

Supporting Information:

Manipulating electrochemical performance through doping beyond the solubility limit

Natav Yatom¹, and Maytal Caspary Toroker^{1,*}

¹Department of Materials Science and Engineering, Technion - Israel Institute of Technology, Haifa 32000, Israel

This supporting information includes the total energies of the bulk in Table S1, the total energies and band positions relative to the vacuum of the surface slabs in Table S2, and afterwards are the unit cells with relaxed geometries.

Table S1-Total energy of the Pure hematite, 1.25at.%Nb doped hematite, and alloyed FeNbO₄ bulk calculations

Stoichiometric unit	Crystal type	Bravais lattice	Number of stoichiometric units in the cell	Total energy [eV]
Fe ₂ O ₃	Hematite	Rhombohedral	2	-68.154
Nb _x Fe _{2-x} O ₃ (x=1/32)	Hematite	Rhombohedral	16	-551.742
FeNbO ₄	Wolframite	Monoclinic	2	-96.795

Table S2- Calculated slabs: phase, number of atoms that converged the highest occupied state (h.o.s) to less than 1 meV/atom, Surface facet and terminated atom, top most atoms, energy levels of valance band maximum (VBM), (h.o.s), lowest unoccupied state (l.u.s) and conduction band minimum (CBM) with respect to the vacuum level and total energy.

Phase	Number of atoms in the slab	Facet/ Terminated atom	Top most atoms (R=bulk)	VBM	h.o.s	l.u.s	CBM	Total energy [eV]
Nb-Fe ₂ O ₃	Nb ₂ Fe ₈ O ₁₅	(0001)/Fe	R-Fe-Fe-O ₃ - Nb	-5.59	-4.04	-3.37	-3.37	-179.896
Nb-Fe ₂ O ₃	Nb ₂ Fe ₈ O ₁₅	(0001)/Fe	R-Fe- Nb -O ₃ -Fe	-5.36	-4.29	-3.10	-3.10	-183.906
Nb-Fe ₂ O ₃	Nb ₂ Fe ₈ O ₁₅	(0001)/Fe	R- Nb -Fe-O ₃ -Fe	-5.84	-4.94	-3.53	-3.53	-183.818
Fe ₂ O ₃	Fe ₁₀ O ₁₅	(0001)/Fe	R-Fe-Fe-O ₃ -Fe	-5.75	-5.40	-3.88	-3.41	-167.158
Nb-Fe ₂ O ₃	Nb ₂ Fe ₁₀ O ₂₁	(0001)/O	R-Fe- Nb -O ₃	-8.14	-7.92	-7.49	-5.85	-235.384
Nb-Fe ₂ O ₃	Nb ₂ Fe ₁₀ O ₂₁	(0001)/O	R- Nb -Fe-O ₃	-8.52	-8.10	-7.59	-6.26	-235.401
Fe ₂ O ₃	Fe ₁₂ O ₂₁	(0001)/O	R-Fe-Fe-O ₃	-8.77	-8.46	-6.59	-6.59	-213.092
Nb-Fe ₂ O ₃	Nb ₂ Fe ₁₀ O ₂₁ H ₆	(0001)/OH	R-Fe- Nb -(OH) ₃	-4.76	-3.81	-2.66	-2.44	-262.540
Nb-Fe ₂ O ₃	Nb ₂ Fe ₁₀ O ₂₁ H ₆	(0001)/OH	R- Nb -Fe-(OH) ₃	-4.82	-3.82	-2.71	-2.44	-263.136
Fe ₂ O ₃	Fe ₁₂ O ₂₁ H ₆	(0001)/OH	R-Fe-Fe-(OH) ₃	-5.71	-5.54	-3.40	-3.40	-249.357
Nb-Fe ₂ O ₃	Nb ₂ Fe ₁₀ O ₁₈	(01-12)/O	R-Fe ₂ -O ₂ -Fe Nb -O ₂	-5.56	-4.75	-3.45	-3.45	-215.381
Nb-Fe ₂ O ₃	Nb ₂ Fe ₁₀ O ₁₈	(01-12)/O	R-Fe Nb -O ₂ -Fe ₂ -O ₂	-5.88	-4.78	-3.70	-3.70	-215.684
Fe ₂ O ₃	Fe ₁₂ O ₁₈	(01-12)/O	R-Fe ₂ -O ₂ -Fe ₂ -O ₂	-5.67	-5.67	-3.65	-3.65	-199.587
FeNbO ₄	Fe ₁₆ Nb ₁₆ O ₆₄	(111)/O	FeNbO ₄	-7.40	-7.05	-5.05	-5.05	-780.324

The geometries below are given according to the following order: title, lattice vectors in Cartesian coordinates, atom types, and numbers, respectively, and atom locations in fractional coordinates with respect to the lattice vectors. The atom coordinates are ordered according to the ordering given in the atom type row according to the format of the VASP simulation package.

Bulk:

Rhombohedral Pure Fe2O3

```

1.0
      5.4876980782      0.0000000000      0.0000000000
      3.1300017913      4.5075483638      0.0000000000
      3.1300000750      1.6371697833      4.1997217046
  O   Fe
  6   4
Direct
      0.749999642      0.444319755      0.055680726
      0.055680603      0.749999642      0.444319636
      0.444319308      0.055680610      0.749999821
      0.250000477      0.555680215      0.944319427
      0.944319367      0.250000358      0.555680335
      0.555680454      0.944319487      0.250000149
      0.854198754      0.854198813      0.854198635
      0.145801365      0.145801127      0.145801321
      0.645801544      0.645801425      0.645801306
      0.354198486      0.354198605      0.354198664

