

## Supplementary Information

### a.) Modified Basis sets

He DZVP-S-ONLY

```
1
2 0 0 4 2
11.042785405048 -0.057709039524 -0.105186433287
2.784477928537 -0.186997538114 -0.390936479220
0.777508803064 -0.356165765185 -0.838063667638
0.22222544418 -0.270871722171 1.442874338563
```

H mod-DZV

```
1
2 0 0 5 2
10.068468228533 -0.033917444900 0.059193775500
2.680222868089 -0.122202212100 0.843318328900
0.791501539122 -0.443818861200 -1.155707115500
0.239116150487 -0.453182186600 0.049479621200
0.082193184441 -0.131612861500 0.522708738000
```

O mod-DZV modified-DZV

```
1
2 0 1 5 2 2
10.389228018317 0.126240722900 0.069215797900 -0.061302037200 -0.026862701100
3.849621072005 0.139933704300 0.115634538900 -0.190087511700 -0.006283021000
1.388401188741 -0.434348231700 -0.322839719400 -0.377726982800 -0.224839187800
0.496955043655 -0.852791790900 -0.095944016600 -0.454266086000 0.380324658600
0.162491615040 -0.242351537800 1.102830348700 -0.257388983000 1.054102919900
```

Fe mod-DZV

```
1
2 0 2 6 3 2 2
8.424366035773 -0.162658565315 -0.035363017559 -0.094078593184 -0.072847050506 -0.005733704721 0.110173914394 -0.070157127293
4.825219529323 -0.376899337900 -0.052967122649 -0.123947729175 0.142729813399 -0.013789178386 0.188638090829 -0.086799612151
2.198939257455 0.782922261822 0.047770046081 -0.097232244128 0.463643359935 -0.102097633738 0.309261422382 -0.268972922540
0.891660670520 0.668791717694 -0.303745487596 -1.526375946562 0.381142099471 -0.120441338124 0.329416033612 -0.034996470754
0.316230539846 0.044155272467 0.241839701006 2.582854093079 0.065337400672 0.562339049496 0.286237082129 0.429744227008
0.103474049912 -0.109124318184 1.110613962319 -1.436336658778 -0.008571808472 0.724515320284 0.085017978924 0.805064206226
```

### b.) Neutral coordinates of systems: cell parameters are given in the paper

#### 1. Optimized coordinates for neutral 7 units one-dim Fe(OH)<sub>2</sub> chain

```
77
Fe 18.3349492144 0.0000007576 0.0000088830
Fe 15.2790010162 0.0000004518 0.0000110067
Fe 12.2234994452 0.0000002531 0.0000092548
Fe 9.1689006748 0.0000000025 -0.0000155245
Fe 6.1144610762 0.0000004777 -0.0000137930
Fe 3.0599564723 -0.0000003633 0.0000083962
Fe 0.0054411568 -0.0000009552 0.0000089075
O 18.3357102616 0.0000063341 2.1492275942
O 18.3357068954 -0.0000039473 -2.1492102802
O 19.8627675229 -1.2603451555 -0.0000005370
O 19.8627688169 1.2603450192 -0.0000046852
O 15.2775569801 0.0000056940 2.1492458436
O 15.2775553627 -0.0000051111 -2.1492226312
O 16.8069625729 -1.2600452152 0.0000058244
O 16.8069622875 1.2600462873 -0.0000093754
O 12.2220377233 -0.0000166497 2.1498754757
O 12.2220122689 0.0000176436 -2.1498473640
O 13.7511618168 -1.2603484147 -0.0000016148
```

O	13.7511615062	1.2603488648	0.0000016921
O	9.1699252435	-0.0000131402	2.1509802399
O	9.1699271574	0.0000128287	-2.1509928769
O	10.6963684520	-1.2602194807	-0.0000053225
O	10.6963681119	1.2602200795	0.0000209162
O	6.1136965806	-0.0000052163	2.1502777432
O	6.1136841349	0.0000024663	-2.1502650548
O	7.6418218188	-1.2600441765	0.0000129579
O	7.6418220281	1.2600446383	0.0000248826
O	3.0589471266	0.0000024472	2.1507110765
O	3.0589694976	-0.0000031056	-2.1506811206
O	4.5869917631	-1.2600634656	0.0000071842
O	4.5869908895	1.2600636699	0.0000082096
O	0.0062342509	0.0000005281	2.1498097408
O	0.0062399863	-0.0000026427	-2.1497865176
O	1.5325777780	-1.2602449535	0.0000003244
O	1.5325774336	1.2602437503	-0.0000015943
H	18.3360500787	-0.7952338376	-2.6987554483
H	18.3360499607	0.7952232609	-2.6987591075
H	18.3360536554	-0.7952387919	2.6987490921
H	18.3360505603	0.7952538858	2.6987458369
H	19.8632672514	-2.2220751546	0.0000049301
H	19.8632702350	2.2220750259	0.0000012057
H	15.2763347320	-0.7952399684	-2.6987724892
H	15.2763936753	0.7952253445	-2.6987789495
H	15.2763961852	-0.7952448926	2.6987710692
H	15.2763352500	0.7952601934	2.6987654228
H	16.8070079802	-2.2217489361	0.0000097073
H	16.8070065390	2.2217499969	-0.0000040147
H	12.2210690973	-0.7950067851	-2.6998838900
H	12.2211573807	0.7950528643	-2.6998685865
H	12.2211492546	-0.7950653130	2.6998540906
H	12.2210642182	0.7950213957	2.6998691442
H	13.7507225122	-2.2220764815	-0.0000003651
H	13.7507226041	2.2220768951	0.0000125189
H	9.1703580091	-0.7950172732	-2.7008053256
H	9.1704025565	0.7950488993	-2.7007969464
H	9.1703973393	-0.7950332664	2.7008134023
H	9.1703581119	0.7950001211	2.7008231009
H	10.6960973729	-2.2219712596	-0.0000121166
H	10.6960971865	2.2219718770	0.0000255637
H	6.1131631428	-0.7950349447	-2.7001547349
H	6.1131785749	0.7950406974	-2.7001535810
H	6.1131735140	-0.7950524198	2.7001520496
H	6.1131653541	0.7950415360	2.7001522358
H	7.6417847681	-2.2217153851	0.0000018518
H	7.6417856211	2.2217157905	0.0000124124
H	3.0577139059	-0.7949049178	-2.7009137765
H	3.0577140166	0.7948963604	-2.7009172338
H	3.0577204248	-0.7949109982	2.7009020193
H	3.0577227988	0.7949177658	2.7008993067
H	4.5870486061	-2.2217371006	0.0000112175
H	4.5870472983	2.2217372598	0.0000061103
H	0.0067910113	-0.7950207345	-2.6997447095
H	0.0067797557	0.7950151403	-2.6997450956
H	0.0067852124	-0.7950338489	2.6997335506
H	0.0067945950	0.7950358489	2.6997322355
H	1.5328878225	-2.2219895563	0.0000064996
H	1.5328864892	2.2219883724	0.0000009069

