# Supporting Information

# Multisites dynamic synergistic oxygen evolution reaction mechanism of Fe-doped NiOOH: A first-principles study

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## 1. Simulation details

The Gibbs free energy is calculated using with calculation hydrogen electrode (CHE) method,[1] as follows:

$$\Delta G = \Delta E_{DFT} + \Delta ZPE - T\Delta S - |e|U + G_{PH} \quad \text{(S1)}$$

$\Delta G$ is the free energy change of each step. $\Delta E_{DFT}$ obtained by DFT calculations is the difference of energy between reactants and products. $\Delta ZPE$ is the zero-point energy correction. Zero point energy can be calculated using vibrational frequencies by applying normal-mode analysis through density functional theory (DFT) calculations. T is the temperature (298 K), and $\Delta S$ is the change in entropy. U is the electrode applied potential relative to reversible hydrogen electrode (RHE). $G_{pH} = -k_B T \ln [H^+] = pH \times k_B T \times \ln 10$ ($k_B$, Boltzmann constant), denoting the correction of pH. In this work, we assumed pH equal to 0, so Gibbs free energy calculation formula is as follow:

$$\Delta G = \Delta E_{DFT} + \Delta ZPE - T\Delta S - |e|U \quad \text{(S2)}$$

According to the standard hydrogen electrode model (SHE) of electrode reaction in fuel cells proposed by Norskov et al[2]. define the electrode potential U=0 V, the free energy of $^{1/2}H_2$ is equal to $H^+(aq) + e^-$.

$$1/2\,H_2(g) \rightleftharpoons H^+(aq) + e^- \tag{S3}$$

Therefore, the OER thermodynamics of the γ-NiOOH surface was evaluated using the CHE method, and the electrochemical potentials of $H^+$ and $e^-$ were estimated by electrochemical equilibrium of the SHE.

$$\mu[H^+] + \mu^{SHE}[e^-] = 1/2\,G^0[H_2] \tag{S4}$$

$\mu[H^+]$ is the electrochemical potential of a proton; $\mu^{SHE}[e^-]$ is the

Electrochemical potential of an electron in SHE; $\mu^{SHE}[e^-]$ is the standard Gibbs free energy for hydrogen.

In the reversible potential of corresponding reaction ($U_{OER}$ = 1.23 V vs RHE), the thermodynamic overpotential (η) is the most unfavorably occurring free energy change, which can represent the catalytic activity exhibited during OER catalysis.[3]

$$\eta = \max[(\Delta G_1 - 1.23\ eV),(\Delta G_2 - 1.23\ eV),\ldots]/e \tag{S5}$$

$\Delta G_n$ (n =1, 2, 3, 4) is the free energy change in the step n; e is the elementary charge. In CHE model, only the thermodynamics of the reaction is calculated, but the kinetic process is ignored. It's not that kinetics is unimportant, but we're only going to look at thermodynamics because thermodynamics dictates the minimum energy required for a reaction in terms of energy.

For Fe atom doping NiOOH to form NiFeOOH, the formation energy $E_f$ can be deduced by the following expression:

$$E_f = E(Ni_{n-1}FeOOH) - E(Ni_nOOH) + \mu_{Ni} - \mu_{Fe} \tag{S6}$$

Where $E(Ni_{n-1}FeOOH)$ and $E(Ni_nOOH)$ separately represent the total energy of the doped and undoped Fe quantum dots. The subscripts “n” mean the numbers of Ni atoms. $\mu_{Ni}$ and $\mu_{Fe}$ are the chemical potentials of Ni and Fe atoms.

## 2. Additional table

**Table S1.** Values used for the entropy and zero-point energy corrections in determining the free energy of reactants, products, and intermediate species adsorbed on catalysts. For the adsorbates, the ZPE values are averaged over all NiOOH (NiFeOOH) catalyst systems since they have rather close value.

| Species | T×S (eV) (298K) | ZPE (eV) |
|---|---|---|
| ***$H_2O$** | 0 | 0.64 |
| ***OH** | 0 | 0.33 |
| ***O** | 0 | 0.05 |
| ***OOH** | 0 | 0.39 |
| ***OO** | 0 | 0.06 |
| **$H_2$(g)** | 0.41 | 0.22 |
| **$H_2O$(g)** | 0.58 | 0.54 |