```

Monoclinic FeNbO4

```

1.0
      4.7112178802      0.0000000000      0.0000000000
      0.0000000000      5.7062559128      0.0000000000
      -0.0499085349      0.0000000000      5.0591853866
  O   Fe   Nb
  8   2   2
Direct
      0.229034200      0.115556479      0.917179048
      0.770965755      0.884443462      0.082820959
      0.770965755      0.115556479      0.582820952
      0.229034200      0.884443462      0.417179048
      0.275250643      0.385083616      0.421349347
      0.724749386      0.614916384      0.578650653
      0.724749386      0.385083616      0.078650653
      0.275250643      0.614916384      0.921349347
      0.000000000      0.168047935      0.250000000
      0.000000000      0.831952095      0.750000000
      0.500000000      0.683595717      0.250000000
      0.500000000      0.316404253      0.750000000

```

Rhombohedral 1.25at.%Nb doped Fe2O3

1.0

11.0010251999	0.0000000000	0.0000000000
6.2659172730	9.0533944357	0.0000000000
6.2740852551	3.2889036380	8.4329460178

O Fe Nb
48 31 1

Direct

0.374579519	0.220758691	0.030272504
0.375738680	0.220860347	0.528864741
0.367139250	0.733437896	0.024597198
0.366249770	0.731074035	0.528235376
0.874323606	0.223659530	0.027420400
0.875059187	0.221578836	0.528752148
0.875081003	0.721886039	0.026826127
0.872807384	0.718269289	0.532112658
0.032041140	0.373799354	0.221382231
0.029922545	0.372959256	0.723157406
0.026695473	0.875578821	0.222843617
0.026454048	0.875892282	0.721760452
0.526663840	0.368907660	0.228938594
0.524785101	0.367356658	0.730721772
0.528094828	0.874508619	0.222535089
0.534168422	0.872226894	0.717176795
0.220524624	0.030436425	0.374832332
0.220916554	0.030531634	0.873668253
0.222110197	0.527747095	0.375970960
0.221951872	0.528181493	0.875080705
0.724469721	0.027394731	0.374521405
0.721747756	0.027745144	0.875586629
0.731137276	0.525270998	0.367836416
0.725956976	0.530195594	0.862939835
0.125443280	0.277603745	0.472054720
0.126378044	0.276836663	0.972227931
0.122108921	0.777779043	0.472999960
0.119990200	0.777987123	0.974827945
0.625083447	0.277955949	0.472946912
0.625667572	0.279211730	0.971801102
0.628920674	0.783957899	0.465818405
0.624224722	0.781498313	0.970307529
0.472087204	0.124098390	0.277472824
0.471836686	0.122454613	0.777962327
0.470305383	0.625594079	0.285642982
0.467786312	0.628247082	0.783413708
0.972366273	0.126235068	0.277040303
0.974687159	0.121194892	0.777816653
0.972450495	0.625776649	0.278488755
0.971153080	0.624227524	0.778314590
0.278416455	0.472851187	0.124527767
0.277731657	0.471844345	0.625296712
0.275845855	0.972995520	0.127199039
0.279025376	0.971978545	0.625656068
0.783246517	0.469815969	0.124209471
0.783681691	0.467210531	0.626165986

Bulk:

Fe₂O₃ (0001) Fe terminated surface

Fe₂O₃ (0001) R-Fe-Fe-O3-Nb

1.000000000000000		
5.0980000496000004	0.000000000000000	0.000000000000000
-2.5490000248000002	4.4149975513999999	0.000000000000000
0.000000000000000	0.000000000000000	25.6149997710999990
O	Fe	Nb
15	8	2
Direct		
0.3141586190234662	0.0154648919936733	0.5003625286515216
0.9691403058435526	0.3276898375099009	0.6882964987810709
0.6410170458424389	0.6741982517103295	0.3145504594231383
0.0080997637321474	0.3213767056346697	0.5002612596158826
0.6642396115153844	0.6432896276643731	0.6862505962159702
0.3246981433987060	0.9769989865424904	0.3125323434695133
0.6978846022336924	0.7053628504117100	0.5002985844898689
0.3466776681031334	0.0152946082058705	0.6857750082539624
0.0121569075570420	0.3557719406259494	0.3146500278315685
0.3595716407046439	0.3482516251310557	0.4083221428603210
0.0175567961776864	0.6734714999210567	0.5900065624600686
0.6677448284104344	0.0256064487355445	0.4105856104645653
0.3406570402634870	0.3651787156435233	0.5922505012445427
0.9904403560541724	0.6602061715171175	0.4095774522479587
0.6524472806574622	0.9961599885916783	0.5911521086905225
0.0055648177488763	0.0142362411426120	0.5566781985365665
0.3387179083041971	0.6865768536910295	0.3735282056282898
0.6592040386662035	0.3312197764549794	0.3562271328904743
0.3405866371270392	0.6825416852750408	0.5344163157965696
0.0078836416359209	0.0134950162861003	0.4439330344901435
0.6789460301841004	0.3442154981096053	0.6272327413474983
0.6753861160460914	0.3482872981217326	0.4662043340748241
0.3223288356012972	0.6627725592781957	0.6442689917028375
0.9949372682691333	0.9958790923747287	0.7084484849492299
0.9935301298996819	0.0039379724270390	0.2922349398830946

