Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information:

The secret behind the success of doping nickel oxyhydroxide with iron

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Table S1. Corrections added to the free energy calculation of molecules involved in water oxidation.[1]

molecule	E_{tot}	ZPE	TS
H_2	-6.77	0.31	0.40
O_2	-9.87	0.10	0.63
H_2O	-14.23	0.60	0.67

Table S2. Corrections added to the free energy calculation of water oxidation on pure NiOOH.[1]

Reaction	delta H	delta ZPE	entropy
A to B	0.04	-0.21	-0.20
B to C	-0.06	0.02	0.47
C to D	0.04	-0.22	-0.20
D to A	0.04	-0.09	-0.16

Table S3. Free energies and overpotentials for NiOOH with or without H or OH vacancies and without pH and voltage corrections (pH=0 and V=0 Volts). Values adapted from ref. 2.

Reaction	No vacancies	H vacancy	OH vacancy
A to B	1.72	1.49	1.12
B to C	1.12	1.34	1.37
C to D	1.43	1.34	1.22
D to A	0.25	0.34	0.81
overpotential	**0.61**	**0.38**	**0.26**

Table S4. Free energies and overpotentials for Fe-doped NiOOH with or without H or OH vacancies and without pH and voltage corrections (pH=0 and V=0 Volts).

Reaction	No vacancies	H vacancy	OH vacancy
A to B	1.42	1.02	1.19
B to C	1.47	1.44	1.65
C to D	1.27	1.21	0.86
D to A	0.35	0.85	0.82
overpotential	**0.36**	**0.33**	**0.54**

Table S5. Magnetizations of the Ni atoms in stoichiometric Fe-doped NiOOH for each intermediate. The Ni atoms are ordered according to their positions in the geometrical coordinate file provided below (POSCAR). The magnetic moment of iron in the reaction intermediates is 3.6, 3.0, 3.8, and 3.4, which we assign to electronic configurations $t_{2g}^3 e_g^1$, t_{2g}^3, $t_{2g}^3 e_g^2$, and $t_{2g}^3 e_g^1$, respectively, and to oxidation states of +4, +5, +3, and +4, respectively.

Ni atom number	Intermediate A	Intermediate B	Intermediate C	Intermediate D
1	1.756	1.758	1.302	1.224
2	0.132	0.178	1.188	1.260
3	1.728	1.719	1.693	1.694
4	1.076	1.118	0.030	0.034
5	0.127	0.126	1.186	1.188
6	1.354	1.320	1.139	1.044
7	0.102	0.140	1.153	1.100
8	1.723	1.720	1.188	1.179
9	1.074	1.093	0.053	0.054
10	0.109	0.134	1.218	1.214
11	1.096	1.118	1.575	1.590
iron	3.603	2.958	3.790	3.418

Table S6. Magnetizations of the Ni atoms in Fe-doped NiOOH with H vacancy for each intermediate. The Ni atoms are ordered according to their positions in the geometrical coordinate file provided below (POSCAR). The magnetic moment of iron in the reaction intermediates is 2.1, 2.9, 3.4, and 2.8, which we assign to electronic configurations $t_{2g}^3 e_g^1$ (low spin), t_{2g}^3, $t_{2g}^3 e_g^1$ (high spin), and t_{2g}^3, respectively, and to oxidation states of +4, +5, +4, and +5, respectively.

Ni atom number	Intermediate A	Intermediate B	Intermediate C	Intermediate D
1	1.360	1.320	1.365	1.283
2	0.072	0.097	1.216	1.204
3	1.689	1.699	1.691	1.699
4	1.085	1.104	0.033	0.034
5	0.132	0.130	1.185	1.189
6	1.421	1.383	1.124	1.058

7	0.131	0.118	1.130	1.098
8	1.731	1.725	1.180	1.188
9	1.098	1.095	0.058	0.058
10	0.108	0.127	1.222	1.218
11	1.086	1.098	1.505	1.605
iron	2.121	2.872	3.373	2.802

Table S7. Magnetizations of the Ni atoms in Fe-doped NiOOH with OH vacancy for each intermediate. The Ni atoms are ordered according to their positions in the geometrical coordinate file provided below (POSCAR). The magnetic moment of iron in the reaction intermediates is 4.1, 2.2, 3.8, and 3.4, which we assign to electronic configurations $t_{2g}^3 e_g^2$, $t_{2g}^3 e_g^1$ (low spin), $t_{2g}^3 e_g^2$, and $t_{2g}^3 e_g^1$ (high spin), respectively, and to oxidation states of +3, +4, +3, and +4, respectively.

Ni atom number	Intermediate A	Intermediate B	Intermediate C	Intermediate D
1	1.747	1.729	1.292	1.286
2	0.008	0.066	1.145	1.244
3	1.722	1.718	1.698	1.696
4	1.081	1.107	0.026	0.033
5	0.141	0.125	1.187	1.187
6	1.377	1.366	1.207	1.041
7	-0.007	-0.028	1.135	1.092
8	1.723	1.727	1.199	1.190
9	1.094	1.094	0.047	0.053
10	0.115	0.133	1.216	1.217
11	1.094	1.102	1.642	1.705
iron	4.107	2.237	3.802	3.387

The relaxed geometries of Fe-doped NiOOH are given below 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 given according to the ordering in the atom type row (format of VASP geometrical coordinates files: POSCAR). There are three different cases: no vacancy, H vacancy, and OH vacancy. There are four intermediate slabs for each case: A, B, C and D.