**Table S2.** Free Energy Changes of Each Elementary Step of the NiOOH Surface by PBE + U

| Step | Chemical equation | $\Delta G_{PBE+U}$ (eV) | $\Delta G_{sol}$ (eV) |
|---|---|---|---|
| **A-1→ A-2** | $^{\delta*}H_2O \rightarrow {}^{\delta*}O^{top}H + (H^+ + e^-)$ | **2.47** | **2.50** |
| **A-2 → A-3** | $^{\gamma*}O^{top}H \rightarrow {}^{\gamma*}O^{top} + (H^+ + e^-)$ | 2.13 | 2.11 |
| **A-3 → A-4** | $^{\gamma*}O^{top} + H_2O \rightarrow {}^{\gamma*}O^{top}OH + (H^+ + e^-)$ | 1.56 | |
| **A-4 → A-5** | $^{\gamma*}O^{top}OH \rightarrow {}^{\gamma*}O^{top}O + (H^+ + e^-)$ | -0.58 | |
| **A-5 → A-6** | $^{\gamma*}O^{top}O \rightarrow {}^{\gamma*} + O_2(g)$ | **0.83** | |
| **A-6 → A-1** | $^{\gamma*} + H_2O + {}^{\delta*}O^{top}H \rightarrow {}^{\gamma*}O^{top}H + {}^{\delta*}H_2O$ | -1.49 | |
| **A-1 → B-2** | $^{\gamma*}O^{br}H + H_2O + {}^{\gamma*}O^{3c} \rightarrow {}^{\gamma*}OOH + {}^{\gamma*}O^{3c}H + (H^+ + e^-)$ | 1.30 | |
| **B-2 → B-3** | $^{\gamma*}O^{br}OH \rightarrow {}^{\gamma*}O^{br}O + (H^+ + e^-)$ | **2.57** | |
| **B-3 → B-4** | $^{\gamma*}O^{3c}H \rightarrow {}^{\gamma*}O^{3c} + (H^+ + e^-)$ | 0.52 | |
| **B-4 → B-5** | $^{\gamma*}O^{br}O + {}^{\gamma*}O^{top}H \rightarrow {}^{\gamma*}O^{br}H + O_2(g) + {}^{\gamma*}$ | -0.60 | |
| **B-5 → A-1** | $^{\gamma*} + H_2O \rightarrow {}^{\gamma*}OH + (H^+ + e^-)$ | 1.13 | |
| **A-3 → C-4** | $^{\gamma*}O^{top} + {}^{\gamma*}O^{br}H + {}^{\gamma*}O^{3c} \rightarrow {}^{\gamma*}O^{br}O + {}^{\gamma*}O^{3c}H$ | -0.90 | -0.88 |
| **C-4 → C-5** | $^{\gamma*} + H_2O \rightarrow {}^{\gamma*}O^{top}H + (H^+ + e^-)$ | 1.24 | 1.27 |
| **C-5 → C-6** | $^{\gamma*}O^{3c}H + {}^{\delta*}O^{top}H + {}^{\delta*}O^{br}O \rightarrow {}^{\gamma*}O^{3c} + {}^{\delta*}O^{br}H + {}^{\delta*}O^{top}O + (H^+ + e^-)$ | 0.36 | 0.40 |
| **C-6 → C-7** | $^{\delta*}O^{top}O \rightarrow {}^{\delta*} + O_2(g)$ | 0.28 | 0.13 |
| **C-7 → A-1** | $^{\delta*} + H_2O \rightarrow {}^{\delta*}H_2O$ | -0.66 | -0.60 |