Fe₂O₃ (0001) R-Fe-Nb-O3-Fe

1.000000000000000		
5.0980000496000004	0.000000000000000	0.000000000000000
-2.5490000248000002	4.4149975513999999	0.000000000000000
0.000000000000000	0.000000000000000	25.6149997710999990
O	Fe	Nb
15	8	2
Direct		
0.3077225254378106	0.0125493854437053	0.5000105593963156
0.9964757117249121	0.3626236577170516	0.6907174450892057
0.6421192137500285	0.6427625230936442	0.3142479300644823
0.0012995912281184	0.3199480202280753	0.5003041481468600
0.6380763790885666	0.6353321929156621	0.6830522655543234
0.3632305862865408	0.9971727981971839	0.3176739390275429
0.6949258387727610	0.7060738000811995	0.5006192748109299
0.3589572945856148	0.0023503239699636	0.6864152535822683
0.0051165174212073	0.3663351235184109	0.3098052630851740
0.3563895218154158	0.3328098927457432	0.4076689777081981
0.0456560520550653	0.6957653195904925	0.5920084024507943
0.6832801926185681	0.0537263639410668	0.4084375710340780
0.3187251427086792	0.3717736108990621	0.5922532729661967
0.9563161124401844	0.6509848484290544	0.4085632163232518
0.6458949145865063	0.9777700224850747	0.5930544371209550
0.9994240159642374	0.0131365464199789	0.5565892784163182
0.3260373563832317	0.6630682083384016	0.3694091775829378
0.9927978925993841	0.9952432070200885	0.7038559014181658
0.3360823300785469	0.6809719204029818	0.5337464884322216
0.0028104417148569	0.0144938533889274	0.4440361922967426
0.6757323269456990	0.3387053889361340	0.6311909376600653
0.0082434862570864	0.0020162472571883	0.2968198439867251
0.6664022056395069	0.3460446148687879	0.4668985090760671
0.6866350293232273	0.3451983803315954	0.3507178740482217
0.3152223375742480	0.6606287567805040	0.6499488867219512

Fe2O3 (0001) R-Nb-Fe-O3-Fe

1.0000000000000000
5.0980000496000004 0.0000000000000000 0.0000000000000000
-2.5490000248000002 4.4149975513999999 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.6149997710999990
O Fe Nb
15 8 2

Direct

0.3322334980046620 0.0168031392693422 0.4996982289809324
0.9842185746310932 0.3529183747451228 0.6857875055004143
0.6245460623651411 0.6547838970835400 0.3153375178828810
0.0103316895469163 0.3386775426571589 0.5009310171935724
0.6476113814041966 0.6305217391931990 0.6853146586376369
0.3469477347465570 0.9914362128235013 0.3148687646727808
0.6955102421781234 0.7020031936662434 0.5003302373121556
0.3722358839935751 0.0167143531222038 0.6859142202523500
0.0106685449630817 0.3794684847106637 0.3147302647051688
0.3606422693591256 0.3624054645231709 0.4055014899186418
0.0158955950120259 0.6441621280821366 0.5959411001224524
0.6381721887236722 0.0230088073548274 0.4047085878340866
0.3553451483245027 0.3667613559629359 0.5951607776088466
0.9802988783733753 0.6361870237373353 0.4058976537177159
0.6290940099786724 0.9863411971976319 0.5947430138835657
0.0125952896062174 0.0073702959373065 0.5553424093979658
0.0016816986803647 0.9998357366816677 0.7030223003227576
0.6607211526221661 0.3412880095415858 0.3504825125719009
0.3401288406178864 0.6855419902699253 0.5332274688918019
0.0011050934356192 0.0192601148285547 0.4452810774959559
0.9938737432656950 0.0089374605913122 0.2976181698845082
0.6791329791824765 0.3467763210417445 0.4674122598671175
0.3341239143555441 0.6667570675755883 0.6501903240647735
0.3275203650988701 0.6759760615126851 0.3658662431665860
0.6689382385304725 0.3335490348905665 0.6347372421134594

Fe2O3 (0001) R-Fe-Fe-O3-Fe

1.0000000000000000
5.0980000496000004 0.0000000000000000 0.0000000000000000
-2.5490000248000002 4.4149975513999999 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.6149997710999990
O Fe
15 10

Direct

0.3078642436629551 0.0075232518484185 0.5003329291123819
0.9867159044941971 0.3529401817314692 0.6815096681913673
0.6430296338873518 0.6622130216908175 0.3191505308103402
0.0009548584136283 0.3143178314757691 0.5003190202094530
0.6543399746595924 0.6483201649502917 0.6815309876168385
0.3475936828413495 0.9944539012715197 0.3191073987841619
0.6939957621455264 0.7005733732980488 0.5003134117002261
0.3588966042925108 0.0206161221659897 0.6814981642277189
0.0151705719829778 0.3666368076795692 0.3191381856736726
0.3572317693744580 0.3405572596081754 0.4089237154669902
0.0230088537350142 0.6742919253745825 0.5917116891499461
0.6684966308283862 0.0304082879570444 0.4089350375231007
0.3333451399187410 0.3631570373038073 0.5917131305705823
0.9788736691207447 0.6519228579669090 0.4089357625578884
0.6446538664891364 0.9846102502526932 0.5917226491300056
0.0004571328238470 0.0073157017318266 0.5564544260687754
0.3351025168888313 0.6743962889258128 0.3694204552776625
0.9999055539832398 0.0072450345000874 0.6911931774802440
0.6685263560815500 0.3410752049914763 0.3552417798110383
0.3341222510742057 0.6740717983808793 0.5344650872940875
0.0013875566225749 0.0075367638449038 0.4441876015311692
0.6667932954303666 0.3406825472632278 0.6312221899488080
0.0019707377399669 0.0078127491611113 0.3094301346075596
0.6677454869890838 0.3408054127754312 0.4661813588540582
0.3333910085197829 0.6740012818501242 0.6454064984019041

Fe₂O₃ (0001) O terminated surface

Fe2O3 (0001) R-Fe-Nb-O3

1.000000000000000		
5.0980000496000004	0.000000000000000	0.000000000000000
-2.5490000248000002	4.4149975513999999	0.000000000000000
0.000000000000000	0.000000000000000	25.6149997710999990