No vacancy

1. A state, no vacancy

5.9784002304000001 0.0000000000000000 0.0000000000000000
1.4945932141000000 6.1742788343999999 0.0000000000000000
0.0000000000000000 0.0000000000000000 27.0132007598999984

H O Ni Fe
14 26 11 1

0.2732178615067931 0.5974419331798311 0.7565884663301814
0.4338706096897316 0.8477968323881283 0.8511026827778162
0.1178984746013753 0.1599519492510363 0.8954720850532045
0.2735158774121233 0.4464312610038730 0.9693698619857248
0.5109167100819155 0.6420764203268863 0.0604747997309626
0.7266849059925619 0.5955792552354507 0.7550321884486365
0.9351717739201226 0.8503435688286859 0.8498797460535117
0.6246546401300647 0.1592513967058043 0.8959732366636444
0.7756787222787173 0.4463261967171681 0.9689731047616948
0.9982555922452765 0.6422016292572993 0.0604328161817218
0.5530172946600095 0.7313817392220988 0.6647141690379976
0.5779896609467853 0.9343872601821915 0.6367244860120973
0.0948693265764774 0.8700040301473595 0.6456169483763811
0.9609643958804837 0.1047290427200618 0.6541262522607419
0.1283152349154602 0.1471573439391757 0.7356867894680827
0.1320470606056216 0.1232840782377392 0.0757983355055577
0.2985502998178581 0.4117565680885579 0.7985555553027149
0.4676795515521069 0.7186687892062071 0.8741520130315915
0.1808943213159938 0.9875303397623991 0.9417084524864052
0.2345186265285185 0.7336628828402514 0.7352232169974882
0.3561334134467121 0.2440537170050037 0.0038097593171110
0.0317958444982883 0.5138123602637049 0.0828992808583343
0.3922676586094203 0.0243285016106061 0.8098243700710266
0.0769391822887995 0.2828120073705766 0.8707458000268913
0.2437392615153969 0.5730961998532074 0.9455370203666675
0.4529116332345319 0.8585014327276310 0.0131093035134147
0.5970637687031903 0.1438797434068979 0.7361229004035655
0.6427997469604328 0.1231275095719330 0.0758312566876245
0.7959968994659457 0.4067167292902963 0.7969092452018781
0.9670262344249811 0.7213732095596257 0.8734662218347654
0.6803634900910356 0.9880858180659690 0.9416348735181648
0.6972429797651568 0.7293602185291599 0.7331857333896741
0.8562963314030909 0.2446554747133299 0.0032725904106006
0.5416834248954886 0.5135456855229037 0.0829160472438399
0.8932134674146213 0.0243047145055560 0.8076909728436711
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0.2731836879288542 0.5010531424967956 0.8713667502486061
0.4595237433660152 0.7824101544678230 0.9440943060363790
0.1550682748053166 0.0541106944903857 0.0085408915757624
0.3353819317295345 0.3232236076850041 0.0749031191061708
0.5951182533156421 0.2147577088456533 0.8029526982223065
0.7733106132539123 0.5019968672590018 0.8708585819734597
0.9592035267393730 0.7830437461215923 0.9437530223692313
0.6560814453136349 0.0543540055703379 0.0084964380719900
0.8355831027922088 0.3221321536101231 0.0747252303460743
0.4118391121782090 0.9437105321973590 0.7380675005432925

Etot = -259.35851424 eV

2. B state, no vacancy

5.9784002304000001 0.0000000000000000 0.0000000000000000
1.4945932141000000 6.1742788343999999 0.0000000000000000

0.0000000000000000 0.0000000000000000 27.0132007598999984
H O Ni Fe
13 26 11 1
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0.3179201996957346 0.4432294977014806 0.9686495922301290
0.4949944245121500 0.6416367529894131 0.0593355884238846
0.7306222360393448 0.6003315888977241 0.7567226083210699
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0.8740132478512876 0.0379894519210993 0.6408451562961304
0.1399634187837577 0.1506206603415947 0.7363387643990151
0.1130696119487453 0.1227189745306418 0.0753079403735128
0.3128424261833089 0.4082050525570864 0.7985789652738475
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0.6095347076847375 0.1483803084149216 0.7353578389614341
0.6215903190768515 0.1228776379933691 0.0753307348408896
0.8101519468317662 0.4015732640501000 0.7971469934645157
0.9859526179232390 0.7174962209166793 0.8730208879710091
0.6414491176956361 0.9840967608573052 0.9412696439515074
0.7061746982065813 0.7396188229286338 0.7372667984782169
0.8386133359661514 0.2422349905742749 0.0026043831324074
0.5266272069464151 0.5128842316298545 0.0818427819913055
0.9076024820063537 0.0208323776193282 0.8062338005629215
0.5952959748250279 0.2748512632714579 0.8705836403391558
0.7824959371256526 0.5708511219204127 0.9446047392393240
0.9353574014365620 0.8550865809290400 0.0122522270995589
0.4059097994064729 0.9695791279690482 0.6656056031432271
0.9740490406204785 0.9141272793333997 0.6570145738049860
0.9307371819549886 0.9298561245685235 0.7334058877437997
0.1089987201180946 0.2122662301500569 0.8021947660922848
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0.4650660628901448 0.7791717196320533 0.9434130806699130
0.1342564355909133 0.0518061338224314 0.0081305852709832
0.3198298268966582 0.3222198294455083 0.0742460559519458
0.6100897773087084 0.2108471875551317 0.8020269107968190
0.7904979805182251 0.4956072123936792 0.8705479083416634
0.9649256479383794 0.7799205116792010 0.9431812236826076
0.6344466963477942 0.0519126678350617 0.0080809782707760
0.8200671624579385 0.3217725440023074 0.0739594269249793
0.4249054363125850 0.9470069396152994 0.7347172131244548

