0.4804385326295062 0.8276822541048716 0.6337311653023576
0.9832859095216975 0.3332059329876316 0.6350900579970542
0.9854638770575832 0.8303532091349695 0.6347757029862748

0.3181125546998445 0.6612826209248226 0.3650065161119471
0.8236827004161995 0.1636406080136155 0.3631853293001868
0.8171722391560436 0.6664441590676375 0.3657709935150137
0.4801711228127203 0.8303871192751870 0.3543245580508980
0.9780283567055150 0.3405410181848865 0.3539428788366621
0.9863189244667652 0.8328902882147489 0.3535346939756536

3) *OH:

Fe2O3 *OH (2x2) (0001) surface, 75% covered Al2O3(0001)- total energy: -741.00638 eV
10.1955165863000001 0.0000000000000000 0.0000000000000000
5.0977577053000003 8.8295767077999994 0.0000000000000000
0.0000000000000000 0.0000000000000000 24.2761898040999995
Fe O H Al
20 60 24 12
0.3216123863304077 0.1545143973989411 0.6500325596582996
0.4884468082351958 0.3285411063638293 0.6343320607365825
0.4848278770408072 0.3279613816708604 0.4658195322837173
0.1501542910990565 0.4963162515838633 0.4390239517666998
0.4865430921984597 0.8278145289010226 0.4664414277553206
0.9851794323272571 0.3263546050852852 0.4663140440247062
0.9868980259629936 0.8267006279446960 0.4663950462567072
0.1515607371874239 0.9937960519853917 0.4392796624799544
0.6519438781691491 0.4954070276949309 0.4384751934828444
0.6554274219659533 0.9928227708255264 0.4388088095707232
0.1510898224023478 0.4955641399035642 0.5612500092426131
0.3178661606569051 0.1621617048803117 0.5345151410362590
0.3194857091688732 0.1582646677623814 0.3654795033590759
0.4860825162672811 0.3335435754310012 0.3506440747687805
0.1520096441231473 0.9942995169863025 0.5616412526156935
0.6540225799790775 0.4939390269914625 0.5607656940815176
0.6543022908132983 0.9902395682224849 0.5610819737770782
0.3199808422128214 0.6618605473023393 0.5335436446659259
0.8185034797662354 0.1601110301943152 0.5335628726295383
0.8196026111032708 0.6598619907165286 0.5337873398316191
0.3340050666265739 0.4978560746476433 0.6871241882616843
0.4758521849588035 0.1803041743940170 0.6922608614594807
0.1376803773291613 0.3233880422322741 0.6842577025279155
0.4682770955738889 0.5111268158990683 0.5955398521352606
0.3227545949383810 0.3121616864366246 0.5947286285887330
0.1560160020752477 0.1689548334682272 0.5958973881974643
0.5005335858840922 0.1454893250042488 0.4999510996982437
0.1514367901350226 0.3430880200955144 0.5000024755199348
0.3037492224259069 0.4948857594845819 0.5002450396144127
0.1352430469241810 0.1795741031445033 0.4048665748350189
0.4770697485737898 0.4919483254958976 0.4043276179423287
0.3325905876570729 0.3255438906698984 0.4052235700695803
0.1485749040614550 0.3116658740838787 0.3130693747577524
0.3217582717278304 0.5154069615891075 0.3135859696337562
0.4746835134706231 0.1687710771743056 0.3109761339135417
0.3424739660086900 0.9719708904580031 0.6866951187182906
0.8376177336350707 0.4883020507410123 0.6834671465346034
0.8429098637512951 0.9868700341685184 0.6841249266796012
0.4737321385769988 0.6737307640594139 0.6823104972488707
0.9753940547277011 0.1777472403397695 0.6829512780526557
0.9695948876313949 0.6804912389591493 0.6834131905601311
0.1478015250625049 0.8157360210639268 0.6819417083949588
0.6633097517720117 0.3090218195800674 0.6853560770004279
0.6487887519031119 0.8105051977499471 0.6816771114091793
0.4743637015333633 0.9979056713890841 0.5965580653349107
0.9690331371260186 0.5037345587342870 0.5964935055723615
0.9713845882487036 0.0019794307524208 0.5965473794543357
0.3256169548651968 0.8109730908520660 0.5961538476650645
0.8252919616249557 0.3095534429407891 0.5961343460927040
0.8274456210763503 0.8084703144645147 0.5961207152361325
0.1611629965968504 0.6680078590241365 0.5966493278177367
0.6692418338243229 0.1605416339278207 0.5957695359415496
0.6622939591766013 0.6671491408896628 0.5958486040046793
0.5017810174755368 0.6460647035383431 0.4998985358498089
0.0003251792519450 0.1447815341164969 0.5001024224073589
0.0011981834095991 0.6450232834107723 0.4999746462870505

0.1524806155252421 0.8431596628906064 0.5001650869455219
0.6511690303391831 0.3428870132934563 0.5001579413775232
0.6537131504811597 0.8420815082003443 0.5001138227805129
0.3039729627044210 0.9951311248653596 0.5001314998802115
0.8039324486210546 0.4937221933608029 0.4999272271090476
0.8045546526828886 0.9926132070891356 0.4999038713376294
0.1412290803137424 0.6797433865915252 0.4041656491166776
0.6470216841350691 0.1746687450952535 0.4041521331635849
0.6432016710251460 0.6767201354567760 0.4037912821452068
0.4858213740426365 0.9767120919229839 0.4040591385126859
0.9798142694395864 0.4839327170970336 0.4029340161610051
0.9790748534820324 0.9841908930071881 0.4040274430318505
0.3347074576649476 0.8218570167711832 0.4038971965619353
0.8337391742780653 0.3209868841002930 0.4035994922275847
0.8360786866884311 0.8191124858657872 0.4036399889246169
0.1530400296191203 0.8146081492216695 0.3174516437793500
0.6719526070120807 0.3063957856397366 0.3133140244872692
0.6569998951567797 0.8062241414304836 0.3170377665918735
0.3372994342482727 0.9884335485761753 0.3130703527178298
0.8330992314872745 0.5006669429251289 0.3159792548519178
0.8346324420372184 0.0009435002685834 0.3162235198477745
0.4675920082714313 0.6723051113447056 0.3185281940944975
0.9731621318460668 0.1718976825102843 0.3188227049694206
0.9673525039747304 0.6764106641353180 0.3181821452890787
0.2375802384033250 0.4984622022854666 0.6875984900611058
0.2273984576416481 0.5118391841939598 0.3129445888980129
0.1118804569465297 0.3224591724814019 0.7226099356961129
0.1619486810157937 0.2569577104744454 0.2788535705201340
0.4277765391171613 0.2466507965108491 0.7237037463156994
0.4307716462782025 0.1878435937168206 0.2743407823187880
0.2452980550476482 0.9738328186791350 0.6871385645357861
0.7413401140789446 0.4893362805992183 0.6867208789812551
0.7453421692562969 0.9911049776391820 0.6877000251604457
0.2422830665554727 0.9861199307505331 0.3125892658291036
0.7383415407497296 0.4988412674691318 0.3129040211352532
0.7382818564370552 0.0022223136643618 0.3129263844869072
0.1303068829533842 0.8075560018863044 0.7206487915983502
0.6433182347340534 0.2831657743429190 0.7216401619176125
0.6297552867195577 0.8104010246172280 0.7206962428164658
0.1681919897758348 0.7694318040457517 0.2811426737152800
0.6850425577306893 0.2524230785060979 0.2788619066324998
0.6690848316079894 0.7705848213831672 0.2793694413159287
0.4475145250653014 0.7146365786884559 0.7193096726904784
0.9408074594330884 0.2216247364900568 0.7192069833473980
0.9398541543701810 0.7227598975281282 0.7201058054505651
0.4438549542338421 0.6785692637647784 0.2796902414092699
0.9463783532721308 0.1782124298060808 0.2802865451901013
0.9489094575817347 0.6758926608204661 0.2791244849209278
0.3180055001181827 0.6608613840361457 0.6461345786887378
0.8261381151653211 0.1552903632712130 0.6460516270724526
0.8205779700199045 0.6572318534279731 0.6459451922853248
0.4874031577416602 0.8225352368952983 0.6349863354242231
0.9831738227093467 0.3292269575724660 0.6351389379969703
0.9853077120175726 0.8274341183714853 0.6349609584944460
0.3154179473766376 0.6654974608478454 0.3654497749451480
0.8231682977926695 0.1591550443612206 0.3652299624161159
0.8192909124856058 0.6597324334730672 0.3646904439159115
0.4864411834063702 0.8257211492201293 0.3537311108783570
0.9822425492230593 0.3316483357411997 0.3536271938622448
0.9827905212113421 0.8313223479531331 0.3543030257308075