O	Fe	Nb
21	10	2

Direct

0.3061755214913546	0.0051060330400077	0.5002691628224127
0.9781537120666570	0.3262676853457052	0.6807929740408198
0.6449845196022679	0.6841562477336112	0.3196592293762066
0.0012242164536218	0.3106359307198545	0.5003445487647724
0.6741543650348305	0.6430511564211940	0.6789749795391131
0.3278826807785080	0.9691628371942045	0.3217150754179343
0.6962032204559208	0.7000963723275788	0.5004298546885479
0.3570214672757643	0.0408618125074511	0.6810183576632625
0.0237667795805123	0.3483015357718529	0.3199146656569170
0.6696171975556169	0.9923261368784253	0.2314835429973741
0.7182342743166785	0.0301073179284401	0.7657157813188959
0.3654047011279999	0.3399239415218460	0.4099465018505839
0.0293200310215127	0.6710555771207822	0.5907911201866938
0.9993886162256658	0.7194178484213509	0.2368758592339049
0.0021891874883408	0.7218243959283228	0.7638309384981028
0.6693318599445846	0.0346696880803208	0.4109165661995959
0.3328958524057910	0.3667928440919965	0.5897826409327322
0.2832287584874322	0.3116297398862358	0.2349858999262509
0.3319246708394843	0.3244695759449954	0.7691754475445478
0.9729397965861111	0.6425650262299243	0.4099085281031805
0.6369108792831710	0.9760381748170914	0.5907395349140145
0.9989229310589067	0.0038559929491200	0.5570198177940711
0.3393250519739226	0.6771575113290140	0.3776353842006657
0.0075358963485144	0.0224241491291224	0.7227665999449684
0.6652154074215133	0.3385062120294364	0.3525491820509501
0.3335104425768947	0.6715370621775847	0.5341138481681398
0.0034076992487968	0.0058491720781291	0.4436702189904622
0.6628482597130940	0.3392924823582106	0.6230691970717714
0.9940200869887690	0.0148433088033073	0.2779220453546429
0.6688918133630892	0.3391368737946650	0.4665857236568201
0.3368214979528830	0.6749653290947037	0.6481407912991486
0.6709390597348133	0.3538430943494930	0.7414613991067469
0.3306245595969770	0.6828090339960227	0.2592325926857484

Fe2O3(0001) R-Nb-Fe-O3

1.0000000000000000

5.0980000496000004	0.0000000000000000	0.0000000000000000
-2.5490000248000002	4.4149975513999999	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.6149997710999990

O	Fe	Nb
21	10	2

Direct

0.3075806534467347	0.0081222890275185	0.5004746471049302
0.9659926919698734	0.3357597923109381	0.6812178058863267
0.6544608188449956	0.6843269143283521	0.3218802725020709
0.0010533102788983	0.3114931205101357	0.5003449409796517
0.6772438577751672	0.6474505897156178	0.6815833912836098
0.3247561434984689	0.9706099700299120	0.3191158584851124
0.6945092852148989	0.7015581218821083	0.5002193634479042
0.3475295584856823	0.0314329336880661	0.6788122400255361
0.0359866452700786	0.3701496305935095	0.3194704882545878
0.6401486959938438	0.9655685535201073	0.2336995005412206
0.7093177378514923	0.0574667085867873	0.7676737195664316
0.3641998252168008	0.3393499220856810	0.4099074300097669
0.0248980219326924	0.6698731060382741	0.5899103320933961
0.0099557437698579	0.7012382108309154	0.2311299736489687
0.9919256243746375	0.6930135612408677	0.7695642459069418
0.6718028356433408	0.0397947683840627	0.4099013340938669
0.3302524866240546	0.3693250793712437	0.5907899872996296
0.2926147875059613	0.3482633204217791	0.2330259420907552
0.3616478103845893	0.3271540325856392	0.7669833606935512
0.9771608423358984	0.6457294920787433	0.4107870500492510
0.6378614875996931	0.9764866634299665	0.5907849456021239
0.9995783210160525	0.0058334168368646	0.5569313353342409
0.6838344706893551	0.3509903335289408	0.7323664851388685
0.3388198004639378	0.6765707216586492	0.3775168755798646
0.6677555687093601	0.3429574407550859	0.3527334451643256
0.3328571190614085	0.6729466325923141	0.5341944158810179
0.0025181975879178	0.0070741999187689	0.4437725261165042
0.6631992392968371	0.3391026701819655	0.6231825426733550
0.3181029274716423	0.6673565236072818	0.2683369921181296
0.6692764213492595	0.3410832986246390	0.4664903114287569
0.3342165574380616	0.6767169927098209	0.6479560600873242
0.0184163023472834	0.0130499932820598	0.7341691522661051
0.9835413735512333	0.9948310956433914	0.2665110386458736

Fe2O3(0001) R-Fe-Fe-O3

1.000000000000000		
5.0980000496000004	0.000000000000000	0.000000000000000
-2.5490000248000002	4.4149975513999999	0.000000000000000
0.000000000000000	0.000000000000000	25.6149997710999990

O Fe
21 12

Direct

0.3071952666367039	0.0051824109801188	0.5002860422717887
0.9737103747308069	0.3311109568328021	0.6814026289965796
0.6441555594103505	0.6807090608844462	0.3191792548937897
0.0013900547754844	0.3105916576892582	0.5003439542889794
0.6705497747358464	0.6414221453594422	0.6797282201533790
0.3314207027937002	0.9711036172048253	0.3209352115820110
0.6955927246374785	0.6993653204577370	0.5004153312569528
0.3577112164075089	0.0382392710015651	0.6815226590176238
0.0281073050311207	0.3574365763117413	0.3193080996816136
0.6419374187867959	0.9422854582754567	0.2339295190766606
0.7381325378870542	0.0762365899468236	0.7654652303173322
0.3659586732460127	0.3395006433031753	0.4096578136215143
0.0274620077015442	0.6710682471069163	0.5909568813600785
0.0461886907040210	0.7373003978900030	0.2372458207108679
0.9549533479352661	0.6929174683953647	0.7634903400785618
0.6722767258558022	0.0363683190660709	0.4103710588360840
0.3301288239462323	0.3656295290436162	0.5903136428008580
0.2630504067209500	0.3375607451775124	0.2352164338870253
0.3593136857198047	0.3024969927225030	0.7667013874721960
0.9749843209909486	0.6445688546545085	0.4097442777576532
0.6365607167357297	0.9751068150243825	0.5910436228624008
0.9980746981333581	0.0034480892234257	0.5569653484767016
0.6726107801216443	0.3542774030603155	0.7334265163073539
0.3410300963740909	0.6778507298264103	0.3775011667770372
0.0053007913747365	0.0221092973829116	0.7231870893527557
0.6680411615947577	0.3410703981372478	0.3518115194226610
0.3332626733861801	0.6712526787395632	0.5344738525647301
0.0045037742741201	0.0064535909692935	0.4437315589351059
0.6612320957024522	0.3382938069447761	0.6231974521349812
0.3287231533462247	0.6812583179290215	0.2672501705291523
0.9960266736610990	0.0164862366620611	0.2775219855159321
0.6695056853650172	0.3392811707590226	0.4662282796086217
0.3339231852771150	0.6746972660377111	0.6488855834510119