## 2. Optimized coordinates for neutral 9 units one-dim Fe(OH)<sub>2</sub> chain

99

i = 15, E = -1700.0026582923  
 Fe -0.0005665282 -0.0000041504 -0.0000004733

Fe	3.0542783547	0.0000166079	-0.0000077169
Fe	6.1096191746	0.0000298370	0.0000084560
Fe	9.1646865398	-0.0001225773	0.0000113038
Fe	12.2203482993	0.0000337933	-0.0000076762
Fe	15.2756313879	0.0000192354	0.0000002092
Fe	18.3305069093	0.0000233904	-0.0000070059
Fe	21.3852352459	0.0000044879	-0.0000030921
Fe	24.4397597877	-0.0000121149	0.0000166657
O	-0.0007244762	-0.0000200761	2.1499340632
O	3.0544753751	-0.0000217410	2.1498908455
O	6.1109922071	-0.0000132991	2.1493832343
O	9.1647827765	-0.0000225493	2.1494190144
O	12.2190905928	0.0000226830	2.1494145236
O	15.2756681665	0.0000014766	2.1499095329
O	18.3308404903	-0.0000095224	2.1499307443
O	21.3853673139	-0.0000089060	2.1499457768
O	24.4396982076	-0.0000011672	2.1499635804
O	-0.0007206456	0.0000004885	-2.1499394638
O	3.0544946263	0.0000037858	-2.1499067146
O	6.1109980930	-0.0000000630	-2.1493604064
O	9.1647836001	-0.0000033688	-2.1494198811
O	12.2190897490	-0.0000057882	-2.1494272371
O	15.2756679889	0.0000052313	-2.1499081929
O	18.3308442799	0.0000256929	-2.1499439844
O	21.3853798145	-0.0000000066	-2.1499556511
O	24.4397073337	-0.0000026869	-2.1499363223
O	1.5266546302	-1.2601683765	-0.0000270229
O	4.5821019663	-1.2601123202	0.0000007446
O	7.6375742990	-1.2605638122	0.0000216313
O	10.6924765124	-1.2604626434	-0.0000127260
O	13.7479385596	-1.2601150246	0.0000105499
O	16.8033752573	-1.2601525670	-0.0000078638
O	19.8580070237	-1.2603281480	-0.0000149108
O	22.9125326364	-1.2604755243	0.0000057119
O	25.9670448220	-1.2603441794	0.0000008478
O	1.5266571482	1.2601622900	0.0000065648
O	4.5821491521	1.2601340635	0.0000138723
O	7.6375147338	1.2605793255	-0.0000037105
O	10.6925348931	1.2604788232	0.0000103011
O	13.7478954773	1.2601477579	-0.0000144718
O	16.8033595182	1.2601887801	0.0000024791
O	19.8580229817	1.2603526431	0.0000010891
O	22.9125390668	1.2604638240	-0.0000009255
O	25.9670317680	1.2603282093	0.0000085624
H	-0.0006438291	-0.7949607037	-2.6998187077
H	3.0545978975	-0.7950115177	-2.6997385200
H	6.1116838530	-0.7950590428	-2.6991164923
H	9.1651784354	-0.7950949994	-2.6991251043
H	12.2181858066	-0.7950454135	-2.6991742811
H	15.2753033592	-0.7950089164	-2.6997271181
H	18.3306092481	-0.7949370147	-2.6998135486
H	21.3851172169	-0.7949763612	-2.6998121603
H	24.4397446450	-0.7949777070	-2.6997964707
H	-0.0006056893	0.7949584676	-2.6998233107
H	3.0546486609	0.7950127993	-2.6997458568
H	6.1117482770	0.7950591965	-2.6991074658
H	9.1651306562	0.7951091782	-2.6990829780
H	12.2182539815	0.7950269885	-2.6991732971
H	15.2752773108	0.7950124914	-2.6997351648
H	18.3305117713	0.7949816852	-2.6998249669
H	21.3852281940	0.7949823662	-2.6998033250
H	24.4398335570	0.7949815581	-2.6997825785
H	-0.0006818402	-0.7949849118	2.6998077147
H	3.0546676512	-0.7950427752	2.6997144202
H	6.1117707104	-0.7950779113	2.6991321781

H	9.1651360874	-0.7951195840	2.6991154460
H	12.2182961670	-0.7950050275	2.6991786577
H	15.2753006119	-0.7950167135	2.6997231167
H	18.3305817750	-0.7949820342	2.6997863983
H	21.3851489508	-0.7949873087	2.6997984523
H	24.4397185270	-0.7949739497	2.6998263215
H	-0.0006009419	0.7949343012	2.6998219106
H	3.0545225208	0.7949825878	2.6997364894
H	6.1116460042	0.7950375044	2.6991437074
H	9.1651522373	0.7950759782	2.6991007424
H	12.2181237636	0.7950662149	2.6991457616
H	15.2752675849	0.7950077709	2.6997390681
H	18.3305190139	0.7949328145	2.6998305912
H	21.3851675172	0.7949701086	2.6997972489
H	24.4398257500	0.7949836609	2.6998085249
H	1.5261589227	-2.2218761699	-0.0000259326
H	4.5822300311	-2.2218542462	-0.0000032635
H	7.6379635489	-2.2222665974	0.0000218522
H	10.6922649657	-2.2221715190	0.0000013878
H	13.7477587745	-2.2218414251	-0.0000001564
H	16.8038365656	-2.2218551679	-0.0000179738
H	19.8583781921	-2.2220457590	-0.0000089903
H	22.9124961758	-2.2221923242	-0.0000001535
H	25.9666016446	-2.2220608415	-0.0000024642
H	1.5261522069	2.2218705649	0.0000016997
H	4.5822018332	2.2218718793	0.0000244110
H	7.6379306016	2.2222776193	-0.0000044933
H	10.6922910577	2.2221812615	0.0000033876
H	13.7477841235	2.2218698239	-0.0000099946
H	16.8038131343	2.2218918165	0.0000085830
H	19.8584057036	2.2220702779	-0.0000075648
H	22.9125049878	2.2221799007	0.0000022804
H	25.9666010518	2.2220450861	0.0000185292

### 3. Optimized coordinates for neutral 11 units one-dim Fe(OH)<sub>2</sub> chain

121

Fe	0.0000553416	0.0000365585	0.0000357493
Fe	3.0544875741	0.0000147019	0.0001884627
Fe	6.1091965203	-0.0000665559	0.0002752119
Fe	9.1643791846	-0.0000898184	0.0003411216
Fe	12.2199747896	0.0000051193	-0.0001268976
Fe	15.2755887878	0.0000760857	-0.0002967581
Fe	18.3307746884	0.0000224789	-0.0004313691
Fe	21.3854737420	-0.0000226979	-0.0001005650
Fe	24.4399141405	-0.0000319498	0.0000548561
Fe	27.4948508608	-0.0000065514	0.0000475410
Fe	30.5501158554	0.0000256520	-0.0000092847
O	0.0038458722	0.0000327296	2.1500953175
O	3.0576656195	0.0000239896	2.1503379054
O	6.1102195324	-0.0001145908	2.1499753402
O	9.1636383115	-0.0001669206	2.1492053038
O	12.2201852566	-0.0000836737	2.1505336534
O	15.2765803655	0.0000509814	2.1485833734
O	18.3296724750	0.0000129392	2.1493116959
O	21.3820754520	-0.0000168897	2.1500663493
O	24.4359924806	-0.0000112730	2.1501427387
O	27.4931273076	0.0000234254	2.1498622225
O	30.5518033916	0.0000261294	2.1498223508
O	0.0040280122	0.0000336107	-2.1501240300
O	3.0578924319	0.0000312981	-2.1500554919
O	6.1100621018	-0.0000213857	-2.1494956226
O	9.1637406970	-0.0000435560	-2.1485310113
O	12.2197783153	0.0001134666	-2.1506946924
O	15.2759865726	0.0001519497	-2.1491553256