4) *O:

Fe2O3 *O (2x2) (0001) surface, 75% covered Al2O3(0001) – total energy: -730.05219 eV
10.1955165863000001 0.0000000000000000 0.0000000000000000
5.0977577053000003 8.8295767077999994 0.0000000000000000
0.0000000000000000 0.0000000000000000 24.2761898040999995
Fe O H Al
20 60 22 12
0.3222273911709621 0.1560087540220607 0.6473317851358047
0.4863102774058987 0.3225687684132410 0.6363425169328920

0.4834137072084985 0.3266836606513834 0.4671737374158127
0.1465979204046874 0.4969741087426627 0.4394441478655082
0.4859129280271546 0.8252490483130757 0.4662353919960296
0.9842080602359715 0.3249945125491323 0.4660327339335950
0.9856421917901912 0.8258970652656927 0.4665456249967761
0.1509479851656295 0.9928785714437183 0.4387303377624647
0.6526603920848189 0.4925789900577584 0.4388227018460498
0.6538198274473004 0.9902832119831118 0.4387767972881704
0.1475685185275140 0.4961785938376835 0.5614669304003570
0.3172737533836525 0.1603606030410916 0.5329886794127390
0.3208846970396380 0.1594931958989179 0.3639055041111874
0.4830986527451699 0.3278405255671615 0.3526770526427896
0.1519306697126979 0.9908203563289888 0.5612894531957835
0.6518014789746900 0.4914166584482800 0.5615925724020698
0.6535986878464115 0.9896306749819672 0.5610317301660928
0.3189297823995361 0.6598215400342582 0.5341859301440621
0.8182088319849825 0.1579229247513751 0.5340488575226914
0.8173169078801763 0.6578328929505091 0.5344079757271416
0.3352630947417339 0.4927695000553669 0.6870773213544510
0.4666668820305517 0.1656416603266493 0.6837449125409165
0.1396412314201712 0.3241574918067442 0.6830743041387493
0.4666107018952772 0.5073231687416140 0.5958156480739945
0.3210917431674147 0.3104144740561452 0.5931883695147349
0.1591958917076823 0.1686987556709809 0.5975557275833694
0.5005795934609267 0.1430639774734317 0.4999866562022817
0.1493169132129495 0.3420278283363700 0.5000076796301514
0.3016727983561864 0.4942492812746337 0.5006681324362177
0.1343061581147040 0.1786050078298231 0.4043172366077457
0.4763244966033824 0.4847787651419182 0.4030946863116043
0.3312335430238562 0.3251758412840715 0.4073769767429667
0.1465162680148069 0.3153481869982997 0.3143446928519964
0.3227994798852905 0.5102829325377840 0.3151432422211116
0.4672787888030712 0.1903130252476046 0.3153460667280612
0.3371616062356537 0.9763652424425615 0.6841446021986286
0.8356979235058972 0.4904790527846004 0.6839291165645349
0.8451597946396916 0.9876246187523208 0.6849414958603290
0.4709812077467319 0.6722076234481875 0.6811877458819566
0.9749238883038061 0.1790324009001694 0.6836414570768099
0.9635383005819449 0.6827857698329538 0.6833899183990297
0.1460856264508337 0.8128015550918946 0.6817457451638731
0.6595623431306734 0.3006163460891642 0.6869303902414643
0.6390510205646223 0.8056161070551155 0.6832414044971387
0.4705542470846211 0.9952892131593103 0.5941404228186826
0.9662459590756072 0.5041979387031645 0.5967220756297422
0.9715942997076539 0.0014047364823497 0.5968854641250374
0.3239740201543313 0.8082949551415339 0.5957171464530617
0.8248187064498254 0.3090867190192270 0.5974046049706558
0.8249720317307805 0.8094042401044632 0.5967504240063732
0.1589509850670012 0.6668688675155892 0.5971325790106761
0.6703598765740324 0.1586871435508428 0.5956594171365666
0.6601414169639597 0.6653577863595146 0.5958821424851450
0.5000710133654209 0.6428893907359239 0.4992025047430815
0.0007408092756336 0.1438806755490134 0.5010608449473608
0.9989365426883552 0.6443718587697873 0.5004085240748353
0.1512721851684944 0.8419621089831040 0.5004118982658170
0.6507861496092673 0.3412057046876953 0.5006300076491783
0.6526485789007737 0.8398521237467662 0.5001895229368429
0.3023676870686955 0.9931725773113698 0.4996254754926213
0.8023537555038516 0.4918427446300626 0.5000394413119480
0.8037233990165049 0.9912207969804712 0.5000442335436830
0.1397736230568185 0.6790095496902566 0.4045335745120866
0.6464921750076300 0.1740459758637698 0.4057426254601140
0.6414642162068986 0.6748402018056794 0.4038219827451854
0.4839161874350566 0.9757030238894302 0.4043741262312608
0.9772723410460031 0.4829456406148793 0.4033964690727174
0.9778193361129155 0.9833023906356360 0.4042171088304869
0.3334956244940273 0.8192291394492628 0.4035011415081442
0.8322227765744685 0.3193779598180058 0.4036671351900125
0.8351704688143826 0.8173863687151766 0.4039269927677722
0.1508918080559880 0.8115634380149217 0.3175324941522675
0.6659860031351741 0.3045328775302210 0.3146311559280548

0.6540853842260645 0.8071312112064888 0.3182231431772493
0.3388190665688242 0.9893832864772136 0.3129489885543535
0.8316845992372706 0.4994945395666051 0.3161135011054128
0.8325501700737448 0.0000915530045660 0.3168792830983946
0.4644391469052209 0.6715606151912610 0.3188073092859014
0.9691931875749802 0.1723914512487426 0.3185112402230956
0.9629563647533814 0.6764107923867826 0.3187782945288404
0.2430410709506958 0.4864569353897679 0.6907589975247390
0.2324934938566798 0.4998303138774958 0.3127177047876017
0.1305162602389629 0.3140680304529724 0.7224137695514941
0.1673949306142006 0.2733538426567748 0.2774128440412866
0.2375063280079317 0.9836082683004506 0.6841397193905152
0.7397835473289263 0.4917214669982428 0.6884884711007402
0.7448473404092155 0.9991831479203555 0.6885778102972466
0.2415369749076035 0.9920933120668280 0.3110734131723376
0.7366081092306729 0.4985982222375327 0.3126605880328128
0.7363374007487948 0.0014021015071819 0.3132128431867898
0.1283458843041672 0.8211241923240209 0.7210355254239786
0.6394267959419082 0.2779701883889416 0.7237526436447013
0.6144351075278038 0.9036758603464747 0.6982638653298494
0.1641466315398148 0.7758567309942066 0.2798313433452861
0.6725615411973678 0.2509055017754349 0.2805995655660709
0.6651495178023339 0.7881724203623790 0.2789776309354437
0.4651152278665194 0.7000782467806417 0.7196222711903886
0.9446592808739496 0.2181245956652944 0.7207132348840020
0.9477945791288036 0.7087340498173660 0.7221157666451603
0.4533071238909940 0.6645989891066719 0.2795471821894395
0.9434455124779291 0.1784183195779718 0.2798680709415891
0.9616887389936295 0.6576511413621162 0.2798364225299110
0.3161081733074198 0.6566111387804909 0.6470443348561261
0.8262678130622731 0.1557358114268794 0.6464508360528569
0.8142459672477287 0.6615461693441276 0.6468202729342849
0.4832641364660759 0.8204163154900073 0.6349244983658409
0.9809850895509626 0.3321658410807871 0.6367221327629835
0.9841282043983668 0.8261227447262485 0.6359097441983650
0.3130554223646058 0.6632655623052131 0.3647874466093413
0.8212993682513172 0.1579643918215012 0.3653617711679900
0.8170904840465383 0.6585523216966536 0.3645219916879512
0.4836495805209466 0.8249426774333202 0.3535591042126995
0.9816031928209696 0.3299864842200861 0.3533139794386599
0.9807900704068899 0.8296547967659365 0.3543359183088128