Fe₂O₃ (0001) OH terminated surface

Fe2O3 (0001) R-Fe-Nb- (OH) 3

1.000000000000000		
5.0980000496000004	0.000000000000000	0.000000000000000
-2.5490000248000002	4.4149975513999999	0.000000000000000
0.000000000000000	0.000000000000000	25.6149997710999990

O	Fe	H	Nb
21	10	6	2

Direct

0.3071915511007148	0.0169635493201241	0.5001890484864262
0.0064020678432186	0.3672691154168746	0.6879168171550347
0.6484676278847985	0.6653403773467303	0.3115082072877300
0.0006957679985362	0.3246950927478665	0.5003365398380879
0.6560543343713832	0.6500324863309430	0.6888491041101545
0.3460870788514256	0.9951401105019855	0.3118739360337983
0.6941782609953293	0.7104665792745877	0.5004988367032581
0.3542891489805697	0.0185501688393401	0.6890345075387785
0.9963584585005947	0.3623289439874213	0.3128863003781603
0.6746896288639661	0.0057181537296529	0.2223677607454988
0.6452416427556784	0.0035283365621765	0.7824460584962196
0.3538718731483428	0.3314955188246458	0.4077593177792878
0.0503093192852830	0.7053526470832168	0.5924432189628348
0.0407622946313069	0.7006034151793870	0.2168853463927860
0.9614419746896630	0.6609098616408886	0.7838390989570101
0.6795103739029997	0.0581440594564384	0.4091242298110132
0.3218092818392719	0.3793097769579958	0.5915384071487679
0.3568005256233917	0.3596434395571180	0.2181677702101439
0.3276377470588940	0.3312074645176892	0.7784047271803942
0.9509911304295784	0.6557406606986333	0.4082867169427615
0.6475529869456409	0.9783075323874968	0.5929013623683019
0.0042262730731650	0.0186730943155098	0.5569232146722740
0.3264209208405262	0.6817915184056673	0.3800658879472394
0.9821875915521261	0.0056620749161453	0.7316194697118092
0.6577412246651164	0.3399727315682384	0.3558851073710088
0.3346639864375192	0.6842655546312386	0.5339157402661883
0.9971993165570865	0.0151880695658804	0.4437490933275754
0.6750862847587698	0.3563550480896964	0.6206220249295455
0.0202495549164325	0.0249836163318591	0.2690193692915201
0.6667323597721335	0.3503109535920501	0.4667607424448548
0.3445194196126451	0.6830660620110081	0.6447835322422719
0.1466393519268721	0.8231722212809558	0.1865933302692895
0.5411630922914696	0.3429574314421018	0.2169436720197453
0.6936325092699533	0.9322078675573380	0.1883380263486174
0.8548268253872848	0.6776498560958046	0.8140185790285202
0.4606698749909341	0.8026711406108404	0.7837508366907926
0.3088662251240990	0.2374746162830803	0.8123062212108394
0.6767682641775110	0.3267066356033013	0.7309683422454469
0.3257179229457634	0.6513472443380905	0.2697184804560493

Fe2O3(0001) R-Nb-Fe-(OH)3

1.0000000000000000
5.0980000496000004 0.0000000000000000 0.0000000000000000
-2.5490000248000002 4.4149975513999999 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.6149997710999990

O Fe H Nb
21 10 6 2

Direct

0.3058984130426552	0.0190162013229624	0.5003785497143411
0.9557748997980795	0.3121902860529389	0.6843330330749779
0.6669694674445878	0.6865982764515337	0.3156690934490385
0.9984504172783346	0.3246270836501637	0.5002881989566816
0.6806373948725906	0.6547942952161421	0.6852818848617375
0.3197292804925524	0.9660690666306238	0.3135879555854046
0.6904230631482520	0.7107078874700079	0.5002322835563078
0.3355020003623039	0.0251436139967467	0.6879897924641440
0.0428682202088808	0.3524989991303755	0.3149488639119085
0.7230978672690469	0.0444397549722453	0.2212031459135915
0.6706718512935979	0.9600917422130024	0.7806636438072800
0.3508844381823195	0.3480693920171021	0.4099537557861055
0.0185662363168859	0.6835223778739135	0.5897957028790017
0.0082141676927776	0.7049339612657377	0.2201759848543929
0.0000060987840556	0.6860077798027007	0.7793726586893825
0.6595151537423405	0.0314839501322695	0.4086010674231488
0.3359819817050322	0.3748540254510075	0.5920684782578078
0.3364275227293945	0.3119582403296945	0.2224585456126391
0.2918829918842789	0.3142571703400847	0.7786808133335086
0.9790422058974926	0.6587460623236865	0.4107928851586280
0.6448912785836072	0.0006638548858930	0.5904888918853928
0.0006619641923393	0.0218908628689718	0.5565726006988854
0.6638706872053177	0.3150881414337547	0.7448265424795011
0.3210475935371804	0.6705794613271365	0.3762712750271575
0.6737107185106552	0.3416737113646207	0.3544455685857528
0.3332497651915176	0.6871971441781142	0.5347494923589409
0.9956629958916778	0.0151601529699406	0.4440168105972759
0.6750116035707450	0.3541284508150966	0.6239267411265530
0.3588556880418565	0.6777301262977247	0.2554929819120915
0.6634457647120868	0.3509179439864738	0.4658071622175228
0.3230453328225380	0.6766406688072308	0.6463639762948930
0.0823768404626151	0.8247906344991520	0.1884656656501775
0.5299973935052193	0.3130135069076943	0.2212626627316894
0.7870420611943629	0.0668787122278474	0.1850720596626303
0.9222058604174421	0.7244848238425305	0.8114025629048029
0.4751701168916540	0.7689501894487094	0.7823758656738278
0.2308756778905590	0.2474101313820114	0.8143274325071701
0.9824434399544515	0.0007427509860136	0.7222264432899408
0.0035435112787283	0.0072541881281865	0.2786693971057375