O	18.3299669489	0.0000082735	-2.1501561290
O	21.3822968121	-0.0000399783	-2.1503209210
O	24.4360762587	-0.0000602341	-2.1500703755
O	27.4931483239	-0.0000144498	-2.1498240406
O	30.5518542448	0.0000117737	-2.1498834468
O	1.5281301622	-1.2603793589	-0.0001027109
O	4.5828882511	-1.2601016973	0.0001031371
O	7.6378126014	-1.2607173034	0.0003230779
O	10.6929788649	-1.2600848113	0.0001633717
O	13.7470415390	-1.2600053431	-0.0001697255
O	16.8021118024	-1.2605831731	-0.0002811223
O	19.8570246365	-1.2600893551	-0.0002289928
O	22.9118145280	-1.2604272453	-0.0000376490
O	25.9668311795	-1.2602104220	0.0000265971
O	29.0224896176	-1.2600276967	-0.0000399810
O	32.0781388948	-1.2601546656	-0.0001412272
O	1.5281645129	1.2604295174	-0.0000910773
O	4.5829535462	1.2600605264	0.0001495795
O	7.6378502157	1.2605591952	0.0003915272
O	10.6929200980	1.2599943690	0.0002902169
O	13.7469867784	1.2600742469	-0.0000719508
O	16.8021638741	1.2606954558	-0.0002663190
O	19.8570661826	1.2600785492	-0.0002573031
O	22.9118303300	1.2603753309	-0.0000849247
O	25.9668227884	1.2601684249	-0.0000173007
O	29.0224797905	1.2600366994	-0.0000705554
O	32.0781479032	1.2602201293	-0.0001376232
H	0.0056534338	-0.7949190915	-2.6999989853
H	3.0589826452	-0.7949099197	-2.6999787592
H	6.1090984284	-0.7949758135	-2.6993004651
H	9.1619768828	-0.7951904341	-2.6982072844
H	12.2196860080	-0.7949480605	-2.7002866588
H	15.2777089873	-0.7949974727	-2.6988618429
H	18.3310304241	-0.7949968708	-2.6998958171
H	21.3814470528	-0.7950262630	-2.7001723499
H	24.4348605635	-0.7950550036	-2.6998804982
H	27.4927790898	-0.7950403443	-2.6996796578
H	30.5527210795	-0.7950020762	-2.6997579032
H	0.0050255120	0.7949828949	-2.7000035922
H	3.0584446584	0.7949838845	-2.6999624826
H	6.1087490448	0.7949705375	-2.6992488821
H	9.1619465293	0.7951330495	-2.6981679635
H	12.2199565642	0.7952210749	-2.7002161605
H	15.2781095286	0.7953378240	-2.6988074057
H	18.3313138240	0.7949996819	-2.6999167405
H	21.3814965318	0.7949357913	-2.7001873051
H	24.4346374615	0.7949107126	-2.6999122821
H	27.4923453981	0.7949933444	-2.6997034978
H	30.5521228890	0.7950148224	-2.6997740139
H	0.0053215403	-0.7949739838	2.6998653012
H	3.0586105506	-0.7949884280	2.7001463285
H	6.1088458907	-0.7950846434	2.6998553199
H	9.1624469944	-0.7952339072	2.6987465426
H	12.2202962197	-0.7950235630	2.7003097153
H	15.2779341087	-0.7950128796	2.6980914282
H	18.3313151582	-0.7949287290	2.6992346723
H	21.3814529926	-0.7949955081	2.6999323184
H	24.4347786592	-0.7949828563	2.6999748671
H	27.4926522710	-0.7949794074	2.6997367637
H	30.5524981947	-0.7949960134	2.6996689148
H	0.0051157270	0.7950397133	2.6998685485
H	3.0583851676	0.7950434717	2.7001396995
H	6.1086224052	0.7948359176	2.6998851773
H	9.1621756478	0.7948848005	2.6987690686
H	12.2200055333	0.7948144607	2.7003708355

H	15.2775626610	0.7950966241	2.6981155432
H	18.3309056284	0.7949487909	2.6992445375
H	21.3810435047	0.7949609924	2.6999283021
H	24.4344645628	0.7949733764	2.6999550685
H	27.4924489396	0.7950367904	2.6997211823
H	30.5523319108	0.7950465458	2.6996698909
H	1.5277814590	-2.2221242776	0.0001347293
H	4.5826045381	-2.2217810277	0.0003587022
H	7.6380287414	-2.2223569390	0.0003933363
H	10.6932860025	-2.2219005688	0.0001395924
H	13.7468011463	-2.2218195384	-0.0002198128
H	16.8019015340	-2.2222212428	-0.0003865779
H	19.8572856949	-2.2217687601	-0.0002052480
H	22.9121601812	-2.2221699584	0.0000703398
H	25.9667926815	-2.2219599289	0.0001079145
H	29.0225030583	-2.2217761455	0.0000620019
H	32.0781924089	-2.2219039371	0.0000267624
H	1.5278243998	2.2221738477	0.0001452425
H	4.5827163083	2.2217391535	0.0004114338
H	7.6380564096	2.2221986688	0.0004984098
H	10.6931673647	2.2218088975	0.0003170225
H	13.7467062024	2.2218887001	-0.0000775733
H	16.8019595199	2.2223367875	-0.0003318822
H	19.8573402985	2.2217574192	-0.0001981291
H	22.9121679386	2.2221184856	0.0000104382
H	25.9667544362	2.2219197181	0.0000718109
H	29.0224723488	2.2217845689	0.0000418391
H	32.0781896370	2.2219692048	0.0000169089