**Table S3.** .Free Energy Changes of Each Elementary Step of the Fe-doped NiOOH Surface by PBE + U

| Step | Chemical equation | $\Delta G_{PBE+U}$ (eV) | $\Delta G_{sol}$ (eV) |
|---|---|---|---|
| **A-1→ A-2** | $*H_2O \rightarrow *O^{top}H + (H^+ + e^-)$ | **1.56** | **1.58** |
| **A-2 → A-3** | $*O^{top}H \rightarrow *O^{top} + (H^+ + e^-)$ | 1.28 | 1.35 |
| **A-3 → A-4** | $*O^{top} + H_2O \rightarrow *O^{top}OH + (H^+ + e^-)$ | 1.08 | |
| **A-4 → A-5** | $*O^{top}OH \rightarrow *O^{top}O + (H^+ + e^-)$ | 0.52 | |
| **A-5 → A-6** | $*O^{top}O \rightarrow * + O_2(g)$ | **0.81** | |
| **A-6 → A-1** | $* + H_2O \rightarrow *H_2O$ | -0.32 | |
| **A-2 → B-3** | $*O^{br}H + H_2O + *O^{3c} \rightarrow *OOH + *O^{3c}H + (H^+ + e^-)$ | 1.51 | |
| **B-3 → B-4** | $*O^{br}OH \rightarrow *O^{br}O + (H^+ + e^-)$ | **1.66** | |
| **B-4 → B-5** | $*O^{3c}H \rightarrow *O^{3c} + (H^+ + e^-)$ | 1.64 | |
| **B-5 → A-6** | $*O^{br}O + *O^{top}H \rightarrow *O^{br}H + O_2(g) + *$ | -1.12 | |
| **A-6 → A-2** | $* + H_2O \rightarrow *OH + (H^+ + e^-)$ | 1.24 | |
| **A-3 → C-4** | $*O^{top} + \gamma*O^{br}H + \gamma*O^{3c} \rightarrow \gamma*O^{br}O + \gamma*O^{3c}H$ | -0.23 | -0.29 |
| **C-4 → C-5** | $\gamma*H_2O \rightarrow \gamma*O^{top}H + (H^+ + e^-)$ | 1.38 | 1.26 |
| **C-5 → C-6** | $\gamma*O^{3c}H + *O^{br}O \rightarrow \gamma*O^{3c} + *O^{top}O + (H^+ + e^-)$ | 1.53 | 1.54 |
| **C-6 → C-7** | $*O^{top}O + \gamma*O^{top}H \rightarrow * + O_2(g) + \gamma*O^{br}H$ | 0.15 | 0.04 |
| **C-7 → C-8** | $* + H_2O \rightarrow *H_2O$ | -0.52 | -0.40 |
| **C-8 → A-1** | $\gamma* + H_2O \rightarrow \gamma*H_2O$ | -0.23 | -0.16 |

**Table S4** . Magnetic moments ($\mu_B$) of the atoms at NiOOH surface

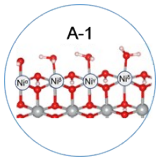
| | | $Ni^{\alpha}$ | $Ni^{\beta}$ | $Ni^{\gamma}$ | $O^{br}$ | $Ni^{\delta}$ |
|---|---|---|---|---|---|---|
| **A-1** |   | -0.01 | 1.05 | 0.99 | -0.02 | 1.91 |

**Table S5**. Magnetic moment ($\mu_B$) of the atoms at NiFeOOH surface.

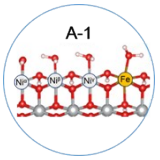
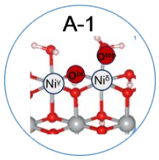
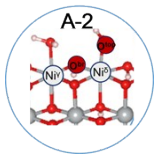
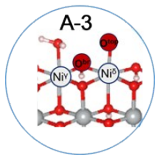
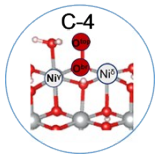
| | | $Ni^{\alpha}$ | $Ni^{\beta}$ | $Ni^{\gamma}$ | $O^{br}$ | Fe |
|---|---|---|---|---|---|---|
| **A-1** |   | 0.10 | 0.98 | 1.64 | 0.156 | 4.22 |

**Table S6.** Atom-projected magnetic moment M ($\mu_B$) - net atomic spin projections - as a function of oxidation state for Ni and Fe[4, 5].

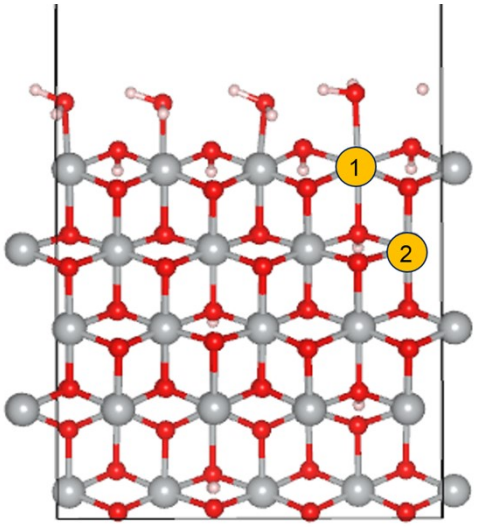
| **Oxidation** | **M(Ni)** | **M(Fe)** |
|---|---|---|
| **State** | **PBE+U** | |
| **2** | 1.70-1.80 | -- |
| **3** | 1.00-1.30 | 4.10-4.20 |

| | | |
|---|---|---|
| **4** | 0.10 | 3.50-3.70 |

**Table S7.** Magnetic moment ($\mu_B$) of the atoms at in NiOOH surface.

| | | $Ni^{\gamma}$ | $O^{br}$ | $Ni^{\delta}$ | $O^{top}$ |
|---|---|---|---|---|---|
| **A-1** |  | 0.99 | -0.02 | 1.91 | 0.03 |
| **A-2** |  | 0.94 | 0.04 | 1.67 | 0.35 |
| **A-3** |  | 0.99 | 0.06 | 0.98 | 0.75 |
| **C-4** |  | 1.71 | 0.27 | 0.99 | 0.39 |