5) *OOH:

Fe2O3 *OOH (2x2) (0001) surface, 75% covered Al2O3(0001) – total energy: -749.08232 eV
10.1955165863000001 0.0000000000000000 0.0000000000000000
5.0977577053000003 8.8295767077999994 0.0000000000000000
0.0000000000000000 0.0000000000000000 24.2761898040999995
Fe O H Al
20 62 24 12
0.3167505374400292 0.1537266763842950 0.6497588586757672
0.4879242785748588 0.3290124416623357 0.6341217176961251
0.4836727784313126 0.3256413660472646 0.4668434076496411
0.1495037395676163 0.4939552421582434 0.4389987082694091
0.4855346544366910 0.8265165775025594 0.4660603335841174
0.9847197020280447 0.3244061350655940 0.4659009786588939
0.9863757440817906 0.8248552802990545 0.4661624130413955
0.1507819265758314 0.9922379330305091 0.4390631506162492
0.6521337639982079 0.4937553101023866 0.4381354634951222
0.6557271287402955 0.9896980998737277 0.4385706850448585
0.1506042485641359 0.4933825354283172 0.5614404887610078
0.3171424218259986 0.1602094531470186 0.5344817998200142
0.3171346057240498 0.1574141618502978 0.3647109997366087
0.4884694832776120 0.3317814670016546 0.3528738482393265
0.1507813947024843 0.9926293581281413 0.5615066156490585
0.6536733987384196 0.4925587765912454 0.5604056724038315
0.6533762708323536 0.9886638837856694 0.5609772484234838
0.3195253084570879 0.6604726365356655 0.5331476704220819
0.8178197224858508 0.1582529781677238 0.5336635338287010
0.8189972877697898 0.6580679210147693 0.5333662999379172
0.3356390788169534 0.4955339365103271 0.6855627144365570

0.4883409102274854 0.1622709780463936 0.6877610073563929
0.1357322533625052 0.3221516352149791 0.6832351286288230
0.4679534797004266 0.5101094503125481 0.5947825055946723
0.3230389087198873 0.3094134945127465 0.5948274283160657
0.1540636651371514 0.1675563850474191 0.5958253689790709
0.5002347293775173 0.1431240225124455 0.5002366914192820
0.1509297304010886 0.3411458884093861 0.5000268487028663
0.3030634756525714 0.4929979099653607 0.5004423178821824
0.1337068561289101 0.1781461415907799 0.4047480636475029
0.4761305083017930 0.4919590581636157 0.4043608244362318
0.3338078429420932 0.3227706447137777 0.4058129612111685
0.1483459381032262 0.3130228290870960 0.3149423119715280
0.3195321550435395 0.5091908994715197 0.3129078784208943
0.4705673043486414 0.1746886541557586 0.3078760067652411
0.4629234630345422 0.2050750741489225 0.7463768480382384
0.4140550155429068 0.2317298103526255 0.2522087320783726
0.3430315505687034 0.9700391256910805 0.6872444484941909
0.8359500391201138 0.4876398324747484 0.6834226082437880
0.8424926681887897 0.9830914453832236 0.6837263751856142
0.4741148773693098 0.6713325631040448 0.6818183368372246
0.9733099714848876 0.1761249320034040 0.6827796890969609
0.9703113961291550 0.6773343207323776 0.6830315479293603
0.1477917967155591 0.8137204560451323 0.6818318107683439
0.6604644205828976 0.3040304772644404 0.6862336483810196
0.6500145959871517 0.8068090651025912 0.6831824484182789
0.4738190138264144 0.9956407248699222 0.5967965177589534
0.9675681130476832 0.5021387772771888 0.5960730562560386
0.9704483341474059 0.0004187334144277 0.5963997712605007
0.3248687467970441 0.8098008682578097 0.5961372700251459
0.8231731620631351 0.3085138503933962 0.5964651283972344
0.8261386259806898 0.8070040295783159 0.5961072129793124
0.1602933103886244 0.6668609950319393 0.5961066916638416
0.6686427186512063 0.1589605223424257 0.5953389787159722
0.6613718174712844 0.6659507708526036 0.5955472218405902
0.5012927730037262 0.6447146372235508 0.4995546747753963
0.9994485276930902 0.1432017238262304 0.4999776390919877
0.0008527871643622 0.6431200536684898 0.4998516803562438
0.1518865981263531 0.8415695625385524 0.4998670251512678
0.6508044451647947 0.3407998457011558 0.4997826352583274
0.6530616455213547 0.8403365790265482 0.4997807913925456
0.3033891920981446 0.9935424441507479 0.4999973434731046
0.8031565477301399 0.4918721579722671 0.4995942838755880
0.8041205429964720 0.9906439382978505 0.4996891929862244
0.1422619815892148 0.6766195807458715 0.4038172668289661
0.6472610887313053 0.1709747683629743 0.4035377217433691
0.6426563037859836 0.6757314850596998 0.4033748098759347
0.4852018572857162 0.9769973797648319 0.4035464346980859
0.9786844664562295 0.4820008524168813 0.4031377026045320
0.9792103843162820 0.9817474860138873 0.4036620318708799
0.3346520701164124 0.8202041052643310 0.4038368611291361
0.8325039154023415 0.3190407547010068 0.4029620736334678
0.8370020804114588 0.8163882172287416 0.4035126668860585
0.1540569807113883 0.8109079538446622 0.3173686506167641
0.6709379415803625 0.3033880676243328 0.3127992538826447
0.6563017395228172 0.8062296395801596 0.3177511190710547
0.3372241869361474 0.9867504470448409 0.3135101693670066
0.8334523139040257 0.4990138329279006 0.3156642758091053
0.8365123982550813 0.9974550669729538 0.3157142321366777
0.4669419469502998 0.6701617693041371 0.3182905079927778
0.9730256778782191 0.1697938606880314 0.3184520753262206
0.9674213925533124 0.6737196975427011 0.3182524110904836
0.2412711937498599 0.4931143894822583 0.6888057932882248
0.2227420065429229 0.5109633115210386 0.3171961460952630
0.1136008104302064 0.3381747839103539 0.7222193977773799
0.1746797931737660 0.2714869637640618 0.2779173471688168
0.4997176790828632 0.1043653012079773 0.7623340547637341
0.3678741043344331 0.3422962523805992 0.2582609445903259
0.2467278517066021 0.9701340639809004 0.6883345774823013
0.7398650683712518 0.4883308113229958 0.6867125500797329
0.7450211688961161 0.9865449766000367 0.6861564687079564
0.2415216786256806 0.9861418560922459 0.3119411467384694