Etot = -254.17909104 eV

3. C state, no vacancy

5.9784002304000001 0.0000000000000000 0.0000000000000000
1.4945932141000000 6.1742788343999999 0.0000000000000000
0.0000000000000000 0.0000000000000000 27.0132007598999984
H O Ni Fe
14 27 11 1
0.2654014994762314 0.5974482029245967 0.7669800835136441
0.4237415921603731 0.8267796798284028 0.8452581178593763
0.1108260292050015 0.1770715708553109 0.9052678938204827
0.2664973966383297 0.4424714295542470 0.9667143107244711
0.4762036812010701 0.6726021904960813 0.0600216779666407

0.7509783159598656 0.6324234989916320 0.7564551083731640
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0.2416448671748234 0.7111953674859712 0.7392296402515715
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0.2370842336219676 0.5749415330569858 0.9431357565612851
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0.9250077776217271 0.8751471871735714 0.0190412448639584
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0.0930821439863350 0.2213889369340520 0.8028367225997337
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0.4056448110435689 0.9313023015461366 0.7381566783693446

Etot = -263.96687972 eV

4. D state, no vacancy

5.9784002304000001 0.0000000000000000 0.0000000000000000
1.4945932141000000 6.1742788343999999 0.0000000000000000
0.0000000000000000 0.0000000000000000 27.0132007598999984

H O Ni Fe
13 27 11 1

0.2685186607804761 0.5939132168253566 0.7678797373489350
0.4432204059641270 0.8104240992053651 0.8419565257019629
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0.4860984852800110 0.6647533783420271 0.0581208525641853
0.7521543503074154 0.6361599321638490 0.7611476205275692
0.9288280258832136 0.8205905091124559 0.8407110689647153
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0.9862864758536233 0.6654574698073672 0.0592066040128420

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0.0203596325105564 0.5311167201283584 0.0807034856358779
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0.9545922560172737 0.7802749147272674 0.9427990180173582
0.6388430485018920 0.0606682991324169 0.0090711820170151
0.8169355453054998 0.3420797355471539 0.0731357972458797
0.9602727504518928 0.9202174468195424 0.7261345687370557
0.4224540904954114 0.9216321001448221 0.7345035718596157

Etot = -259.06473908 eV

H vacancy

1. A state, H vacancy
5.9784002304000001 0.0000000000000000 0.0000000000000000
1.4945932141000000 6.1742788343999999 0.0000000000000000
0.0000000000000000 0.0000000000000000 27.0132007598999984
H O Ni Fe
13 26 11 1
0.4369004344633333 0.8301117513742042 0.8479233343525762
0.1244988597949750 0.1499604944042454 0.8962882448173182
0.2782276527715778 0.4396971824378788 0.9683444072932639
0.5122726007812380 0.6372056369414071 0.0608289251763906
0.7442243079148044 0.6123981157295948 0.7554967681375842
0.9372182009572190 0.8399759367919738 0.8494101933994306
0.6229119257840818 0.1478141906173295 0.8959510241102101
0.7745778049139422 0.4401374871525038 0.9686745009388249
0.9964237816332888 0.6365296679883238 0.0606664133686081
0.5659964194347590 0.7563741387556091 0.6699899441526543
0.5681658183236378 0.9771880292381390 0.6471036051558722
0.0837864775980054 0.9038637659263341 0.6460481726966345
0.9451919138637560 0.1368955505751185 0.6560186528274357
0.1154076007200327 0.1571104912516810 0.7357213868200222
0.1292044946016789 0.1159205299360764 0.0750391505397763

0.3001856778425259 0.3998873823289231 0.7987180682182371
0.4683546997986600 0.7091179371730244 0.8725547396290069
0.1819260125649784 0.9812248536134746 0.9409402030355516
0.2189618855544183 0.7716177710914767 0.7340383083803704
0.3554000486524703 0.2387610998724777 0.0033634679803448
0.0301094955031887 0.5076942756861765 0.0828853758581856
0.3935728483182245 0.0128776344132841 0.8045483053538077
0.0815927726343991 0.2721594603004808 0.8710680717618312
0.2475147736425997 0.5663170388873946 0.9443728055254855
0.4519046695446112 0.8533214525346208 0.0126527283217344
0.6111671751430362 0.1444399635438451 0.7355124952873500
0.6439167911705505 0.1158684144047932 0.0750650373481729
0.7982484400229249 0.4022368566788402 0.7983854659659725
0.9686236707675971 0.7127791302308109 0.8732159166402786
0.6777259021385378 0.9808218638171071 0.9408710093643641
0.7114905874901553 0.7362551692730930 0.7314320557723291
0.8551979431549217 0.2390014753272429 0.0025207219590826
0.5429330378215331 0.5076882406081128 0.0829015844867252
0.8947202476946966 0.0178719591952460 0.8072872212903920
0.5806681687852150 0.2701717319978473 0.8708118511998291
0.7442986055377940 0.5671283273786578 0.9447862181169048
0.9516984546918739 0.8517821847499999 0.0115992399681706
0.4595735980939676 0.8928625566135265 0.6584417886754010
0.9261315810045663 0.9894363191047005 0.6514037658497407
0.9154115474237533 0.9455988968743890 0.7351922566011985
0.0951553694940013 0.2106273470053215 0.8027761651295534
0.2746914478108837 0.4914165770463106 0.8705601182352620
0.4599716662017259 0.7762919224034002 0.9432150794741371
0.1542561315836560 0.0486102268816891 0.0078887157285409
0.3348457713083850 0.3172196886803572 0.0746420254887243
0.5986537872215923 0.2089123713015669 0.8026802902769016
0.7748174626088770 0.4919467495303740 0.8711432266433918
0.9599195455204131 0.7768203595147395 0.9429553067801002
0.6547756494093788 0.0485201113529777 0.0078820210213492
0.8350296717828852 0.3158022516566022 0.0742170672137007
0.4072087569978129 0.9489853266268147 0.7364180553010958