#### 4. BLYP+U optimized coordinates for neutral Hematite (U= 6 eV)

270

Fe	0.0327953032	2.9279869393	13.7702780148
Fe	2.4860884043	4.3451380723	4.9258241221
Fe	2.4860922474	1.5117150461	9.3475739697
Fe	2.4862439091	4.3452012468	2.0879342973
Fe	2.4864716114	1.5118717238	6.5096911500
Fe	0.0322194094	2.9289227680	10.9329397915
Fe	0.0324673630	2.9285543457	4.2989447544
Fe	2.4859303361	4.3452626269	8.7210497034
Fe	2.4871497417	1.5111849689	13.1438665332
Fe	2.4867099577	1.5117075440	2.7140750983
Fe	0.0323326926	2.9287257390	7.1367812660
Fe	2.4868399839	4.3453498289	11.5591153614
Fe	4.9406153423	2.9287966564	13.7700685070
Fe	7.3942513808	4.3453155788	4.9256070271
Fe	7.3944512234	1.5113616147	9.3479254846
Fe	7.3948487327	4.3463285843	2.0883365668
Fe	7.3949965442	1.5115901013	6.5097161421
Fe	4.9407207974	2.9288269905	10.9324697349
Fe	4.9405335041	2.9283975935	4.2988437783
Fe	7.3949040865	4.3456483049	8.7211626193
Fe	7.3952036416	1.5115370081	13.1436279758
Fe	7.3944801784	1.5122712103	2.7135578023
Fe	4.9405758381	2.9288766302	7.1371773710
Fe	7.3953268223	4.3447644604	11.5599943209
Fe	9.8487660764	2.9284378332	13.7704252647
Fe	12.3032689134	4.3453122033	4.9259096688
Fe	12.3027780822	1.5121390393	9.3471702061
Fe	12.3030062102	4.3456136455	2.0884471405
Fe	12.3026576500	1.5116014581	6.5095317171
Fe	9.8491286462	2.9287844931	10.9307627540
Fe	9.8484398503	2.9279374002	4.2978589739
Fe	12.3026006476	4.3452608028	8.7207508253
Fe	12.3026727737	1.5114792279	13.1440094651
Fe	12.3032931018	1.5118245115	2.7148726230
Fe	9.8486031913	2.9286971175	7.1369383041

Fe	12.3031932225	4.3454824695	11.5600045053
Fe	-2.4215668385	7.1788510872	13.7702568657
Fe	0.0321078763	8.5957109967	4.9258233069
Fe	0.0324536064	5.7623372817	9.3479601565
Fe	0.0318629272	8.5964705812	2.0880696736
Fe	0.0320465022	5.7625661934	6.5101205788
Fe	-2.4220429773	7.1788281167	10.9313710328
Fe	-2.4223890182	7.1796534381	4.2989564898
Fe	0.0319379348	8.5961111073	8.7212838964
Fe	0.0330053643	5.7627214069	13.1437867417
Fe	0.0324575128	5.7621033646	2.7143491424
Fe	-2.4215542629	7.1796312269	7.1369916183
Fe	0.0317636112	8.5958768901	11.5596233534
Fe	2.4864842783	7.1792268951	13.7700453111
Fe	4.9410655834	8.5956043788	4.9257434118
Fe	4.9411654496	5.7616569831	9.3482529910
Fe	4.9399778427	8.5958334469	2.0886961169
Fe	4.9400349979	5.7623759997	6.5096075360
Fe	2.4862761790	7.1795304324	10.9321244449
Fe	2.4861305496	7.1794479264	4.2985530498
Fe	4.9403889724	8.5964525675	8.7213381483
Fe	4.9406634041	5.7628207855	13.1445141909
Fe	4.9405750914	5.7619672885	2.7138512621
Fe	2.4874202386	7.1792049533	7.1370575630
Fe	4.9409908910	8.5961956342	11.5595373052
Fe	7.3953507003	7.1797374737	13.7697269338
Fe	9.8495675251	8.5962974700	4.9249682575
Fe	9.8486992646	5.7624808169	9.3475870309
Fe	9.8484342659	8.5956080876	2.0877549216
Fe	9.8486810341	5.7619641755	6.5089818821
Fe	7.3941256273	7.1795834308	10.9312883949
Fe	7.3953605836	7.1791879980	4.2985079578
Fe	9.8477505887	8.5961568913	8.7211359205
Fe	9.8483295603	5.7632974469	13.1441824474
Fe	9.8493722123	5.7614451826	2.7140084005
Fe	7.3946356316	7.1792152911	7.1371400752
Fe	9.8491045911	8.5972448192	11.5599969357
Fe	-4.8755886276	11.4295175952	13.7712468235
Fe	-2.4222819531	12.8470168938	4.9256002271
Fe	-2.4221399752	10.0132361584	9.3478210031
Fe	-2.4213238192	12.8466571042	2.0883962401
Fe	-2.4223489980	10.0134760874	6.5092937057
Fe	-4.8757797715	11.4301588665	10.9329896495
Fe	-4.8765238582	11.4300759147	4.2987622052
Fe	-2.4219408348	12.8468110377	8.7216157553
Fe	-2.4217122209	10.0131177991	13.1436113203
Fe	-2.4219112500	10.0130717226	2.7144281662
Fe	-4.8757213775	11.4304946734	7.1375289683
Fe	-2.4220658606	12.8464382392	11.5594482116
Fe	0.0320237577	11.4299699019	13.7700501662
Fe	2.4864772293	12.8467759108	4.9255736977
Fe	2.4863458793	10.0132763028	9.3479284344
Fe	2.4864752200	12.8471889911	2.0869840813
Fe	2.4859348482	10.0130818673	6.5097282246
Fe	0.0327095230	11.4299584427	10.9328230166
Fe	0.0322100181	11.4297710107	4.2982857917
Fe	2.4862873116	12.8468746229	8.7213931971
Fe	2.4868803352	10.0128093708	13.1434401969
Fe	2.4861194673	10.0129767827	2.7139554660
Fe	0.0322677129	11.4296602300	7.1373199740
Fe	2.4863646156	12.8463425436	11.5600434786
Fe	4.9413247956	11.4291844554	13.7712958228
Fe	7.3946695466	12.8466739508	4.9256706026
Fe	7.3952543459	10.0135814373	9.3477413051
Fe	7.3945866459	12.8471520295	2.0876462645
Fe	7.3940272320	10.0126061400	6.5091337529
Fe	4.9411466606	11.4298133604	10.9317945726
Fe	4.9406043210	11.4302202552	4.2981530951
Fe	7.3940491242	12.8472220873	8.7215018033
Fe	7.3946768220	10.0132543469	13.1434150125