0.7382956643487049 0.4985473427743514 0.3115001664613217
0.7408338370171919 0.9981874814518363 0.3112747534660727
0.1305373438552309 0.8038305487149486 0.7204322000287746
0.6326925068472562 0.2786777969737173 0.7214163045228190
0.6361560675190674 0.7806940414790802 0.7202660862085679
0.1680702967176728 0.7700286554258966 0.2803891813508486
0.6792844637497382 0.2510242973568424 0.2783022156383126
0.6651385293391172 0.7904181595199447 0.2783205615261934
0.4489037980586303 0.7068512086015843 0.7194842289552597
0.9436272964911296 0.2162824820900013 0.7197447190917288
0.9385849872905112 0.7216931870582002 0.7193720613237673
0.4451262534219893 0.6768847823722481 0.2792677950074207
0.9505345607716080 0.1734413227163998 0.2795749486895147
0.9563390064109356 0.6648270310387616 0.2790958481976631
0.3172017839111945 0.6596025152153118 0.6455667833664620
0.8239530402781412 0.1534036728564345 0.6465321622060145
0.8204020626442130 0.6555138658690041 0.6453564002680778
0.4871037675924228 0.8211681353084046 0.6350428409031679
0.9805784213467490 0.3278307896110988 0.6354910661135094
0.9852505424815448 0.8253044213141720 0.6346960619960669
0.3156841246028037 0.6639508678567196 0.3651865396002947
0.8237865827629136 0.1563946591126140 0.3641760099733844
0.8189299688054490 0.6576620697722504 0.3641341894013763
0.4858452699060933 0.8243647728358923 0.3534395824843202
0.9816247661923825 0.3295099478446488 0.3529663490464969
0.9834354072249809 0.8284037912624740 0.3540816924654067

6. Relaxed geometry of pure Fe_2O_3(0001) (1x1) surface slabs at different reaction steps:

1) *Vacancy:

Fe2O3 *vac (1x1) (0001) surface, pure – total energy: -158.06793 eV
4.4147882200000002 2.5488791700000002 0.0000000000000000
0.0000000000000000 5.0977583400000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 24.2761897900000001
O Fe H
13 8 4
0.6903016877787920 0.8960434313124424 0.6930495361067059
0.2780866377481317 0.6434080579570320 0.6912366619728658
0.9326725420921917 0.0201317191880435 0.5969250349142570
0.6265221861966381 0.6288796009057549 0.5956594476571695
0.3045743473362350 0.3222781015906548 0.5954388156885528
0.9811321571257565 0.2979903272823634 0.5001913805301612
0.2855816021919964 0.6833126747677483 0.5000136677102844
0.5946467890433667 0.9927765758269871 0.5002221976837546
0.2554354045303882 0.3477499481086852 0.4027729077329809
0.9527469553416452 0.9791336611775421 0.4049009588197450
0.6460259299636277 0.6539440420758709 0.4048704252861981
0.3702221333318718 0.6128979855975771 0.3082645567687408
0.6536218190755108 0.0126096060592715 0.3058266243717114
0.6205912019075583 0.2955592432540328 0.6559161016242783
0.9569493069191068 0.6634222656964184 0.6291094160429935
0.9492326271308897 0.6582899008909351 0.4633460837455772
0.2879576417312251 0.9883694566950183 0.4409865869717180
0.2922908264596913 0.9881650841944989 0.5593407751402992
0.6213669957914618 0.3279782631645389 0.5369235728452182
0.6112223579583045 0.3256213802079628 0.3706651226649313
0.9745201602050670 0.6663482671690133 0.3451315297993531
0.5096017744380177 0.8734551486970901 0.6941275465118792
0.4888324363262839 0.9661493191631081 0.3029960587766780
0.1863809599978339 0.6428271520800024 0.7263024517517138
0.4281429076742924 0.4786037663752651 0.2763660049578434

2) *OH2:

Fe2O3 *OH2 (1x1) (0001) surface, pure – total energy: -187.96179 eV
4.4147882200000002 2.5488791700000002 0.0000000000000000
0.0000000000000000 5.0977583400000004 0.0000000000000000

0.0000000000000000 0.0000000000000000 24.2761897900000001
O Fe H
15 8 8
0.6799122381264056 0.9356985033985623 0.6908868853872647
0.9936157948086404 0.2456938311111756 0.7169647217243522
0.2652497696482854 0.6646867836027468 0.6966242668272855
0.9271765838169443 0.0483179932368429 0.5953018975351299
0.6136513571484556 0.6630196436566891 0.5945790909563939
0.2972448237235810 0.3539710568030614 0.5952623117498419
0.9702204859584356 0.3300117226964900 0.4989145256886545
0.2767640371263980 0.7134425180410773 0.4986156343669705
0.5846615925924965 0.0235137341388594 0.4991564640775366
0.2488225734646790 0.3739252221883831 0.4017405218939771
0.9411824918847529 0.0036360161833002 0.4035608506909298
0.6349870975802006 0.6848070413090426 0.4036176580488799
0.3425283840573030 0.6741864076841324 0.3097760090851693
0.6857330410567641 0.0646532651597269 0.3003252776582457
0.0610303865437487 0.2620010380541586 0.2889249934512534
0.6262031925755664 0.3412031292829312 0.6552354598380603
0.9447322029530341 0.6945652698462581 0.6277434209432400
0.9400621581040767 0.6908014958162028 0.4618890651737857
0.2744708967281397 0.0195780199753202 0.4398790337731810
0.2815728663054600 0.0232715677829916 0.5580114863210852
0.6102598287121097 0.3589496795695126 0.5359665464566703
0.6029561271413115 0.3562866392360746 0.3701983584310184
0.9454162098562691 0.6738384192252695 0.3421324111046289
0.4900074474124736 0.9342585939947057 0.6910024769466361
0.4971301538004766 0.1070276783116455 0.2825396652414938
0.1873462568586106 0.5771560352767011 0.7232639393270759
0.3794923938968324 0.5827833335609895 0.2733744405167968
0.8828722542260721 0.3005604908078183 0.7515966474633302
0.8866381257441276 0.2384207493556616 0.2770005788145014
0.0958422934039547 0.0136693001645867 0.7137773249907653
0.1892769147444042 0.0460648005290452 0.3035599455158575

3) *OH:

Fe2O3 *OH (1x1) (0001) surface, pure - total energy: -180.50668 eV
4.4147882200000002 2.5488791700000002 0.0000000000000000
0.0000000000000000 5.0977583400000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 24.2761897900000001
O Fe H
15 8 6
0.6664474990320883 0.9647714450179095 0.6922443170034640
0.9654016580927021 0.3479035331416114 0.6925080303341673
0.2963289043438166 0.6531916658648882 0.6892703644307545
0.9495424845612703 0.0110848470001557 0.5961268741672328
0.6431962829042135 0.6253468182099908 0.5956640475690662
0.3315479952140521 0.3207607914920203 0.5959472773517476
0.0018869278441898 0.2939317993878987 0.5000040616218868
0.3073173419229249 0.6835645820112362 0.5001219966561834
0.6130850291945791 0.9886390381120052 0.5000418220445226
0.2807974024094335 0.3518126311592624 0.4043740061545122
0.9725751808609573 0.9660053401741848 0.4039692385220874
0.6643371594569842 0.6566708995884269 0.4041461383214653
0.3258224724750036 0.6292153252477064 0.3076455104594373
0.6442919871113730 0.0123247509373172 0.3077715285491465
0.9620209531002786 0.3236903476677995 0.3108442093220702
0.6464783296995193 0.3097484806485653 0.6525636307197260
0.9748109220217174 0.6517664773419298 0.6352645413309048
0.9743133406168241 0.6554407532310194 0.4647803740855920
0.3065279975835864 0.9915106824931712 0.4399727301325456
0.3087242342805823 0.9858906772238925 0.5601090684782619
0.6408599551671728 0.3220919343076147 0.5352976645159373
0.6388876078997896 0.3253255793038008 0.3649000102565267
0.9686913562651824 0.6671795681122461 0.3474545076183304
0.4717269086944071 0.9679867248401948 0.6923439026998466
0.4527552537260604 0.0091465726194926 0.3075912799159468
0.2439543672514404 0.6167174688440156 0.7258624305116683
0.3619292610342058 0.4975567804198775 0.2759911600409595

0.8697026678003965 0.4795110628262123 0.7241778319772720
0.8730984994352511 0.3578800627755712 0.2742798152087218

4) *O:

Fe2O3 *O (1x1) (0001) surface, pure – total energy -169.30815 eV
4.4147882200000002 2.5488791700000002 0.0000000000000000
0.0000000000000000 5.0977583400000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 24.2761897900000001
O Fe H
15 8 4
0.6590407803697644 0.9658906162616603 0.6909216258998185
0.9223299957718822 0.3384000322241292 0.6856788024571046
0.2851625894348189 0.6298943448457024 0.6887398927401094
0.9357465196049333 0.0004526526754276 0.5951154824135969
0.6325915840534293 0.6195095836717073 0.5944277694141675
0.3302840625037575 0.3152726592670447 0.5974486850687128
0.9945407869588152 0.2839527838839047 0.5001288129631547
0.2950569995620214 0.6777258633890284 0.5001975480341656
0.6013660326548376 0.9827678369766915 0.4996959606537033
0.2741545081673280 0.3454650870728457 0.4050114964897276
0.9639994058049126 0.9488221337345735 0.4020388746166219
0.6565333804878790 0.6443530080712989 0.4060200582722473
0.3096600907143667 0.6280682808076534 0.3104123224175126
0.6473226082786923 0.9959036303454596 0.3103460569871856
0.9360705859322636 0.3623216383379955 0.3137384314673213
0.6411790760196752 0.3073195509671578 0.6504435489454679
0.9582506513456153 0.6424941004668767 0.6386336220624500
0.9638435355004233 0.6476432509609182 0.4652845515870467
0.2969229224262406 0.9824423959116118 0.4395658832955149
0.2968786482986800 0.9805175059787175 0.5605360440637668
0.6299640527074004 0.3149343713179675 0.5346400424636855
0.6351693403401839 0.3178632954852816 0.3621321961149775
0.9616975881650589 0.6442477701921305 0.3490728305506039
0.4662438540346230 0.9660530703029835 0.6929633554348555
0.4590281282401776 0.9894734176790507 0.3056001931752519
0.2617449002216077 0.5959106849817388 0.7274544905898566
0.3422773424006493 0.5389670841904461 0.2737521218213956

5) *OOH:

Fe2O3 *OOH (1x1) (0001) surface, pure – total energy: -188.55886 eV
4.4147882200000002 2.5488791700000002 0.0000000000000000
0.0000000000000000 5.0977583400000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 24.2761897900000001
O Fe H
17 8 6
0.6616463724304182 0.9541336501282984 0.6903721779133676
0.9854908409829903 0.3060955144835447 0.6865819464389986
0.2827962654094307 0.6342259409986681 0.6924393448939270
0.9398749488997424 0.0061288135461410 0.5955294741308421
0.6317105907094458 0.6203832293236076 0.5964177737055962
0.3210274521060015 0.3179624924942530 0.5947026260952484
0.9936368224582353 0.2849939927955347 0.4999637098050442
0.2986094983922882 0.6748540841103434 0.4996685619539036
0.6050179186418987 0.9796810608530464 0.4998244455640020
0.2727866001524362 0.3385000976467722 0.4037341246764328
0.9652187279358060 0.9590825015141462 0.4032735004984787
0.6598372933169827 0.6413618387891589 0.4043529514731503
0.3200286198005600 0.6193512806682904 0.3093213571736939
0.6386145361428746 0.9871543405524363 0.3073454528199164
0.9524418068552194 0.3185319352395197 0.3080847652308236
0.9600919212400569 0.3701182565861671 0.7458672250978822
0.8617635263434380 0.4036547333782039 0.2506988359133331
0.6256527449388045 0.3100778868605971 0.6525236433270578
0.9641941263377518 0.6522304830724721 0.6349312426061502
0.9652796183385206 0.6448315128806499 0.4648909926465024
0.3001899271838084 0.9785396779392173 0.4397207523213780
0.2992017289897362 0.9801170199423623 0.5599117163054999
0.6316083980011911 0.3141602940645924 0.5350991199686135
0.6306240488009962 0.3132946982356160 0.3630646681796890

0.9665211267351737 0.6542461819483094 0.3488002590861825
0.4737006220175317 0.9453315546707586 0.6916454822856366
0.4428884796320247 0.9924225058311720 0.3082770750167825
0.2278112443394278 0.5633585957135878 0.7256909532260778
0.3724074966142226 0.5149441919410833 0.2738321479011887
0.0566379013673668 0.1612480939846463 0.7596503770652276
0.7665499282939408 0.6270935309310488 0.2526184645281973

7. Relaxed geometry of pure Fe_2O_3(0001) (2x2) surface slabs at different reaction steps:

1) *Vacancy:

Fe2O3 *vac (2x2) (0001) surface, pure – total energy: -699.86091 eV
10.1955165863000001 0.0000000000000000 0.0000000000000000
5.0977577053000003 8.8295767077999994 0.0000000000000000
0.0000000000000000 0.0000000000000000 24.2761898040999995
Fe O H
32 58 22
0.515455 0.669896 0.464372
0.670799 0.844823 0.652901
0.848945 0.00276834 0.43917
0.517968 0.665388 0.635092
0.0153597 0.66923 0.465131
0.1873 0.824494 0.652731
0.350327 0.000916544 0.440366
0.00841294 0.669022 0.636173
0.516177 0.168964 0.463666
0.692132 0.330282 0.652543
0.844223 0.504468 0.440541
0.512994 0.178536 0.629966
0.016046 0.169443 0.464812
0.185266 0.335822 0.653358
0.350179 0.50329 0.440288
0.0250098 0.162521 0.637161
0.518624 0.664988 0.347322
0.682244 0.836642 0.535386
0.852534 0.000306294 0.559679
0.673224 0.845445 0.361755
0.00640671 0.672882 0.346943
0.182249 0.836312 0.535675
0.348216 0.00189183 0.559822
0.186797 0.827503 0.365059
0.504616 0.180583 0.346216
0.682809 0.33524 0.534903
0.8491 0.502471 0.560597
0.687699 0.33007 0.364794
0.02296 0.161521 0.347519
0.181568 0.33682 0.536124
0.348687 0.504965 0.559843
0.177476 0.34316 0.37069
0.857299 0.827666 0.401721
0.524539 0.996038 0.595047
0.520279 0.510792 0.403975
0.67993 0.683957 0.595578
0.668177 0.671637 0.403632
0.829766 0.841886 0.597793
0.832222 0.686433 0.307781
0.00135842 0.849358 0.500163
0.68866 0.505584 0.691
0.658207 0.00282335 0.304212
0.847267 0.657318 0.49982
0.513809 0.819444 0.690355
0.518594 0.833154 0.308405
0.696413 0.00223478 0.499417
0.846422 0.682589 0.692389
0.361797 0.81931 0.40522
0.0323095 0.986732 0.596248
0.0105513 0.518991 0.405486

0.178505 0.680043 0.596273
0.16692 0.667482 0.404276
0.338062 0.831049 0.595216
0.345136 0.67289 0.308786
0.502004 0.850044 0.499829
0.162473 0.514407 0.694386
0.197539 0.984164 0.311489
0.349154 0.654914 0.500127
0.00896417 0.834756 0.689721
0.0331808 0.827362 0.307085
0.196068 0.00268072 0.500269
0.363361 0.660907 0.690327
0.866511 0.320647 0.403494
0.533302 0.485572 0.595762
0.509784 0.0201368 0.402352
0.685271 0.180472 0.5951
0.670561 0.173026 0.40588
0.842785 0.332989 0.597523
0.845988 0.179018 0.307947
0.0021814 0.349375 0.500262
0.61369 0.033319 0.695909
0.700102 0.494127 0.310359
0.851135 0.154789 0.500298
0.517306 0.327561 0.688923
0.52977 0.339036 0.306673
0.696614 0.502001 0.499957
0.864296 0.164444 0.691069
0.357067 0.326753 0.404998
0.0254991 0.495964 0.594096
0.0204255 0.0105983 0.403861
0.187246 0.179971 0.5976
0.173388 0.167922 0.403954
0.335737 0.338604 0.59558
0.50179 0.349483 0.50019
0.194432 0.994608 0.689418
0.179106 0.488357 0.311157
0.348568 0.156194 0.49997
0.0456943 0.293083 0.697284
0.0616386 0.306635 0.306956
0.196067 0.502831 0.500031
0.62901 0.538608 0.724813
0.636636 0.962748 0.271205
0.0994208 0.530373 0.726686
0.175526 0.966824 0.274079
0.553033 0.0311841 0.726465
0.675393 0.474387 0.273668
0.146292 0.0305511 0.725171
0.15036 0.458862 0.277055
0.82097 0.601296 0.693254
0.364157 0.564064 0.691724
0.87449 0.0631633 0.691843
0.354969 0.571816 0.307684
0.802651 0.608008 0.306068
0.848772 0.081492 0.305236
0.406284 0.89986 0.693062
0.944957 0.371874 0.708616
0.410882 0.913336 0.308603
0.964044 0.39541 0.298294
0.0268073 0.791913 0.726595
0.0984408 0.779479 0.275294
0.552929 0.266729 0.722345
0.592339 0.29093 0.274342