Etot = -253.14192378 eV

2. B state, H vacancy

5.9784002304000001 0.0000000000000000 0.0000000000000000
1.4945932141000000 6.1742788343999999 0.0000000000000000
0.0000000000000000 0.0000000000000000 27.0132007598999984

H O Ni Fe
12 26 11 1

0.4573599411060126 0.8332841122207028 0.8480036716233013
0.1129992376611575 0.1517103639636305 0.8964447951771406
0.3177922327358998 0.4417982053995167 0.9682834858044925
0.4971997022934691 0.6408292636542459 0.0597537861411747
0.7340513761532171 0.6095713235253385 0.7566798738122157
0.9586047739061012 0.8380917353964541 0.8484637151128713
0.6135157471984204 0.1503656736916325 0.8959078832600516
0.8160699321245424 0.4426480212824457 0.9683977646583292
0.9845026273161344 0.6401794566133313 0.0596591739729417
0.3985250956246611 0.1262134231058235 0.6605801999744381
0.1320535366730008 0.9376526842322344 0.6552182476138283
0.8670641557615537 0.0315459122820194 0.6412998797160765
0.1373566258578372 0.1623224289200759 0.7363607868079827
0.1117087252855337 0.1206550666480200 0.0750413399626112
0.3161733947655175 0.4006158819913943 0.7989020150564348
0.4883601569149181 0.7117525902572355 0.8725562153298052
0.1438241508785398 0.9828931689820238 0.9410196248397363
0.2312024096739038 0.7685464693470979 0.7386823708313089
0.3384582058516793 0.2412126569476947 0.0030665827892661
0.0179254797177786 0.5118063105821028 0.0821188120840809
0.4115818939750630 0.0143375753687872 0.8042952234398876
0.0951794892304332 0.2730038985642480 0.8711063539446691
0.2846891614450539 0.5685112179463453 0.9443431541434656
0.4347891302298353 0.8557611520218356 0.0126147371397715
0.6289927219158107 0.1455709854210904 0.7350228567005116
0.6236707420536686 0.1205887132106853 0.0749366709485807

0.8128668465118295 0.4030045858825818 0.7980188115994957
0.9888132142910397 0.7135914921678551 0.8728190536662642
0.6413005722371509 0.9829935791208205 0.9408864135143523
0.7060468306232001 0.7438618849140514 0.7354971398398729
0.8383251390052751 0.2415985939570363 0.0024334833122379
0.5282787376091757 0.5118184942405569 0.0820816172506514
0.9109097449114412 0.0176307648213789 0.8056364625452400
0.5966174233498255 0.2719314082986645 0.8706233946150206
0.7830057883362852 0.5696137664917422 0.9445415646411205
0.9349798054590036 0.8544100708349074 0.0117804780019095
0.3984827762627808 0.9732109193964013 0.6651548658179475
0.9707749822499492 0.9152731268847863 0.6592195386443401
0.9272036334863244 0.9452624788255766 0.7343692772369416
0.1123404904436320 0.2115405117633191 0.8026875224859780
0.2924889640415615 0.4921252763411916 0.8705426497074935
0.4648687939865644 0.7783244479122243 0.9430620484020551
0.1339616860146942 0.0511147959348603 0.0078873734629032
0.3196602989158112 0.3211887043350593 0.0742580933810327
0.6134692172123454 0.2094735784709206 0.8021772270510238
0.7920160550360742 0.4936813045439686 0.8707814722756629
0.9649257013356906 0.7787858749530093 0.9429496911907945
0.6344550175248168 0.0511899040721519 0.0078274772962930
0.8200585073272966 0.3201705287438893 0.0739085974072616
0.4172557395636020 0.9448463611170539 0.7342632293312819

Etot = -248.36242293 eV

3. C state, H vacancy

5.9784002304000001 0.0000000000000000 0.0000000000000000
1.4945932141000000 6.1742788343999999 0.0000000000000000
0.0000000000000000 0.0000000000000000 27.0132007598999984