Fe	7.3948255820	10.0129570747	2.7142276687
Fe	4.9407273006	11.4297770702	7.1373514784
Fe	7.3949137133	12.8467969527	11.5591859726
O	-0.9087776064	4.3454438828	3.5074156478
O	3.9996685953	1.5112038804	7.9286527861
O	1.5460829876	2.9280067792	12.3510783412
O	4.1851664132	1.4054897261	3.5056666964
O	1.7307436765	2.8221631828	7.9283537379
O	-0.7231954236	4.2396108747	12.3515435365
O	1.7291989844	3.0349347848	3.5058070681
O	-0.7244131132	4.4516280242	7.9293999766
O	4.1836881911	1.6184668383	12.3506649092
O	0.9737031692	1.5109780713	14.5625775312
O	3.4272404947	2.9280125045	5.7174152283
O	0.9734977641	4.3449003619	10.1399085451
O	0.7889370573	4.4519633519	14.5624741531
O	0.7891769148	1.6183666069	5.7177559771
O	3.2430292573	3.0348826276	10.1398636220
O	3.2427308238	2.8223914293	14.5623898401
O	0.7885876422	4.2396791715	5.7178350188
O	0.7882258000	1.4057884879	10.1399135585
O	3.9996537593	4.3450065561	3.5064732820
O	8.9076830685	1.5116116787	7.9289189072
O	6.4537701072	2.9282521258	12.3521174288
O	9.0929670899	1.4051194407	3.5054036947
O	6.6387218960	2.8218535176	7.9288126672
O	4.1848133644	4.2397250968	12.3511162977
O	6.6372792811	3.0346211252	3.5062444096
O	4.1840020205	4.4517545686	7.9297417653
O	9.0923305497	1.6182766205	12.3508729809
O	5.8816046763	1.5112150739	14.5622292683
O	8.3354061258	2.9279299769	5.7172139386
O	5.8821987152	4.3447163528	10.1405402205
O	5.6975330099	4.4513548519	14.5634420532
O	5.6969611304	1.6184248043	5.7183458513
O	8.1506740118	3.0348666316	10.1404289346
O	8.1508183419	2.8229853794	14.5623259510
O	5.6970164267	4.2395422662	5.7176373586
O	5.6967252104	1.4053523368	10.1401693504
O	8.9079429403	4.3451146047	3.5067560832
O	13.8163315333	1.5115646061	7.9285985241
O	11.3614587354	2.9284872353	12.3520035844
O	14.0017435528	1.4056100408	3.5059824027
O	11.5471124100	2.8220731132	7.9279886631
O	9.0937596407	4.2392335321	12.3511967983
O	11.5456930150	3.0349300376	3.5064012770
O	9.0922593167	4.4516603435	7.9293019874
O	14.0001055878	1.6182854626	12.3510523157
O	10.7905249860	1.5117225353	14.5626924588
O	13.2446507374	2.9276004547	5.7171770713
O	10.7906820512	4.3451044050	10.1400739407
O	10.6056553080	4.4520576504	14.5622979365
O	10.6053097124	1.6183732200	5.7180392622
O	13.0588079314	3.0345353598	10.1413122129
O	13.0594698696	2.8222608257	14.5628530746
O	10.6054988565	4.2392888260	5.7172405506
O	10.6057208549	1.4050998987	10.1403285594
O	-3.3627267269	8.5960419770	3.5068069169
O	1.5459671205	5.7620965657	7.9285607461
O	-0.9086979797	7.1788826051	12.3518589753
O	1.7309619647	5.6561045643	3.5053213595
O	-0.7238828941	7.0729628914	7.9291124606
O	-3.1771189704	8.4898830711	12.3511011648
O	-0.7252893283	7.2855586754	3.5063297180
O	-3.1784768069	8.7024049677	7.9294447378
O	1.7297781877	5.8688599844	12.3508201463
O	-1.4801698755	5.7614803885	14.5623953889
O	0.9735362687	7.1785972426	5.7174594412
O	-1.4806028949	8.5950908474	10.1392726713
O	-1.6653630531	8.7029322438	14.5627952269



O	-1.6646536554	5.8692182256	5.7175338496
O	0.7888734364	7.2855454027	10.1402567304
O	0.7891728440	7.0734544231	14.5632543375
O	-1.6653270037	8.4898125871	5.7183025543
O	-1.6653130941	5.6553552702	10.1401090087
O	1.5453302964	8.5955424114	3.5058073627
O	6.4537011664	5.7616260898	7.9290240755
O	3.9999325392	7.1785428600	12.3509127087
O	6.6389153289	5.6565466239	3.5057913780
O	4.1847693175	7.0727793522	7.9294651920
O	1.7302928055	8.4899796990	12.3507648122
O	4.1839377143	7.2856638009	3.5065435996
O	1.7293348851	8.7021441100	7.9288309589
O	6.6380274602	5.8685559742	12.3514835098
O	3.4274918697	5.7618370147	14.5626471261
O	5.8816228635	7.1783490876	5.7178395355
O	3.4274880024	8.5957819919	10.1396814301
O	3.2434229573	8.7027332407	14.5622566629
O	3.2432778344	5.8686450841	5.7173866777
O	5.6972255025	7.2853438706	10.1402924256
O	5.6971047183	7.0731770301	14.5629370517
O	3.2429493627	8.4903338515	5.7170981863
O	3.2428729962	5.6565536278	10.1392614213
O	6.4540462251	8.5957412465	3.5066963146
O	11.3619771843	5.7624905623	7.9293342176
O	8.9077855996	7.1783997708	12.3501925797
O	11.5468664342	5.6556356363	3.5066820567
O	9.0928803737	7.0728412893	7.9278212534
O	6.6385469799	8.4896841594	12.3519682132
O	9.0918945554	7.2855490369	3.5055489901
O	6.6378651467	8.7027778922	7.9294033736
O	11.5455030011	5.8692416220	12.3511826168
O	8.3352952768	5.7616940725	14.5619455799
O	10.7900148290	7.1787324726	5.7172356243
O	8.3364514276	8.5955993399	10.1398640154
O	8.1520662499	8.7025226046	14.5625571544
O	8.1516765415	5.8688935263	5.7173919615
O	10.6048829421	7.2857359311	10.1406058551
O	10.6055128629	7.0725832044	14.5628723512
O	8.1517565130	8.4900216654	5.7173916833
O	8.1513916989	5.6557670850	10.1404724705
O	-5.8169592970	12.8458350183	3.5057002372
O	-0.9087876681	10.0126200200	7.9287798883
O	-3.3628463185	11.4298814014	12.3515308827
O	-0.7236297253	9.9066598161	3.5057479013
O	-3.1778104608	11.3233046741	7.9289158751
O	-5.6315027878	12.7406158457	12.3514274569
O	-3.1790025927	11.5367341441	3.5060818002
O	-5.6330833490	12.9535718735	7.9289687259
O	-0.7249758981	10.1189135407	12.3514070075
O	-3.9345663257	10.0118466088	14.5623421692
O	-1.4804798824	11.4299061123	5.7175890808
O	-3.9350992782	12.8457572862	10.1392491497
O	-4.1189964847	12.9535150202	14.5629582693
O	-4.1193483525	10.1200731556	5.7180006640
O	-1.6644371275	11.5365544513	10.1397390676
O	-1.6647867146	11.3235593724	14.5629994355
O	-4.1197696803	12.7403150214	5.7176263364
O	-4.1195195164	9.9067549726	10.1406127243
O	-0.9085063252	12.8461397696	3.5056607805
O	3.9993227219	10.0122867835	7.9283116885
O	1.5454055159	11.4298129684	12.3519810919
O	4.1846370528	9.9067958366	3.5059472585
O	1.7305713112	11.3239490209	7.9282469770
O	-0.7235054217	12.7404834447	12.3505614827
O	1.7296427847	11.5364749291	3.5061221123
O	-0.7252302092	12.9531069659	7.9287212573
O	4.1833528431	10.1191371052	12.3505056860
O	0.9731185464	10.0124123237	14.5622535819
O	3.4274633670	11.4292402345	5.7174231946