2) *OH2:

Fe2O3 *OH2 (2x2) (0001) surface, pure – total energy -729.47420 eV
10.1955165863000001 0.0000000000000000 0.0000000000000000
5.0977577053000003 8.8295767077999994 0.0000000000000000
0.0000000000000000 0.0000000000000000 24.2761898040999995
Fe O H

32 60 26
0.518449 0.668261 0.464078
0.677986 0.841638 0.653009
0.853796 0.00157493 0.439193
0.523082 0.661115 0.634562
0.0184597 0.667122 0.464978
0.191437 0.826871 0.651683
0.352694 0.0010973 0.44011
0.0153675 0.666906 0.635167
0.519995 0.164405 0.46212
0.692892 0.326809 0.651415
0.848159 0.501358 0.440399
0.519287 0.174074 0.627891
0.0200013 0.168784 0.464463
0.191855 0.332639 0.655813
0.353993 0.49802 0.438913
0.0224814 0.167658 0.635326
0.528822 0.662074 0.347402
0.685018 0.835062 0.535129
0.857452 0.997344 0.558977
0.679668 0.845491 0.363229
0.0116958 0.676395 0.347067
0.186568 0.834153 0.535049
0.351133 0.00085485 0.559418
0.195565 0.824719 0.364819
0.514017 0.179881 0.344648
0.686003 0.333281 0.533424
0.852983 0.501595 0.560248
0.685072 0.328154 0.363473
0.0176422 0.161531 0.347767
0.185337 0.335478 0.537141
0.352044 0.502567 0.558798
0.172097 0.344183 0.367829
0.8651 0.823709 0.403251
0.528708 0.991887 0.594536
0.522759 0.510389 0.403201
0.684507 0.681325 0.59578
0.674067 0.669294 0.403757
0.834488 0.839502 0.597207
0.837616 0.693995 0.307015
0.00615352 0.846999 0.499815
0.693031 0.498681 0.69021
0.685708 0.999681 0.309018
0.850994 0.655144 0.499873
0.529319 0.804975 0.691567
0.53507 0.826256 0.307661
0.700354 0.999994 0.499186
0.855848 0.684488 0.69301
0.367426 0.819183 0.403985
0.0366042 0.986368 0.595496
0.0137028 0.517978 0.405164
0.183545 0.67966 0.59549
0.173442 0.66527 0.403067
0.341928 0.831487 0.596234
0.354157 0.67602 0.307346
0.504787 0.847564 0.500011
0.169034 0.517673 0.693863
0.203847 0.99742 0.307887
0.352625 0.653422 0.499435
0.0122524 0.838032 0.688128
0.047164 0.825436 0.306112
0.199661 0.00102752 0.499695
0.365259 0.662417 0.689941
0.866788 0.318162 0.403948
0.535716 0.483656 0.594893
0.516059 0.013758 0.404094
0.688907 0.178074 0.593246
0.674695 0.169686 0.405518
0.84253 0.331993 0.595527
0.844042 0.175237 0.307843
0.0062944 0.347483 0.500274

0.619614 0.0302922 0.694232
0.71017 0.49226 0.309756
0.855594 0.152033 0.499459
0.521189 0.322032 0.68813
0.527304 0.353529 0.304255
0.699519 0.500767 0.499441
0.865315 0.15943 0.689401
0.356533 0.326194 0.40119
0.0293181 0.49392 0.594283
0.0259902 0.00637979 0.402692
0.191115 0.176924 0.598274
0.173937 0.167497 0.402782
0.340532 0.336028 0.594987
0.329577 0.174853 0.297649
0.504896 0.346951 0.498486
0.185745 0.00116717 0.694756
0.165019 0.491603 0.305848
0.351084 0.155312 0.499543
0.0228069 0.310099 0.693566
0.0282972 0.325678 0.308203
0.199773 0.500621 0.499462
0.316762 0.157228 0.724981
0.635007 0.53167 0.724348
0.677726 0.958752 0.273804
0.102904 0.540156 0.725675
0.177152 0.971931 0.272522
0.535505 0.0484993 0.718771
0.683874 0.473244 0.273228
0.111164 0.0297406 0.724306
0.100807 0.480318 0.278537
0.265379 0.0962799 0.715296
0.836381 0.599917 0.695852
0.358712 0.569475 0.69183
0.875782 0.0579282 0.688132
0.372302 0.571402 0.304799
0.810599 0.614746 0.302647
0.836896 0.0823646 0.306166
0.282692 0.107423 0.298061
0.426155 0.881743 0.701142
0.915713 0.386149 0.698308
0.42789 0.903952 0.30591
0.9192 0.402268 0.307754
0.0241093 0.797602 0.725191
0.115644 0.769954 0.275813
0.561651 0.255134 0.719989
0.582908 0.312096 0.270119
0.280184 0.248943 0.26837
0.258003 0.219635 0.755971

3) *OH:

Fe2O3 *OH (2x2) (0001) surface, pure - total energy: -722.27368 eV
10.1955165863000001 0.0000000000000000 0.0000000000000000
5.0977577053000003 8.8295767077999994 0.0000000000000000
0.0000000000000000 0.0000000000000000 24.2761898040999995
Fe O H
32 60 24
0.515849 0.668417 0.464877
0.675935 0.841853 0.65302
0.849623 0.000862954 0.439802
0.521962 0.662056 0.634845
0.0158132 0.667401 0.464539
0.191405 0.825303 0.652375
0.347791 0.00194091 0.440248
0.00945978 0.672988 0.635757
0.515814 0.167401 0.464539
0.691405 0.325303 0.652376
0.847791 0.50194 0.440248
0.509459 0.172988 0.635757
0.0158494 0.168417 0.464877
0.175935 0.341852 0.653019

0.349623 0.500863 0.439802
0.0219622 0.162056 0.634845
0.520319 0.66188 0.347817
0.682763 0.83469 0.535463
0.849303 0.00177888 0.560074
0.675297 0.841276 0.363849
0.0057348 0.675635 0.346884
0.181937 0.834417 0.535188
0.349214 0.000608048 0.560014
0.187685 0.828207 0.365497
0.505736 0.175635 0.346884
0.681938 0.334417 0.535189
0.849214 0.500608 0.560014
0.687685 0.328207 0.365497
0.0203197 0.161879 0.347816
0.182763 0.33469 0.535462
0.349303 0.501778 0.560074
0.175297 0.341277 0.363849
0.858385 0.824884 0.403397
0.525885 0.992335 0.595997
0.520124 0.509523 0.404107
0.682528 0.681346 0.595477
0.669779 0.668781 0.404014
0.832691 0.83823 0.596395
0.8301 0.696701 0.30692
0.00137396 0.848061 0.499986
0.6949 0.499559 0.68987
0.671707 0.00176913 0.309043
0.848759 0.654586 0.499982
0.524736 0.810613 0.691778
0.524802 0.828237 0.30897
0.696238 0.00125737 0.499916
0.851331 0.681928 0.692671
0.363013 0.81915 0.404967
0.0327207 0.985122 0.595589
0.0124715 0.51721 0.404084
0.180487 0.679635 0.596028
0.168242 0.667783 0.404267
0.34001 0.830756 0.59579
0.344635 0.675681 0.308845
0.502042 0.848947 0.500079
0.159187 0.517887 0.69301
0.200311 0.990955 0.310321
0.349475 0.653375 0.500094
0.0145709 0.83407 0.689242
0.0323919 0.834125 0.308438
0.196455 0.00103725 0.500091
0.366411 0.661561 0.690239
0.863014 0.31915 0.404967
0.532721 0.485122 0.59559
0.512472 0.0172104 0.404084
0.680487 0.179635 0.596029
0.668242 0.167783 0.404267
0.840009 0.330756 0.59579
0.844636 0.175681 0.308845
0.00204172 0.348947 0.500078
0.659187 0.0178871 0.69301
0.700311 0.490956 0.310321
0.849476 0.153375 0.500094
0.51457 0.334071 0.689242
0.532393 0.334124 0.308438
0.696455 0.501037 0.500091
0.866411 0.161561 0.690239
0.358385 0.324884 0.403397
0.0258847 0.492335 0.595997
0.0201243 0.00952288 0.404107
0.182527 0.181346 0.595477
0.16978 0.168781 0.404014
0.332691 0.33823 0.596395
0.330101 0.196701 0.30692
0.501375 0.348061 0.499986