Fe2O3(0001) R-Fe-Fe-(OH)3

1.0000000000000000
4.4149975084930704 -2.5489999999999999 0.0000000000000000
0.0000000000000000 5.0979999999999999 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.6149998092651003

O Fe H
21 12 6

Selective dynamics

Direct

0.3061405007624529	0.0064594586372948	0.5002944104331988
0.9743215539803529	0.3417574879095469	0.6819595219668457
0.6461691147552600	0.6770317349376498	0.3188661661981058
0.0005745859835997	0.3114230620521354	0.5002923540903197
0.6684832292018470	0.6499305233573764	0.6815370087247388
0.3336997454566628	0.9814098532972864	0.3191876271378646
0.694946757431072	0.7008582323446291	0.5003117764819436
0.3563743542125835	0.0329349398997323	0.6817233903109994
0.0290520035772985	0.3681503625927292	0.3188327274529712
0.6815950054513564	0.0149440998126735	0.2310354788634967
0.6911409791861658	0.0147321323124459	0.7730709964977436
0.3633440955610538	0.3413390417621613	0.4097560912996485
0.0270682623683172	0.6723454934683701	0.5907369273814567
0.0099642088157523	0.7042622457824237	0.2276302459991655
0.9906058074211899	0.6970920921749553	0.7733353020567222
0.6685406115981678	0.0353331777028529	0.4097594736426942
0.3330167570441702	0.3679950089688333	0.5908338977400263
0.3110896889862360	0.3233142707992940	0.2275803830355301
0.3216984861759471	0.3324467346463962	0.7702190254481849
0.9743515624551691	0.6455822554165067	0.4098926414566577
0.6382945601066865	0.9793543814734846	0.5908740020401169
0.9995118532313967	0.0060353610209276	0.5570233059726348
0.6717991816457243	0.3397942010271962	0.7353972940281608
0.3357122287741277	0.6749971734211471	0.3762554486934206
0.9996087303856100	0.0087009295585503	0.7190140878992679
0.6685902384142963	0.3413727011066214	0.3528228723145688
0.3333737353270081	0.6727341195942955	0.5342171258625399
0.0017475140211474	0.0069012796751409	0.4435794420204644
0.6658406888279771	0.3407187347032803	0.6243590382056894
0.3315487805330477	0.6686096010220339	0.2651257859898877
0.0032703546196728	0.0094572778758462	0.2817505598997201
0.6676483060880898	0.3398171680008701	0.4663685297028763
0.3338891273822426	0.6748473440668192	0.6477968168678814
0.1007295448980230	0.8332375189758494	0.1971908707976766
0.5062031200879247	0.3272591581374940	0.2277528249215450
0.7360054284175916	0.9912524077760807	0.1957135534959420
0.8945098314894437	0.7340553085470489	0.8031680841326363
0.4954152742431788	0.8243479884515068	0.7731591392662907
0.2717760390105397	0.2423706567656367	0.8048162872173705

Fe₂O₃ (01-12) O terminated surface

```
Fe2O3 (0001) R-Fe2-O2-FeNb-O2
1.0000000000000000
 19.6922664641999994    0.0000000000000000    0.0000000000000000
  0.0000000000000000    5.0980000496000004    0.0000000000000000
  0.0000000000000000    0.0000000000000000    5.4933905601999999
 O      Fe      Nb
 18     10      2
Selective dynamics
Direct
0.8020749689911781 0.0835141769935177 0.8086015177610619
0.8665609350433101 0.6025486289452857 0.9466641177321264
0.0552524286212019 0.0962694649629441 0.3744426872641426
0.2494715403367067 0.6159138262846398 0.7981046397805187
0.2033028020646839 0.0573962843190259 0.6689933075224204
0.1322694173702672 0.6099275565782349 0.5476505234160243
0.9394004945370042 0.1032376579809693 0.1181850210623452
0.7387181707754564 0.5782724498591847 0.7110674765974423
0.1979296562857655 0.9165754258865206 0.1913975093930915
0.1334708448908160 0.3974493203494305 0.0532928461227229
0.9447717239030951 0.9037122116159750 0.6256129593667481
0.7504686145515436 0.3841162688381559 0.2019151891665132
0.7966647703519740 0.9425444667055345 0.3311221347824542
0.8676758660361585 0.3899196512624030 0.4522481944823795
0.0606219261845027 0.8967464783167287 0.8819776636060510
0.2612670158261992 0.4218543157447527 0.2889075378154971
0.9988316344487487 0.5612740041288617 0.2499656262961736
0.0012144197835013 0.4387196114550065 0.7499042653972552
0.8450934058384263 0.7636819397424475 0.6058340732395067
0.0403260958391343 0.2488770027873102 0.0303480757172352
0.1526156757374295 0.7486087456551331 0.9190433887708593
0.9639531239743135 0.2426661658592835 0.4692715419296789
0.7666733516390849 0.7437825335197488 0.0390282650930374
0.1549067790307674 0.2362301389704911 0.3941786732935029
0.9597051668230208 0.7511257922243857 0.9697012645652521
0.8474010817855486 0.2514525436460247 0.0809307626101088
0.0360466840106710 0.7573689654676130 0.5307483967023501
0.2333458108487889 0.2562860817967803 0.9609976778998899
0.2252071452499322 0.6930042178623808 0.4728625785075238
0.7747583982207686 0.3069240512412748 0.5270020651060463
```