H O Ni Fe
13 27 11 1

0.4259810306297753 0.8240699476898293 0.8447067130551937
0.1096065086894380 0.1745395072005906 0.9047893881184444
0.2660047897317650 0.4447235229098551 0.9667795311316655
0.4756430948750214 0.6728512574287340 0.0599508951897564
0.7458009690232792 0.6299921065217223 0.7568548055473172
0.9222096003050663 0.8272024677900921 0.8414444858201381
0.6356180375340637 0.1735067644369433 0.9052641483298846
0.7955591038879215 0.4428945867114067 0.9656103400109544
0.9755370022145862 0.6736339886285039 0.0610275085188476
0.5908515621809898 0.7482426375775730 0.6605324556079438
0.0575037883512540 0.6512392408330738 0.6588575965138159
0.1659222016332567 0.8390631462630550 0.6435295082711687
0.5496079177826536 0.9641187857346708 0.6317575622774032
0.1467224190738542 0.1264717005674848 0.7265986039525790
0.1075139034360464 0.1519892489668578 0.0772182048390204
0.2975751051816079 0.4209129561301166 0.8067784880213320
0.4538664723602089 0.7087669469125514 0.8709955863596393
0.1318852252086032 0.9949428499174918 0.9445830918202009
0.2460203967064328 0.7190794206809602 0.7399066270393229
0.3275318119729171 0.2589871508268182 0.0029655033950436
0.0098132340763535 0.5394593641593828 0.0825797233678986
0.4106905697093109 0.0211616835755155 0.8054887052351242
0.0855420883962152 0.2895809715256896 0.8772906984923420
0.2369075368468366 0.5765371473204765 0.9430815016151110
0.4250708997116805 0.8771388317920593 0.0172599483256028
0.5375011491078879 0.2129494099771372 0.7265426435202130
0.6038915130021175 0.1521778845025652 0.0769466480463442
0.7888475860849264 0.4333571967110841 0.8038327661741035
0.9528385277054360 0.7135335278457284 0.8682876290177135
0.6608880532304368 0.9932651737276278 0.9444004987066870
0.7105038267046425 0.7502502613135205 0.7317280606590679
0.8292260610082011 0.2618287769267754 0.0042360980260842
0.5080554335843116 0.5401081497385398 0.0819553849916970
0.8867397848440801 0.0327925552420931 0.7989832854606973
0.5950079195801171 0.2917004876728173 0.8784245124965409
0.7593582915273837 0.5745755384705080 0.9420741036839189
0.9242709252008191 0.8761443392726561 0.0187667728862465
0.7212140561910642 0.1676728333725466 0.6989169732290333

0.4695730990178586 0.8580529595268003 0.6443422577125507
0.0159632369005731 0.8059097518957217 0.6512858864874822
0.0927681887840931 0.2235742185357933 0.8031222826759392
0.2700713236416068 0.4969112682493518 0.8738332522128126
0.4451565703571067 0.7918570630284665 0.9444563361471937
0.1244217644249307 0.0687567878192876 0.0109210353992650
0.3062932085989404 0.3499650056642880 0.0743772557981297
0.5969656968245198 0.2288276061713756 0.8051044604046564
0.7734400254831862 0.5020316649003651 0.8723669143077589
0.9459210415195911 0.7894931597441605 0.9446381869674971
0.6286906338846906 0.0694378321302191 0.0107794615359188
0.8063613417765539 0.3502612773316333 0.0750095299413753
0.9496488343209198 0.9235665102132206 0.7276925085171575
0.3998483832468879 0.9201195911090359 0.7404202119116901

Etot = -258.19950435 eV

4. D state, H vacancy

5.9784002304000001 0.0000000000000000 0.0000000000000000
1.4945932141000000 6.1742788343999999 0.0000000000000000
0.0000000000000000 0.0000000000000000 27.0132007598999984

H O Ni Fe
12 27 11 1

0.4404977076305368 0.8075766422702257 0.8411826562660092
0.1183011803938755 0.1611769707528399 0.9018733750848300
0.2761899895013406 0.4334636204233607 0.9644602385949589
0.4847445077988932 0.6644235973411192 0.0577528381437749
0.7497654290882815 0.6411852083736428 0.7625471895716379
0.9310355348014167 0.8190121318051083 0.8404471611916052
0.6421725765664711 0.1602765542209113 0.9032610979027482
0.8038288715045008 0.4311759309617502 0.9636380929238083
0.9846087459962972 0.6649899984500659 0.0588380802701876
0.5561130691079896 0.7660183265639294 0.6600265734162958
0.1875159827865875 0.8581615677605490 0.6517058551622292
0.9310727213202867 0.9598727966289295 0.6328516152752227
0.1611288453060921 0.1334298418135639 0.7300213526167245
0.1167483387037341 0.1431015609923836 0.0748916889123115
0.3058536226696082 0.4095214613357936 0.8050814497436525
0.4622061351444232 0.6986705959533775 0.8687574524782732
0.1412395517536452 0.9858742767413299 0.9421680408457616
0.2577670651513205 0.7217585358242797 0.7461614875266307
0.3373234568872505 0.2495325317675199 0.0006986402071459
0.0188736579223796 0.5305063360257528 0.0802962622325820
0.4338154806436424 0.0041721659677644 0.8002634756636791
0.0930592332270068 0.2781256238864137 0.8744643021273598
0.2461747094540153 0.5659038742774858 0.9408532497778350
0.4341586798595237 0.8678231513895627 0.0151637423350079
0.5582047811487779 0.2676732654604347 0.7247403288717938
0.6133291732501093 0.1434738600794462 0.0747649422822549
0.7919371696381121 0.4312379671451571 0.8037200033624874
0.9619284053866493 0.7046491343229666 0.8668643560704656
0.6705752355669753 0.9824686645050601 0.9424052608609228
0.7203934272766677 0.7515794834961805 0.7349960109861420
0.8384818509539753 0.2523452872499936 0.0019799912495934
0.5173493099087981 0.5313318791334940 0.0796834846720686
0.8972029279437325 0.0301236240846659 0.7974973569694314
0.6011474175090834 0.2787300559910682 0.8764942506527761
0.7680144493700629 0.5633611496012524 0.9400859647761487
0.9341149348055318 0.8667866092534787 0.0165980096693916
0.7334443942456519 0.1946407799551116 0.6978626012551297
0.4314970763900591 0.8946545590491449 0.6654958258276952
0.0197860439919355 0.8455768766738981 0.6538105413270270
0.1059596462092104 0.2140637374343091 0.8014016654942842
0.2783218826310025 0.4871883973719849 0.8718164361378991
0.4539707817709663 0.7824033566197700 0.9423273398097819
0.1339082733977811 0.0596117270856038 0.0086214664099450
0.3155237474035538 0.3412134856757127 0.0721130778511899
0.6066569185654327 0.2221656980914334 0.8032120783904483
0.7801931506987640 0.4923812122298164 0.8709990590290675