O	0.9736777027	12.8458364908	10.1396287291
O	0.7894802575	12.9539673571	14.5623278187
O	0.7887853141	10.1194161185	5.7173098684
O	3.2435422101	11.5366677600	10.1400071755
O	3.2427579973	11.3236908254	14.5623646621
O	0.7885074986	12.7403342480	5.7170912739
O	0.7884568270	9.9070358665	10.1398832951
O	3.9992281484	12.8460574936	3.5055430598
O	8.9079795820	10.0124463381	7.9289633126
O	6.4541462822	11.4293751134	12.3511754342
O	9.0925919860	9.9062022732	3.5066606568
O	6.6388436082	11.3232620507	7.9285462655
O	4.1853336985	12.7393560571	12.3512587020
O	6.6382110717	11.5366320140	3.5061982479
O	4.1832158080	12.9527350793	7.9287636864
O	9.0913708849	10.1196662094	12.3515689929
O	5.8818651223	10.0123654204	14.5630651479
O	8.3362008172	11.4294632230	5.7175174620
O	5.8816784561	12.8469388851	10.1396609078
O	5.6973360221	12.9536375067	14.5626957766
O	5.6977049489	10.1197120874	5.7170746377
O	8.1518669029	11.5366927490	10.1402565730
O	8.1514572701	11.3237436556	14.5634799501
O	5.6965402205	12.7405433181	5.7169580574
O	5.6977689780	9.9063835633	10.1403226053

## 5. Optimized coordinates for neutral TiO<sub>2</sub> (U = 6 eV)

270

Ti	0.0020400584	-0.0011155041	0.0012499146
Ti	2.3123458556	2.3109387797	1.4890731665
Ti	4.6273068783	0.0043065723	0.0010424451
Ti	6.9345797239	2.3115738042	1.4912346635
Ti	9.2441296507	0.0014382667	0.0010886040
Ti	11.5565201179	2.3118481996	1.4889508456
Ti	-0.0021055202	4.6240277012	0.0012508238
Ti	2.3123810903	6.9335985199	1.4884597875
Ti	4.6244408372	4.6211277628	0.0010886260
Ti	6.9348528045	6.9335166963	1.4889514508
Ti	9.2418966296	4.6188958088	0.0010410061
Ti	11.5557629792	6.9327601886	1.4874746969
Ti	0.0001398394	9.2461380410	0.0011578138
Ti	2.3134232254	11.5594200485	1.4875040346
Ti	4.6218929396	9.2480388277	0.0012501037
Ti	6.9339387924	11.5583464336	1.4890744579
Ti	9.2470214660	9.2438976869	0.0012510562
Ti	11.5566025561	11.5583750192	1.4884603700
Ti	-0.0017148265	0.0030689943	2.9767527391
Ti	2.3132856994	2.3107740026	4.4679142246
Ti	4.6226732997	-0.0003281758	2.9781547322
Ti	6.9345884427	2.3115760407	4.4695086403
Ti	9.2474048330	-0.0007297919	2.9775991218
Ti	11.5570704046	2.3135622687	4.4678262469
Ti	0.0023408911	4.6205044192	2.9767219001
Ti	2.3105791230	6.9364934221	4.4663885604
Ti	4.6222776334	4.6243987366	2.9775986592
Ti	6.9365636940	6.9340738938	4.4678228070
Ti	9.2465684360	4.6235637853	2.9780981248
Ti	11.5597868495	6.9367411084	4.4655950280
Ti	0.0001373085	9.2461311939	2.9757494234
Ti	2.3093790709	11.5553830363	4.4656533175
Ti	4.6260589546	9.2442752995	2.9767522809
Ti	6.9338076749	11.5592389402	4.4679093048
Ti	9.2435205869	9.2483382964	2.9767195170
Ti	11.5595173835	11.5565790301	4.4663873478
Ti	0.0025315855	-0.0005035019	5.9587076266

Ti	2.3095067156	2.3170603175	7.4544515475
Ti	4.6216019656	-0.0014617758	5.9620239462
Ti	6.9346617596	2.3116468057	7.4540463311
Ti	9.2472887796	0.0023129989	5.9595476477
Ti	11.5635693107	2.3100243977	7.4544466012
Ti	0.0009753958	4.6269990271	5.9587180192
Ti	2.3145573102	6.9357931656	7.4544731737
Ti	4.6253176055	4.6242695303	5.9595476170
Ti	6.9329978263	6.9405613515	7.4544467385
Ti	9.2477197462	4.6247268194	5.9619895332
Ti	11.5572530872	6.9341855599	7.4544756890
Ti	0.0001075833	9.2460953648	5.9604519519
Ti	2.3120047411	11.5580068182	7.4544752670
Ti	4.6225073363	9.2485511782	5.9587051975
Ti	6.9401678005	11.5554456653	7.4544517423
Ti	9.2500442912	9.2469037863	5.9587117157
Ti	11.5587749540	11.5605078041	7.4544732288
Ti	0.0025217733	-0.0004663501	8.9503424725
Ti	2.3133258954	2.3107521721	10.4412323601
Ti	4.6216389459	-0.0014248304	8.9466149524
Ti	6.9345881883	2.3115756849	10.4387917800
Ti	9.2472696351	0.0023364175	8.9492155016
Ti	11.5570271587	2.3135792595	10.4413110438
Ti	0.0009916055	4.6269675492	8.9503302025
Ti	2.3106105034	6.9364592855	10.4428048353
Ti	4.6253409620	4.6242501824	8.9492154910
Ti	6.9365806378	6.9340305565	10.4413148172
Ti	9.2476828684	4.6246898953	8.9466479479
Ti	11.5597655320	6.9367196933	10.4435802425
Ti	0.0001074998	9.2460952475	8.9484620769
Ti	2.3093988818	11.5554029047	10.4435189572
Ti	4.6225446302	9.2485415571	8.9503452783
Ti	6.9337859598	11.5592791721	10.4412377501
Ti	9.2500127165	9.2469199051	8.9503369785
Ti	11.5594833473	11.5566103248	10.4428061142
Ti	-0.0017129639	0.0030799579	11.9326248128
Ti	2.3123501429	2.3109044464	13.4202915867
Ti	4.6227114855	-0.0002898413	11.9307980131
Ti	6.9345793908	2.3115734418	13.4172668130
Ti	9.2474034748	-0.0007270908	11.9314540397
Ti	11.5565163807	2.3118831104	13.4204065601
Ti	0.0023387040	4.6204931948	11.9326565374
Ti	2.3123873359	6.9335885295	13.4209608395
Ti	4.6222803185	4.6243972409	11.9314544937
Ti	6.9348877594	6.9335129544	13.4204062873
Ti	9.2465301542	4.6235254852	11.9308517370
Ti	11.5557420084	6.9327392058	13.4219115006
Ti	0.0001375135	9.2461313121	11.9334538024
Ti	2.3134462851	11.5594430971	13.4218766151
Ti	4.6260698686	9.2442770793	11.9326256525
Ti	6.9339043048	11.5583507409	13.4202907333
Ti	9.2435092667	9.2483362264	11.9326593982
Ti	11.5565926431	11.5583811488	13.4209603128
O	1.4079953227	1.4079521548	-0.0002406149
O	3.2150560579	3.2148744448	-0.0002380040
O	0.9034979798	3.7195987435	1.4868868039
O	3.7195940583	0.9035417960	1.4866684194
O	6.0309416564	1.4079413904	-0.0002009817
O	7.8380593405	3.2150588380	-0.0002006686
O	5.5264434452	3.7195651606	1.4865097589
O	8.3425651812	0.9034433249	1.4865096239
O	10.6539289183	1.4081123751	-0.0002374442
O	12.4609860289	3.2150217331	-0.0002404382
O	10.1494058925	3.7194673056	1.4866792579
O	12.9655049423	0.9034075506	1.4868852279