Fe2O3(0001) R-FeNb-O2-Fe2-O2

1.000000000000000		
19.6922664641999994	0.000000000000000	0.000000000000000
0.000000000000000	5.098000049600004	0.000000000000000
0.000000000000000	0.000000000000000	5.493391037000003

O Fe Nb
18 10 2

Selective dynamics

Direct

0.8054590209317141	0.0587946622320104	0.7961264485458983
0.8679733117256134	0.6240882112272956	0.9521914758758072
0.0626654646426630	0.0999061818816571	0.3873136615068375
0.2506684483828039	0.6078571722905295	0.8022176626239172
0.1964015859034092	0.0869076996188554	0.6916031504027345
0.1285376826518458	0.5826198632859345	0.5358385459666692
0.9452590577282152	0.1033334840090347	0.1252510933065167
0.7511488070255723	0.6160210010864304	0.7060144974208029
0.1945395718156959	0.9412016375990291	0.2038761916167076
0.1320271984316364	0.3759112024052556	0.0478064325152801
0.9373341833614504	0.9000959005864146	0.6126919818054262
0.7493318354918728	0.3921479114980997	0.1977810940602325
0.8036009227706984	0.9130940449154323	0.3083954670869744
0.8714622960689411	0.4173784585261799	0.4641626587270622
0.0547410066878129	0.8966674909514296	0.8747559183325748
0.2488514586050457	0.3839759127961457	0.2939817937292304
0.0005304345466115	0.5610922911928498	0.2522104060612875
0.9994686055211162	0.4389101283905390	0.7477984182883759
0.0391748178517872	0.2467329432254033	0.0226853360468979
0.2331133785319750	0.7212800650747013	0.4754742529043625
0.1529492823981542	0.7613419013814422	0.9098997607562396
0.9611182265399734	0.2511010958975177	0.4645404890456390
0.7703582777395113	0.6984779605111271	0.0400233283468978
0.9608245606694794	0.7532682259436072	0.9773197274849466
0.7668856888279194	0.2787130168530609	0.5245231727579025
0.8470514330658361	0.2386614520404891	0.0900874917877701
0.0388815159967493	0.7489017737109762	0.5354685882791728
0.2296415471029007	0.3015261478651539	0.9599688148653200
0.8401713783570557	0.7562368677037057	0.5936223790927571
0.1598279376259342	0.2437542952997092	0.4063678667597799

Fe2O3(0001) R-Fe2-O2-Fe2-O2

1.000000000000000		
19.6922656094624671	0.000000000000000	-0.0000000000000020
0.000000000000000	5.0980000000000034	0.000000000000000
0.000000000000000	0.000000000000000	5.4933905052484668

O Fe
18 12

Selective dynamics

Direct

0.8056726110587604	0.0631401289639939	0.8105898837574657
0.8695956757575587	0.6014626478502691	0.9531481260458747
0.0580100182666428	0.1027621472486402	0.3809523317294818
0.2449993277696549	0.5983037987626432	0.7974186750031720
0.1943294489891656	0.0631293423316990	0.6894054416382644
0.1304038819985607	0.6014550408873518	0.5468528319592281
0.9419904661680647	0.1027623801028668	0.1190464216616576
0.7550005291639224	0.5983115489123279	0.7025817943477861
0.1943280998180725	0.9368572075151604	0.1894097930894247
0.1304046254275377	0.3985333371173212	0.0468503258608237
0.9419902594532559	0.8972404657183688	0.6190476471562931
0.7550006613255960	0.4016870640716448	0.2025791128002865
0.8056712351019044	0.9368628056178991	0.3105896076417807
0.8695960491584955	0.3985432997147456	0.4531473314963961
0.0580101539114324	0.8972394516220987	0.8809538681896996
0.2449990865429612	0.4016881389933573	0.2974216428678176
0.0000006963724388	0.5604794494344603	0.2499990918712740
0.9999999727734945	0.4395249100516025	0.7500013107088250
0.8468227680272236	0.7630486420092808	0.5946971765423612
0.0384484840162287	0.2486457935458688	0.0297580176197698
0.2243449486169169	0.7114081066315805	0.4675203374597103
0.1531761462543386	0.7630358521548288	0.9053021474274558
0.9615512162776412	0.2486470151807865	0.4702403575640446
0.7756546471593992	0.7114075584778163	0.0324844159474722
0.1531751681764888	0.2369613647121369	0.4052991585935146
0.9615502475544773	0.7513543437852377	0.9702413361727977
0.7756549008089024	0.2885984397256607	0.5324824990781210
0.8468244751124345	0.2369655090131744	0.0946992697318976
0.0384480789243256	0.7513586894559907	0.5297622436299321
0.2243461200140828	0.2885855203911873	0.9675178024073929

FeNbO₄ (111) O terminated surface

FeNbO4(111) R-Fe2Nb2-O3
1.00000000000000
6.6582457565451714 3.2287397729529732 -0.0000000000000020
0.0000000000000000 6.9472070052878721 0.0000000000000000
-0.00000000000000040 -0.00000000000000040 37.8345640978416498