0.9551739245858107 0.7793347060296482 0.9425190568768307
0.6382010855819332 0.0597999090504983 0.0086706388617200
0.8155249667760497 0.3414912901365314 0.0727185179078856
0.9575580917935286 0.9229155923340739 0.7274977930209998
0.4110318551290945 0.9118457363939236 0.7354127713917797

Etot = -253.22749506 eV

OH vacancy

1. A state, OH vacancy
5.9784002304000001 0.0000000000000000 0.0000000000000000
1.4945932141000000 6.1742788343999999 0.0000000000000000
0.0000000000000000 0.0000000000000000 27.0132007598999984
H O Ni Fe
13 25 11 1
0.4382151256963788 0.8442269982336105 0.8501704740804119
0.1216481422170831 0.1559689276760654 0.8952836065797858
0.2752350833575700 0.4451391595413099 0.9688546001008317
0.5107389210918180 0.6409708636072485 0.0606630918451988
0.7360374547827642 0.5974172613800394 0.7534729279388632
0.9337900558383603 0.8477288025563254 0.8496080541260497
0.6229409251738994 0.1571268988628435 0.8957487004457333
0.7750047411226523 0.4449383502346352 0.9688842501761338
0.9979390985090104 0.6407916254921062 0.0605787087903252
0.5733602698093231 0.7361890335450302 0.6725411308144562
0.5400925860332724 0.9245779221309163 0.6341544546670637
0.1015493703515527 0.8834234279810933 0.6459374714764996
0.9537764873315243 0.1086253508223903 0.6593840159524051
0.1180027138102286 0.1246418899376735 0.7351821362204376
0.1306691248963557 0.1215000944474802 0.0756226348311675
0.2956869392918833 0.4098708852353988 0.7979852098236286
0.4687968223624357 0.7169806693843122 0.8734957715114887
0.1810561740889342 0.9862242796723795 0.9414622833856613
0.3554511186825748 0.2431508281956398 0.0037164146344089
0.0311400846736576 0.5124563144365923 0.0830471043241564
0.3978061310855787 0.0234285883363208 0.8078501214797523
0.0798401070722374 0.2788083095060718 0.8704501471746238
0.2449469000806145 0.5716337239791383 0.9449507641504611
0.4521155353987827 0.8573813839543649 0.0130143960687048
0.6098643473587789 0.1795100500379300 0.7345422347745830
0.6426792439643140 0.1213701395024614 0.0756797783949544
0.8003837194536786 0.4101535833275756 0.7978237544929684
0.9679528344736698 0.7194204077110591 0.8733193572129928
0.6788272165044816 0.9866786459764773 0.9414015821526307
0.7004171313673324 0.7260861486375558 0.7302392424144220
0.8553206947031746 0.2437106304125658 0.0030799308688469
0.5416192369395857 0.5123003480891158 0.0830608391953582
0.8908497451458509 0.0217883544022159 0.8076072035254084
0.5808807278389855 0.2808256079900376 0.8711178246749938
0.7448176425302422 0.5723655959956938 0.9451642665440014
0.9515396250956970 0.8567225677758584 0.0124100585662069
0.4515822271879927 0.8424213717140077 0.6534627924759244
0.9420977259622708 0.9590641634077014 0.6538259401897086
0.8952359605619606 0.9449713732385883 0.7358203090255929
0.0967836763407714 0.2123524846580934 0.8022805628325623
0.2736024921375379 0.4991669347608231 0.8705313679935365
0.4595009314385394 0.7809758564268491 0.9437873338109722
0.1543792809710148 0.0530312291786345 0.0083800971315008
0.3348313889608391 0.3218995901582302 0.0749047079034369
0.5970795006639776 0.2224471292602284 0.8028194431223831
0.7753629767512527 0.4997578845438807 0.8710690985297207
0.9593129177508821 0.7819289893554320 0.9435178994960866
0.6551329944050174 0.0531324425064585 0.0083500478673494
0.8350103636035042 0.3207634040609155 0.0746248698764662
0.4302390470947626 0.9735484917024787 0.7363492670014791