O	1.4079829649	6.0311154630	-0.0002450669
O	3.2148713160	7.8380041313	-0.0002448641
O	0.9033549786	8.3426524851	1.4870336324
O	3.7194314471	5.5265765870	1.4867116104
O	6.0311125362	6.0309286976	-0.0002374691
O	7.8380219260	7.8379860945	-0.0002404632
O	5.5264074287	8.3425047273	1.4868852237
O	8.3424672135	5.5264058277	1.4866788430
O	10.6540367483	6.0310364929	-0.0002306205
O	12.4609075458	7.8379073309	-0.0002400287
O	10.1493356236	8.3425359375	1.4867535288
O	12.9655357533	5.5263356712	1.4867538945
O	1.4080816814	10.6540814052	-0.0002403703
O	3.2149595708	12.4609595331	-0.0002300334
O	0.9034787966	12.9656775675	1.4867471911
O	3.7196773800	10.1494786680	1.4867472332
O	6.0309521239	10.6539948974	-0.0002406496
O	7.8378747629	12.4610558832	-0.0002380328
O	5.5265416722	12.9655941894	1.4866673999
O	8.3425986677	10.1494982049	1.4868870754
O	10.6541156920	10.6539827400	-0.0002450722
O	12.4610044886	12.4608711330	-0.0002448672
O	10.1495764985	12.9654312952	1.4867115431
O	12.9656525022	10.1493551717	1.4870334999
O	1.4078954957	1.4081429212	2.9744380875
O	3.2146736389	3.2148133272	2.9745461712
O	0.9032589533	3.7195683484	4.4643155811
O	3.7193486013	0.9029095739	4.4635750921
O	6.0309831086	1.4079818396	2.9736685322
O	7.8380302267	3.2150297349	2.9736925787
O	5.5261592608	3.7199149540	4.4632950173
O	8.3429158097	0.9031593230	4.4632945593
O	10.6543115966	1.4081774564	2.9745934393
O	12.4611053795	3.2148392005	2.9744157452
O	10.1497711053	3.7202052890	4.4635800763
O	12.9659187062	0.9036173623	4.4643022176
O	1.4082300088	6.0309969175	2.9747381647
O	3.2149832647	7.8377426882	2.9747129072
O	0.9033922424	8.3426682491	4.4640547602
O	3.7196508222	5.5264814773	4.4641664640
O	6.0311778850	6.0313112476	2.9745937307
O	7.8378396589	7.8381044747	2.9744162915
O	5.5266179600	8.3429186604	4.4643031043
O	8.3432057876	5.5267708332	4.4635807901
O	10.6542614024	6.0312603418	2.9744630451
O	12.4609447932	7.8379434176	2.9748195871
O	10.1494091216	8.3427672016	4.4642934812
O	12.9657665672	5.5264100030	4.4642921802
O	1.4080498166	10.6540496808	2.9748011558
O	3.2147462644	12.4607458618	2.9744616941
O	0.9033159996	12.9656699434	4.4642657090
O	3.7196705474	10.1493157137	4.4642661367
O	6.0311439555	10.6538945700	2.9744386719
O	7.8378143748	12.4606721523	2.9745462288
O	5.5259083408	12.9653482228	4.4635766803
O	8.3425673185	10.1492587743	4.4643157666
O	10.6539979370	10.6542289718	2.9747374243
O	12.4607429396	12.4609828243	2.9747136655
O	10.1494820967	12.9656510586	4.4641665699
O	12.9656685370	10.1493923938	4.4640547375
O	1.4081083873	1.4079621819	5.9573040071
O	3.2151306611	3.2149131814	5.9553602534
O	0.9044427793	3.7198925132	7.4527537418
O	3.7199353230	0.9036736620	7.4529491382
O	6.0312024948	1.4081980017	5.9549730131

O	7.8378511011	3.2148503864	5.9549000221
O	5.5266896771	3.7195974934	7.4529807267
O	8.3425984403	0.9036893161	7.4529806990
O	10.6538208047	1.4080305754	5.9550989776
O	12.4608437579	3.2149706425	5.9575691505
O	10.1492362273	3.7194988844	7.4529502986
O	12.9649203962	0.9034456169	7.4527600135
O	1.4079290938	6.0311090934	5.9564001919
O	3.2148463857	7.8380302825	5.9564750653
O	0.9037235788	8.3425172873	7.4528073084
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O	6.0310312840	6.0308205424	5.9550995470
O	7.8379738205	7.8378417552	5.9575705213
O	5.5264459501	8.3419188046	7.4527597390
O	8.3424989078	5.5262341288	7.4529502944
O	10.6538960526	6.0308935467	5.9565871428
O	12.4611254999	7.8381220231	5.9558510317
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O	1.4079197334	10.6539193876	5.9558289611
O	3.2151473674	12.4611444385	5.9565610166
O	0.9037751810	12.9650748997	7.4527795953
O	3.7190758589	10.1497754751	7.4527794968
O	6.0309648813	10.6541047022	5.9573053795
O	7.8379168192	12.4611266424	5.9553600831
O	5.5266731790	12.9659381661	7.4529494765
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O	1.4080768043	1.4079548465	8.9485373424
O	3.2151103524	3.2149243835	8.9507113142
O	0.9032343833	3.7195739849	10.4418555477
O	3.7193191795	0.9028944699	10.4427647404
O	6.0311813823	1.4081768971	8.9513976400
O	7.8378722708	3.2148715501	8.9514730129
O	5.5261336954	3.7199426049	10.4430630823
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O	10.6538449825	1.4080236636	8.9509661256
O	12.4608808166	3.2149838370	8.9482817730
O	10.1498012996	3.7202212107	10.4427602027
O	12.9659467977	0.9036166164	10.4418737917
O	1.4079179520	6.0310956877	8.9494728651
O	3.2148635563	7.8380451583	8.9494290267
O	0.9033908908	8.3426671876	10.4421401236
O	3.7196330507	5.5264997082	10.4421183552
O	6.0310243440	6.0308447228	8.9509654465
O	7.8379869481	7.8378788379	8.9482799131
O	5.5266172743	8.3429467962	10.4418727044
O	8.3432216795	5.5268010934	10.4427594453
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O	12.4611341661	7.8381306333	8.9501022009
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O	1.4079109586	10.6539105999	8.9501322881
O	3.2151485872	12.4611456827	8.9494198801
O	0.9033193354	12.9656760167	10.4419102358
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O	6.0309576651	10.6540730512	8.9485353398
O	7.8379281335	12.4611062664	8.9507114415
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O	8.3425729536	10.1492340906	10.4418550197
O	10.6540996818	10.6539145462	8.9494694337
O	12.4610460284	12.4608634909	8.9494317276