0.1949 0.999559 0.689869
0.171706 0.50177 0.309043
0.34876 0.154586 0.499982
0.024736 0.310613 0.691778
0.0248019 0.328238 0.30897
0.196238 0.501258 0.499916
0.35133 0.181929 0.692671
0.639366 0.533011 0.72453
0.651551 0.966688 0.274453
0.0981027 0.533482 0.725881
0.175908 0.969967 0.273771
0.598102 0.0334827 0.725881
0.675907 0.469968 0.273771
0.139366 0.0330104 0.72453
0.15155 0.46669 0.274453
0.328712 0.0990253 0.693708
0.828713 0.599025 0.693708
0.369608 0.563367 0.691175
0.869607 0.0633673 0.691175
0.346657 0.57824 0.307383
0.806917 0.615715 0.300455
0.846659 0.0782394 0.307383
0.306918 0.115715 0.300455
0.417711 0.885158 0.698295
0.91771 0.385158 0.698295
0.41647 0.905327 0.308634
0.91647 0.405327 0.308634
0.028876 0.793045 0.726302
0.0926065 0.786888 0.275535
0.528875 0.293045 0.726303
0.592608 0.286887 0.275535

4) *O:

Fe2O3 *O (2x2) (0001) surface, pure – total energy: -710.98750 eV
10.1955165863000001 0.0000000000000000 0.0000000000000000
5.0977577053000003 8.8295767077999994 0.0000000000000000
0.0000000000000000 0.0000000000000000 24.2761898040999995
Fe O H
32 60 22
0.3258037661864179 0.1589183926508255 0.6500250756463046
0.3228415203766133 0.6555067612989092 0.6525708346555561
0.8213599228361019 0.1551842896739828 0.6531794627454488
0.8226201216151168 0.6565568522408398 0.6522892519329133
0.4844045226367442 0.3250923778518029 0.6367692030092371
0.4862664207060661 0.8278855398847611 0.6351912992078752
0.9855468707961634 0.3272737196342916 0.6366643890668868
0.9876351093747004 0.8263196548511047 0.6354023496639982
0.4865704237836965 0.3273457196645069 0.4659768848017833
0.4872139497250885 0.8260677739171882 0.4644520394188021
0.9869962211803909 0.3271230029494134 0.4642290232943651
0.9869480477083243 0.8279819889905582 0.4649004963720813
0.1515634360111946 0.4963493199579361 0.4400725950041746
0.1539225192289848 0.9954637796502013 0.4394975909136534
0.6548316094053632 0.4933260736087988 0.4398332070004898
0.6529552051755516 0.9937531365893051 0.4398512964554513
0.1517960837407060 0.4948788640441393 0.5599064106147154
0.1549186554972337 0.9923429309875615 0.5601506215618741
0.6534829904493762 0.4926805680593844 0.5604655288669846
0.6549025699106181 0.9938781974549897 0.5601534121731433
0.3202473764931995 0.1611441047818474 0.5338954210453863
0.3199051594581803 0.6608733971245400 0.5354792669295279
0.8208282420959847 0.1607688207149920 0.5357927363480783
0.8190241286802546 0.6607981965341949 0.5352242371589568
0.3219853632844405 0.1636993073404724 0.3634740272363430
0.3196165202374814 0.6597619044019893 0.3640572347800273
0.8202713479158064 0.1608915450998083 0.3644544970235941

0.8188995012179277 0.6615132806690838 0.3644868382028719
0.4857339663657712 0.3253540029380133 0.3496530900771120
0.4831772916381354 0.8326901702870586 0.3475170173626339
0.9857687579757624 0.3317937894847347 0.3467146038821838
0.9848832919843815 0.8312738508398070 0.3476720943888552
0.3329575473402215 0.4846157413297831 0.6916979949300099
0.3342969652944561 0.9873464686612436 0.6908928543397224
0.8320801893576188 0.4848027741582257 0.6926449829518191
0.8315485174903472 0.9813742744265639 0.6919204264226693
0.4662098643812200 0.1735180705529729 0.6852590532210314
0.4832211436250518 0.6751103979967468 0.6919922654838970
0.9817929022299694 0.1742066883865903 0.6927363732149914
0.9829663872330912 0.6737485857565844 0.6921370174631463
0.1497877772592773 0.3273499057691680 0.6872948354369726
0.1478729869791451 0.8276057382540216 0.6891276318595274
0.6438241934632671 0.3179143547247207 0.6914598725988057
0.6477892285289713 0.8294970725688700 0.6883343398133661
0.4720529513088678 0.0054930016739974 0.5941920396103981
0.4744563850453787 0.5053031917817066 0.5965191039395208
0.9752210575544282 0.0064193206929701 0.5964618381572677
0.9733874973940289 0.5057220741811221 0.5961643735772526
0.3208794450073924 0.3131411778333941 0.5935855627239377
0.3215946436582726 0.8132773299823555 0.5954772765487633
0.8211155381688755 0.3135067068417143 0.5966605764668103
0.8216458792804104 0.8130488843003789 0.5954010754205470
0.1693716541405621 0.1611122159220386 0.5979876604367860
0.1648812342679093 0.6614667752572529 0.5956080884316393
0.6664216262083968 0.1609773363170532 0.5956045857093173
0.6646970795434726 0.6612891832163541 0.5956621350618718
0.0020126076751623 0.1472108045796006 0.5007185756477028
0.9999074729278234 0.6471002888475184 0.4999920181971191
0.5022060944435864 0.1452194004510261 0.4999070083411610
0.5000259885464260 0.6450477651949313 0.4991415321879202
0.1519783391599816 0.3419942043161939 0.4999687218288926
0.1531679175822518 0.8422097467584848 0.5002748343016279
0.6537703976278522 0.3415894591055419 0.5003508332433171
0.6530450134366959 0.8409901760304024 0.4999008457173488
0.3055686803898112 0.4951902539445854 0.5000922866796316
0.3060052855367417 0.9941366599159664 0.4994748399488742
0.8057979061536145 0.4938391564569002 0.4997855710775312
0.8069164336747647 0.9941591872572744 0.5001786090553111
0.1408660436765317 0.1754109835467403 0.4037325545064689
0.1404128747080122 0.6753914476420562 0.4045829877619980
0.6422860208429313 0.1756507745579228 0.4056509863836766
0.6398403501512675 0.6743929230209034 0.4042490504347498
0.4872073169410811 0.4769334890426222 0.4021596534686438
0.4864197615208923 0.9819045001809030 0.4038200234203373
0.9854393885634494 0.4825564329193881 0.4039070333792480
0.9867765540890261 0.9820420525544122 0.4039267530095856
0.3331628225602898 0.3269530578061577 0.4065306662297132
0.3320408604612481 0.8259657253031421 0.4037560759444645
0.8326840138401295 0.3267063510374513 0.4038656704631194
0.8325775334572612 0.8268240703004750 0.4043654012375626
0.1622681960120502 0.3202342745521918 0.3090095683097616
0.1642481266740035 0.8101262703936030 0.3073121339155165
0.6602719760753573 0.3113344196408292 0.3087594830398288
0.6613784710420845 0.8185700006777452 0.3088129874290502
0.3248409731922663 0.0073016335945013 0.3077974692426153
0.3253821054631914 0.4990745412007556 0.3103413515593800
0.8227551267130480 0.0038248583908924 0.3080971583239531
0.8213160113013771 0.5055246297784848 0.3078596642004214
0.4742519955600955 0.1833433813514205 0.3144806436959939
0.4818613438275392 0.6603635205437612 0.3105124504822143
0.9811281127765739 0.1606367199018095 0.3103698269814146
0.9797824253564045 0.6613033162101942 0.3108232268979236
0.2388760420768818 0.4802907416061615 0.6937443019970573
0.2343364357249413 0.9943602124904629 0.6904739812226737
0.7333251715744140 0.4895703904562012 0.6933295509058794
0.7361903622055976 0.9788165782012328 0.6910721673342337
0.2265578388717913 0.0110011669400265 0.3066463737449041
0.2339942507310155 0.4893982776204240 0.3080723456825964