Etot = -248.53911169 eV

2. B state, OH vacancy

```
   5.9784002304000001   0.0000000000000000   0.0000000000000000
   1.4945932141000000   6.1742788343999999   0.0000000000000000
   0.0000000000000000   0.0000000000000000  27.0132007598999984
 H   O   Ni   Fe
 12  25  11   1
0.4583263790563646  0.8378005536932797  0.8485797728254889
0.1121971211570349  0.1519428199199626  0.8959853379270842
0.3163534636606525  0.4424173987375740  0.9687010452054716
0.4970470800115918  0.6382661529857746  0.0603540453679346
0.7179318394138062  0.6411094614224139  0.7578581086707030
0.9538163072296131  0.8430247281665081  0.8491448250238075
0.6137429428876252  0.1529995837377673  0.8959516821601693
0.8151246540147450  0.4423596691871167  0.9687998066612963
0.9855220909299329  0.6376564969585742  0.0602893124614894
0.3817464648492666  0.1418522519299875  0.6528546377485293
0.1545807346559591  0.9279312436453372  0.6548529134566838
0.8934936757465816  0.9118063261814784  0.6379303049466909
0.1357255091226305  0.1405941618425293  0.7364629174865456
0.1119872984163648  0.1186986121835750  0.0756829779232515
0.3077988317321858  0.4093444561474682  0.7992071371234749
0.4862606931653600  0.7155371739729632  0.8728267430076790
0.1429198613675935  0.9833737102805151  0.9415513931597347
0.3378196236714113  0.2402862003083319  0.0036402170599725
0.0186310725927610  0.5095086110781054  0.0827829124861490
0.4137128071670391  0.0205262882888825  0.8035562571824728
0.0935566223308474  0.2743377504614544  0.8710248129297843
0.2831746361985166  0.5692468902912597  0.9448717886052961
0.4343184781716679  0.8546433404956550  0.0131149692779318
0.6120139463253961  0.1850059181844775  0.7353120722419135
0.6230684312016918  0.1186582765918975  0.0755704205365880
0.8106901046728412  0.4104332977907257  0.7983975161072530
0.9859326267312309  0.7174433460289026  0.8732722713304377
0.6403875556132337  0.9834220752769319  0.9414622432234475
0.6932922935115213  0.7580185214172166  0.7321658750336474
0.8378484358456998  0.2406486308113390  0.0030523496130457
0.5281757651091993  0.5096579905238974  0.0827647188644673
0.9056423638713408  0.0215409506255114  0.8051891171240553
0.5938427180448076  0.2765014497664144  0.8712885881416359
0.7819664330156373  0.5698548463584630  0.9450844644053675
0.9345655774236411  0.8535943294798839  0.0124090009093000
0.4031662736755107  0.9901636058059957  0.6625773867502016
0.0123023112121909  0.8720346236129050  0.6630722900618480
0.9109988521657212  0.9548427259427874  0.7328935490633013
0.1098002649791621  0.2136897271274516  0.8027868965637444
0.2889147711814612  0.4959686302059403  0.8709389648037023
0.4638020182756505  0.7787627309082514  0.9435696837224461
0.1335350588775257  0.0500902595643320  0.0084434594829041
0.3199082955130526  0.3189711198391244  0.0748653618535675
0.6084824232356582  0.2211010431127884  0.8027897487867542
0.7904282021726881  0.4965421447509938  0.8712806280410041
0.9636996969140145  0.7795874888162938  0.9434904315695549
0.6339163629202591  0.0501776769786937  0.0083718576983950
0.8202042902902537  0.3179676691256986  0.0745351826025449
0.4329863398052363  0.9904333569164596  0.7321638522588665
```