O Fe Nb
64 16 16
Selective dynamics
Direct

0.8794990214309664	0.7978190142764490	0.7070858908598865
0.1481922857704703	0.1582120428413916	0.7880183484059771
0.4191652190884980	0.4929513875769445	0.8659175735321298
0.9526108602774599	0.1745458813507312	0.0204590483819729
0.6866384836585482	0.8330357776309825	0.9429852993153460
0.2174136702101706	0.5171915685757824	0.0978985029059345
0.4848983350283405	0.8550239628984500	0.1751103884791760
0.7513916561057528	0.1911971783395288	0.2562027707420782
0.5721984170580185	0.2373946501335951	0.6990485704910938
0.8408396813996717	0.5798924290750733	0.7739015783097543
0.1055795287216910	0.9249410531634013	0.8511652820006219
0.3715783032897448	0.2642312988430078	0.9291328904632365
0.6369604612068045	0.6061041878445010	0.0065975688032580
0.9017962002203248	0.9484993791299701	0.0840000753550214
0.1689674420166014	0.2876815354958993	0.1617875203399706
0.4341123348478604	0.6259272900969393	0.2355881497194119
0.9523262744808463	0.2031537273822437	0.7217079127477319
0.2091583751892969	0.5559162521677266	0.8035157176531129
0.4765243321676849	0.8928742087417945	0.8816370070360975
0.7422199178186730	0.2347176080327884	0.9589678407930933
0.0071658155596950	0.5764927913104430	0.0365073209584921
0.2732654500698999	0.9184728121215144	0.1138063773915476
0.5395777812286369	0.2524809153778733	0.1921279102181401
0.8071197836809390	0.6026323843901480	0.2762729311810119
0.6068154996264070	0.5975115603186651	0.7063800549512962
0.8665366639793888	0.9587255246107986	0.7803767016772341
0.1328932468604833	0.3047164231672070	0.8595098429559442
0.3976629054756700	0.6450860321195151	0.9367830021685393
0.9305162822515385	0.3276887146899341	0.0919130327111546
0.6637388289588415	0.9865945002401304	0.0143708785013317
0.1966214027405613	0.6666499108800679	0.1686754864871531
0.4659297856409239	0.0071491802707371	0.2475033109787645
0.1205007581415742	0.2021798531029546	0.2929141263608557
0.8518089320642019	0.8417862503184352	0.2119816277611406
0.5808347260271347	0.5070493764447335	0.1340822961174126
0.0473897898776130	0.8254549706443655	0.9795410039866681
0.3133618138099195	0.1669652465675071	0.0570147035914985
0.7825859493151057	0.4828107649220712	0.9021014901520843
0.5151012072056602	0.1449770716437939	0.8248896891630935
0.2486089783069900	0.8088005842832686	0.7437971040492073
0.4278007989897077	0.7626033947003350	0.3009513895233056
0.1591596855515149	0.4201064230689298	0.2260984962900849
0.8944199337678853	0.0750589767745424	0.1488347931171177
0.6284219755252209	0.7357693493854853	0.0708671514322603
0.3630394661862439	0.3938969664967900	0.9934024765440839
0.0982036274501326	0.0515014454625486	0.9159999505672971
0.8310328567890934	0.7123186513553534	0.8382124861090574
0.5658866509479452	0.3740719127072012	0.7644119839400432
0.0476739834112578	0.7968443378461600	0.2782921226390656
0.7908409447449429	0.4440834812518943	0.1964843599269912
0.5234752533193614	0.1071270584196071	0.1183629892682845
0.2577805211359774	0.7652835991832347	0.0410322375570118
0.9928342255742351	0.4235079945520326	0.9634927514836917
0.7267342970383055	0.0815289286588197	0.8861935845905933
0.4604214477072972	0.7475193080052094	0.8078720716017429
0.1928798298605514	0.3973652922604458	0.7237269747090238
0.3931830509626835	0.4024872931806485	0.2936195189004067
0.1334627522457481	0.0412745329643229	0.2196234730172648
0.8671064912045097	0.6952834285547880	0.1404901064692581

0.6023372297964755	0.3549146845735294	0.0632169553786071
0.0694839240982716	0.6723121609086462	0.9080869750081604
0.3362618055520628	0.0134059400556694	0.9856292215510791
0.8033787798119789	0.3333501275576083	0.8313243944596849
0.5340723186376906	0.9928484883403002	0.7524968963035477
0.8836199950753993	0.5266757145989800	0.7227178194002448
0.1421100867767322	0.8714809512538366	0.7976325589611122
0.4118296659881509	0.2082412978357695	0.8774505905469425
0.6766529576755929	0.5512734394234116	0.9547689889752959
0.9432228007054988	0.8919147545718360	0.0321534414070115
0.2095078352309940	0.2350079984975721	0.1098350925599618
0.4780150375489995	0.5653615310482110	0.1846324925242016
0.7584195652610859	0.8915609967221556	0.2612674590432604
0.1163789751608348	0.4733229666753971	0.2772820609638558
0.8578892118302974	0.1285176314258507	0.2023675951315198
0.5881694948490352	0.7917601325339305	0.1225494773440587
0.3233472320193655	0.4487277200467830	0.0452310668351998
0.0567777519304116	0.1080859682192923	0.9678466402327146
0.7904923292032606	0.7649940456078497	0.8901648808311222
0.5219845615070611	0.4346398124221622	0.8153674042180654
0.2415816600469967	0.1084370798867837	0.7387323553947809
0.4180342985431409	0.5197872983753768	0.7258884279054953
0.9009473681146645	0.2130830221073197	0.8785055049267072
0.6346416684882215	0.8827903489344848	0.7995336672487099
0.1671996505521705	0.5560253966418145	0.9559606703396497
0.4321387981794373	0.8975504753584715	0.0335079046372684
0.7019256809046439	0.2341165782023253	0.1110204521650218
0.9695544810582106	0.5679899652016971	0.1873504269499335
0.2227272512598049	0.9416974423462676	0.2711598749938702
0.5819649461071350	0.4802111383845258	0.2741113867083627
0.0990527933768917	0.7869188781961469	0.1214946397776373
0.3653593323248217	0.1172090596752966	0.2004666262774606
0.8328004296942098	0.4439753173905956	0.0440393954028906
0.5678619790322657	0.1024504353099047	0.9664922171510355
0.2980744595516356	0.7658838478113452	0.8889795761589596
0.0304459019372132	0.4320072505460075	0.8126492602828250
0.7772735492481075	0.0583024274631256	0.7288398566196719