0.7281085458820868 0.0001884763986340 0.3075006113549463
0.7248985697717174 0.5052503795727148 0.3078202131320822
0.1417907869871229 0.3055411790039955 0.7257571744368576
0.1229824644329440 0.8098616140102024 0.7260022587088031
0.6139581759062196 0.2991479900099421 0.7273501469312933
0.6206527529092014 0.8173667217649694 0.7255825344334355
0.1929290141012387 0.2644182234841566 0.2744234112212780
0.1793752315705817 0.7485537023376310 0.2746388491051519
0.6720803462284408 0.2490582657445870 0.2765240024925504
0.6779621910081630 0.7612197279267363 0.2748939610243255
0.4385189073185671 0.7370290228220355 0.7247369170312581
0.9391534887684116 0.2360932876921353 0.7256317157851910
0.9374085000557599 0.7379421177526098 0.7243351014439341
0.4399658379191180 0.6776303375638548 0.2735313108580542
0.9390446787434286 0.1766811257742305 0.2734375329813190
0.9381785540217891 0.6781287935891811 0.2738207708173022

5) *OOH:

Fe2O3 *OOH (2x2) (0001) surface, pure – total energy: -730.43806 eV
10.1955165863000001 0.0000000000000000 0.0000000000000000
5.0977577053000003 8.8295767077999994 0.0000000000000000
0.0000000000000000 0.0000000000000000 24.2761898040999995
Fe O H
32 62 24
0.517219007 0.668142021 0.464426011
0.677762985 0.844281971 0.652858019
0.850965977 0.000742601 0.439406991
0.520466030 0.667315006 0.634988010
0.017909700 0.667527020 0.464343011
0.191103995 0.823098004 0.652778029
0.350834012 0.000394065 0.439987004
0.010613900 0.670773983 0.635783970
0.517071009 0.167467996 0.464783996
0.690825999 0.331501007 0.652316988
0.848694980 0.502516985 0.439994007
0.515856028 0.174070001 0.633858979
0.017817000 0.167939007 0.464827001
0.176173002 0.338690996 0.652300000
0.351976991 0.500819981 0.439936012
0.022699200 0.159429997 0.636274993
0.517683029 0.670575976 0.347052008
0.684464991 0.834347010 0.535172999
0.851653993 0.000996590 0.559567988
0.679675996 0.841414988 0.363490999
0.009944630 0.668385029 0.346320003
0.183625996 0.834469020 0.535337985
0.350585997 0.001063550 0.560144007
0.187287003 0.826197028 0.364813000
0.514894009 0.176124007 0.347427011
0.683965981 0.334455013 0.535080016
0.849730015 0.500824988 0.559916973
0.689101994 0.333813012 0.364831001
0.022026500 0.158160999 0.347575009
0.183757007 0.334789991 0.535210013
0.350915015 0.501594007 0.560217023
0.181059003 0.335828990 0.366167009
0.862394989 0.822937012 0.402992010
0.528499007 0.993789017 0.595031977
0.520999014 0.511394978 0.403780013
0.683175027 0.682428002 0.595143974
0.670787990 0.670122981 0.403797001
0.834981024 0.837409019 0.595956028
0.833139002 0.690066993 0.307384998
0.003190280 0.847986996 0.499861985
0.693243027 0.505787015 0.690330029
0.679409027 0.001748080 0.308840990
0.850735009 0.654219985 0.499646991
0.520331025 0.820686996 0.690142989
0.526118994 0.835318983 0.309368998
0.698279023 0.000948869 0.499354005

0.850759029	0.680840015	0.692385018
0.363260001	0.819513977	0.404787987
0.032903399	0.984798014	0.595552981
0.015321600	0.513720989	0.403964996
0.181484997	0.678249002	0.596010029
0.169991001	0.666009009	0.404651999
0.339177996	0.832383990	0.595836997
0.347716004	0.672406018	0.308613986
0.503337026	0.848969996	0.499792010
0.160312995	0.512296975	0.693159997
0.191303998	0.983121991	0.310757995
0.351016015	0.653257012	0.500129998
0.015909100	0.828130007	0.689478993
0.036023799	0.823720992	0.307029992
0.198045000	0.000982835	0.500176013
0.368221998	0.660767972	0.690190971
0.866005003	0.319985986	0.403930992
0.533725023	0.487410009	0.595438004
0.514858007	0.018350800	0.403618008
0.683570981	0.181450993	0.595162988
0.671531975	0.170038000	0.403854996
0.841829002	0.331741005	0.596525013
0.843533993	0.179529995	0.308117002
0.003413560	0.348327994	0.500133991
0.664318025	0.020501699	0.691519022
0.699007988	0.496623009	0.309709996
0.851200998	0.153733000	0.499778003
0.513760984	0.336988986	0.687996984
0.532503009	0.336573005	0.307529002
0.698253989	0.500882030	0.499745995
0.861562014	0.165574998	0.690968990
0.362879992	0.321821004	0.404240996
0.027233999	0.490673006	0.595883012
0.020558400	0.008881780	0.404053986
0.184334993	0.179899007	0.596557975
0.171207994	0.166933000	0.404383004
0.334246010	0.336511999	0.596105993
0.341042995	0.173650995	0.310613006
0.503160000	0.348132014	0.500063002
0.181750998	0.998592973	0.691107988
0.182082996	0.491521001	0.312213004
0.349886000	0.154420003	0.499945015
0.028351700	0.307846010	0.693674982
0.040221501	0.314918995	0.305712998
0.197933003	0.500667989	0.499852002
0.357106000	0.166146994	0.688674986
0.379022986	0.189991996	0.746873975
0.300873995	0.219749004	0.253169000
0.636331975	0.538425028	0.724744976
0.656476974	0.968730986	0.274289995
0.097778603	0.528518975	0.725655019
0.167999998	0.962948978	0.273966014
0.606226981	0.039230201	0.725570977
0.671684027	0.477640003	0.273342997
0.121844001	0.028301800	0.724815011
0.191532001	0.449458987	0.275344014
0.823944986	0.600638986	0.692837000
0.374805987	0.560892999	0.690289974
0.856450021	0.071665198	0.691662014
0.356638014	0.571711004	0.308887005
0.803647995	0.612375975	0.303344995
0.839909971	0.084953099	0.306297988
0.418444008	0.909942985	0.692635000
0.922513008	0.385127991	0.700248003
0.425805986	0.927385986	0.307850003
0.936487973	0.398104012	0.300303996
0.031506799	0.786432028	0.726454973
0.101761997	0.774495006	0.275451005
0.521449983	0.300574988	0.725552022
0.592207015	0.291339993	0.274354011
0.319624990	0.149603993	0.764050007

0.193351001 0.243466005 0.255903006