Etot = -243.59301458 eV

3. C state, OH vacancy

```
   5.9784002304000001   0.0000000000000000   0.0000000000000000
   1.4945932141000000   6.1742788343999999   0.0000000000000000
   0.0000000000000000   0.0000000000000000  27.0132007598999984
 H   O   Ni   Fe
 13  26  11   1
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0.4186954841522240 0.8277236072757893 0.8428548922328148
0.1096143709528387 0.1822419297190520 0.9047208335677938
0.2656285401196126 0.4469880303892886 0.9652635794708853
0.4737757594549613 0.6764769865776420 0.0592827656462947
0.7271874637672314 0.6380365345740679 0.7611512487419759
0.9147423631027395 0.8344295350844217 0.8414412943249562
0.6305212194141868 0.1802983695453745 0.9049324196061090
0.7918361238943105 0.4464397703387009 0.9649770019703685
0.9737989091346168 0.6769981309984411 0.0603657028411103
0.6085360386316766 0.7363078630016993 0.6662899418013987
0.0980041476647033 0.5790634172906721 0.6734621191725405
0.2036170384812369 0.7698031972370988 0.6540595583449144
0.5482485989392127 0.9517719446802615 0.6362238341937115
0.1327752965640205 0.1118512014708690 0.7225057773538885
0.1056908769497502 0.1555540453907682 0.0765203610353706
0.2921139466074520 0.4317864976140189 0.8049487752111184
0.4496939021268843 0.7139743212388302 0.8693293709848111
0.1306408203219965 0.9988865391549334 0.9439334437876375
0.3263344238649229 0.2625192073518537 0.0022164773294350
0.0078530159900387 0.5429063601608434 0.0819098882039051
0.3953669142988976 0.0323106308394512 0.8019328470134340
0.0850540687827207 0.2962161109506835 0.8770229924261154
0.2356275927926781 0.5793928696487080 0.9417130465111844
0.4234194823521980 0.8805086813526983 0.0167061330673596
0.5402005839980762 0.2449631318174607 0.7187964617021652
0.6024221183286834 0.1557371223374641 0.0763691984590734
0.7910143806827129 0.4375051196398863 0.8038079322252185
0.9487886802785556 0.7196995160223068 0.8679335906417426
0.6588610175803528 0.9971383323939179 0.9438629596948214
0.6999195020981233 0.7491155538141470 0.7338051016101674
0.8275805578367520 0.2654449421565445 0.0035291226018839
0.5062276897380756 0.5435535759025106 0.0812700733085603
0.8825469091137980 0.0377527675746889 0.7980777726344406
0.5908059935737587 0.2978900731978340 0.8781175949593382
0.7559064721269889 0.5788063643054311 0.9415669275415746
0.9231922613877820 0.8794080040046860 0.0180793043112808
0.7212039614256769 0.1499006420407070 0.6874708672860568
0.4792270749169482 0.8389914969936157 0.6499304493748255
0.0622763551109514 0.7346276836273840 0.6671271714476829
0.0898242682966570 0.2304022151425628 0.8024612952086529
0.2670565102928936 0.5026555380082901 0.8725945343416291
0.4429558145607930 0.7961311763589903 0.9436495194113874
0.1230696832653626 0.0722604021463549 0.0102428127162954
0.3044472696084219 0.3534308444777327 0.0736916484264706
0.5922124821786654 0.2371972852901310 0.8040293092352371
0.7710755969580059 0.5065359348408320 0.8721616281964850
0.9439403221027138 0.7935498757643843 0.9439746972519119
0.6271479070804817 0.0726774027325843 0.0101950093348581
0.8044852600399615 0.3537732712238035 0.0743043972784642
0.9268491157480783 0.9290689378090643 0.7289809473647447
0.4266787322212530 0.9871531895104888 0.7321906062825136

Etot = -253.21460815 eV

4. D state, OH vacancy

5.9784002304000001 0.0000000000000000 0.0000000000000000
1.4945932141000000 6.1742788343999999 0.0000000000000000
0.0000000000000000 0.0000000000000000 27.0132007598999984

H O Ni Fe
12 26 11 1

0.4438163338923856 0.8102646403683370 0.8415459055367385
0.1178782826498359 0.1610651083085121 0.9012563812396147
0.2754255654597221 0.4351320634208226 0.9645008712665052
0.4849470443676214 0.6644749508675176 0.0578491809813043
0.7474851812329018 0.6418165377303063 0.7631858554802471
0.9280003043505494 0.8208410713893339 0.8407264858834040
0.6408619448519289 0.1635590928137947 0.9036848041087131
0.8039921281479300 0.4318058630198255 0.9638555244908362
0.9851077786016846 0.6650948760439790 0.0589131556974776

0.5576118857994179 0.7548532455694830 0.6609465461164724
0.1887858868458350 0.8481458225712187 0.6527658920419603
0.9321354886292459 0.9461539072147798 0.6333825543655206
0.1577922082738476 0.1185939197376733 0.7318414906749099
0.1169436164498138 0.1433202256635290 0.0750434007157049
0.3064454134217416 0.4131776393876100 0.8041431328817199
0.4622286718144395 0.7014032070618892 0.8690527886062966
0.1409043144912767 0.9869573401704295 0.9422153296674426
0.3373972489433261 0.2500492741409337 0.0008728408548776
0.0192811634579997 0.5307407437207541 0.0804187492406471
0.4378726863776781 0.0025766794482111 0.8001467507384308
0.0926338191072532 0.2784344850014300 0.8739848541501604
0.2456876643348432 0.5670651757922244 0.9408575717448058
0.4339387035860195 0.8682841963777764 0.0152879655482897
0.5502405636371305 0.2436521910072922 0.7250551312823492
0.6136393443590977 0.1436733385528831 0.0749519050092103
0.7890602665047235 0.4339095849252225 0.8036208917493430
0.9612322204652803 0.7053123797962615 0.8668777365214905
0.6702039760799614 0.9833529090329111 0.9425348045792475
0.7248796970660535 0.7476843248913003 0.7345743875789028
0.8384769039805340 0.2527903580146158 0.0021488802886306
0.5176279990182169 0.5315023085088398 0.0798143055405108
0.8977134072553504 0.0295087170429052 0.7980088453710910
0.6002725640078884 0.2821608004262857 0.8769724170904099
0.7680813256106213 0.5640173921234064 0.9402984156957532
0.9343075362257763 0.8672502059677382 0.0167075232798094
0.7385008237924232 0.2102010000155100 0.6970734238001377
0.4290809881499161 0.8805377383769034 0.6658558554155086
0.0212446424245633 0.8354560813006725 0.6551939358258932
0.1053789253436259 0.2146140096717170 0.8016666428046656
0.2781077869341497 0.4889125618680382 0.8714509840094004
0.4537190079176251 0.7832944356691895 0.9425440380660471
0.1339034565858989 0.0602312301707921 0.0087353959428153
0.3158483490185133 0.3413614690836718 0.0722808012634719
0.6068408535932943 0.2248672238438153 0.8035892728069649
0.7794412600028268 0.4940709100955285 0.8711654372474874
0.9550115638127030 0.7801443300328661 0.9427034216901558
0.6381888600834795 0.0602404706062395 0.0088270302466316
0.8158530723475582 0.3416980112939025 0.0728858257705144
0.9381446969704342 0.9384431903457812 0.7263988221849904
0.4437257148975030 0.9564911819237358 0.7327284544604475

Etot = -248.59326485 eV

1. Li, Y.-F.; Selloni, A., Mechanism and Activity of Water Oxidation on Selected Surfaces of Pure and Fe-Doped NiOx. *ACS Catalysis* **2014**, *4*, 1148-1153.
2. Fidelsky, V.; Caspary Toroker, M., Enhanced Water Oxidation Catalysis of Nickel Oxyhydroxide through the Addition of Vacancies. *The Journal of Physical Chemistry C* **2016**.