O	10.1495003435	12.9656333010	10.4421183089
O	12.9656674825	10.1493910253	10.4421401017
O	1.4078861350	1.4081483893	11.9319697836
O	3.2146483323	3.2148060106	11.9318559958
O	0.9035022333	3.7195989216	13.4195926863
O	3.7195867625	0.9035362100	13.4198673942
O	6.0309780480	1.4079767687	11.9328892870
O	7.8380353155	3.2150348266	11.9328650105
O	5.5264269659	3.7195826642	13.4200200304
O	8.3425826840	0.9034268303	13.4200201515
O	10.6543399495	1.4081878962	11.9318046641
O	12.4611187387	3.2148382772	11.9319966635
O	10.1494131689	3.7194728458	13.4198569495
O	12.9655014257	0.9034081436	13.4195952137
O	1.4082321974	6.0310026471	11.9316399748
O	3.2149790788	7.8377420812	11.9316674854
O	0.9033533430	8.3426537222	13.4194545175
O	3.7194231999	5.5265858278	13.4198083336
O	6.0311883337	6.0313396254	11.9318042710
O	7.8378387257	7.8381178503	11.9319960401
O	5.5264080137	8.3425012039	13.4195951754
O	8.3424727461	5.5264131089	13.4198573544
O	10.6542825263	6.0312814352	11.9319579460
O	12.4609522379	7.8379508299	11.9315772932
O	10.1493246229	8.3425483703	13.4197215026
O	12.9655482105	5.5263246463	13.4197211699
O	1.4080421098	10.6540419641	11.9315965620
O	3.2147257092	12.4607253102	11.9319619329
O	0.9034672108	12.9656895640	13.4197289063
O	3.7196893676	10.1494670812	13.4197288065
O	6.0311494591	10.6538851613	11.9319691298
O	7.8378070610	12.4606467624	11.9318558151
O	5.5265361122	12.9655868722	13.4198684259
O	8.3425988752	10.1495024355	13.4195923342
O	10.6540036603	10.6542311447	11.9316406970
O	12.4607423521	12.4609786265	11.9316667587
O	10.1495857366	12.9654230298	13.4198084232
O	12.9656537433	10.1493535269	13.4194546327

## 6. Optimized coordinates for neutral BVO ( $U = 6$ eV)

216

Bi	2.5892879171	1.2733465487	10.2349646176
Bi	2.5552404793	6.3667327551	10.2349646638
Bi	2.5211930769	11.4601192917	10.2349647176
Bi	7.7848878139	1.2733465633	10.2349646515
Bi	7.7508404323	6.3667327725	10.2349647351
Bi	7.7167929516	11.4601192517	10.2349647605
Bi	12.9804878521	1.2733464853	10.2349646309
Bi	12.9464403682	6.3667327341	10.2349645773
Bi	12.9123929678	11.4601192924	10.2349646498
Bi	2.5722642591	3.8200394799	1.4695385203
Bi	2.5382168578	8.9134258972	1.4695385114
Bi	2.5041695046	14.0068122936	1.4695386307
Bi	7.7678642391	3.8200394800	1.4695385025
Bi	7.7338168030	8.9134259286	1.4695385054
Bi	7.6997694347	14.0068123083	1.4695385683
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Bi	12.9294168080	8.9134259064	1.4695385360
Bi	12.8953692808	14.0068122425	1.4695386780
Bi	-0.0085113858	1.2733472590	7.3217858921
Bi	-0.0425588120	6.3667335040	7.3217859296
Bi	-0.0766062111	11.4601199551	7.3217859117
Bi	5.1870885244	1.2733472699	7.3217859799
Bi	5.1530411074	6.3667335088	7.3217860135

Bi	5.1189936437	11.4601199010	7.3217860232
Bi	10.3826883606	1.2733472713	7.3217860753
Bi	10.3486408700	6.3667335086	7.3217860313
Bi	10.3145934402	11.4601198500	7.3217860674
Bi	-0.0255356555	3.8200398692	4.3827169214
Bi	-0.0595830783	8.9134262153	4.3827168912
Bi	-0.0936304863	14.0068125754	4.3827168396
Bi	5.1700642308	3.8200398448	4.3827168177
Bi	5.1360167901	8.9134262400	4.3827168066
Bi	5.1019694662	14.0068125422	4.3827168524
Bi	10.3656640355	3.8200398143	4.3827168609
Bi	10.3316166568	8.9134262179	4.3827167904
Bi	10.2975692038	14.0068125567	4.3827168965
O	3.8906724503	1.9862587349	0.5232396451
O	3.8566249936	7.0796450159	0.5232396386
O	3.8225775465	12.1730311980	0.5232396653
O	9.0862718988	1.9862586940	0.5232397499
O	9.0522243877	7.0796449714	0.5232397758
O	9.0181769383	12.1730311046	0.5232397583
O	14.2818721816	1.9862588069	0.5232395983
O	14.2478246723	7.0796450503	0.5232396232
O	14.2137772545	12.1730312151	0.5232396298
O	3.3054281938	2.5466904059	3.4480127709
O	3.2713807684	7.6400766510	3.4480127275
O	3.2373334460	12.7334629455	3.4480126986
O	8.5010276910	2.5466904894	3.4480127511
O	8.4669802636	7.6400767332	3.4480127084
O	8.4329328882	12.7334630189	3.4480127029
O	13.6966282541	2.5466904038	3.4480126934
O	13.6625807384	7.6400766415	3.4480126794
O	13.6285334049	12.7334629303	3.4480126445
O	1.2758500370	4.5329581549	6.3754866245
O	1.2418027244	9.6263447945	6.3754866365
O	1.2077552975	14.7197311575	6.3754866261
O	6.4714502611	4.5329582549	6.3754864599
O	6.4374029563	9.6263449151	6.3754864765
O	6.4033555381	14.7197312759	6.3754864746
O	11.6670502271	4.5329582095	6.3754865249
O	11.6330029778	9.6263448578	6.3754865433
O	11.5989554609	14.7197312131	6.3754865330
O	0.7246513168	-0.0000006355	9.3002601201
O	0.6906039681	5.0933856046	9.3002600729
O	0.6565565008	10.1867721757	9.3002601826
O	5.9202517094	-0.0000007515	9.3002601184
O	5.8862043373	5.0933854994	9.3002600912
O	5.8521568062	10.1867720243	9.3002601774
O	11.1158513832	-0.0000007118	9.3002601370
O	11.0818040467	5.0933855161	9.3002600973
O	11.0477566221	10.1867720748	9.3002601850
O	1.7710053753	15.2801618087	3.4480124555
O	1.8391002616	5.0933889525	3.4480124827
O	1.8050527579	10.1867755957	3.4480124203
O	6.9666058078	15.2801616832	3.4480125045
O	7.0347006267	5.0933888241	3.4480125174
O	7.0006531507	10.1867754677	3.4480124496
O	12.1622053150	15.2801617384	3.4480124971
O	12.2303001136	5.0933888691	3.4480124924
O	12.1962526883	10.1867755390	3.4480124450
O	0.7076270813	2.5466925176	2.4042405770
O	0.6735796449	7.6400787044	2.4042405997
O	0.6395322907	12.7334651136	2.4042406334
O	5.9032274309	2.5466923905	2.4042405907
O	5.8691800178	7.6400785882	2.4042406141
O	5.8351326461	12.7334649714	2.4042406480
O	11.0988273112	2.5466924192	2.4042405988

O	11.0647798960	7.6400786093	2.4042406176
O	11.0307324331	12.7334649998	2.4042406418
O	4.4539244073	2.5466942614	9.3002598012
O	4.4198769968	7.6400806011	9.3002598307
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