## 3. Additional Figure.




| site | $E_f$ (eV) |
|---|---|
| **1** | -1.86 |
| **2** | -1.61 |

**Fig. S1**. Dopant site search of Fe dopant on γ-NiOOH surface. Here we considered two different possible dopant sites on NiOOH (see above) and found that Fe prefers to substitute the $Ni^{\delta}$ (site 1). Red, gray, white, and brown balls represent O, Ni, H, and Fe, respectively.

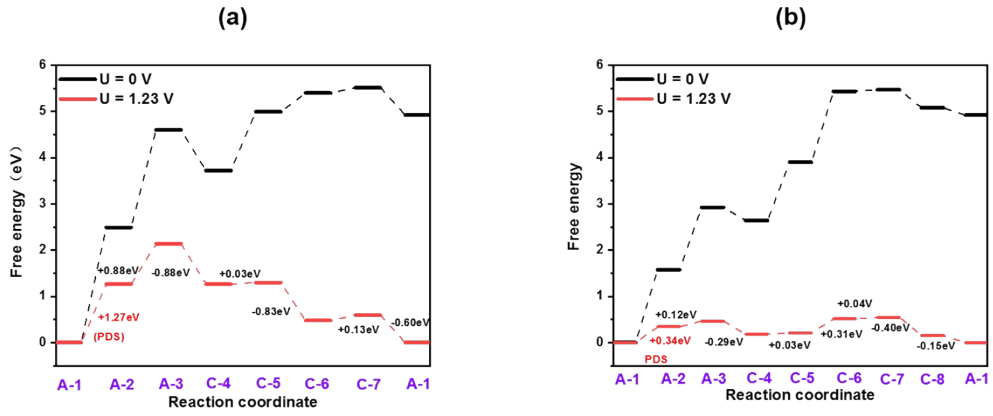



**Fig. S2.** Free energy diagram corrected for implicit solvation of NiOOH and NiFeOOH models toward OER. Pathway C (the designed MDSM mechanism) for NiOOH (a) and NiFeOOH (b).

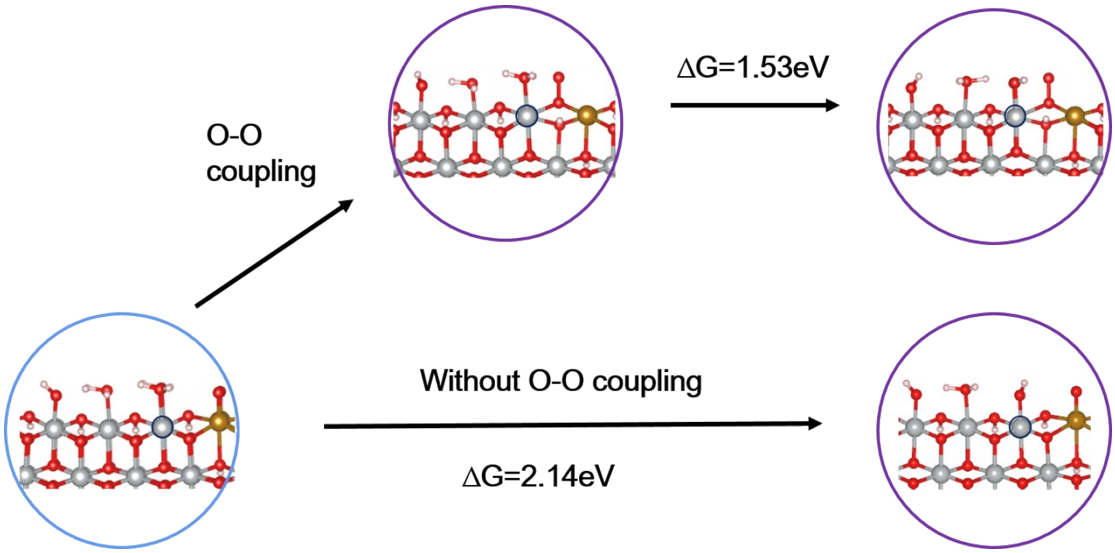



**Fig. S3.** Schematic diagram of the Ni$^{\gamma}$ site deprotonation process. The dark cycles represents the Ni$^{\gamma}$ that will participate in the reaction.

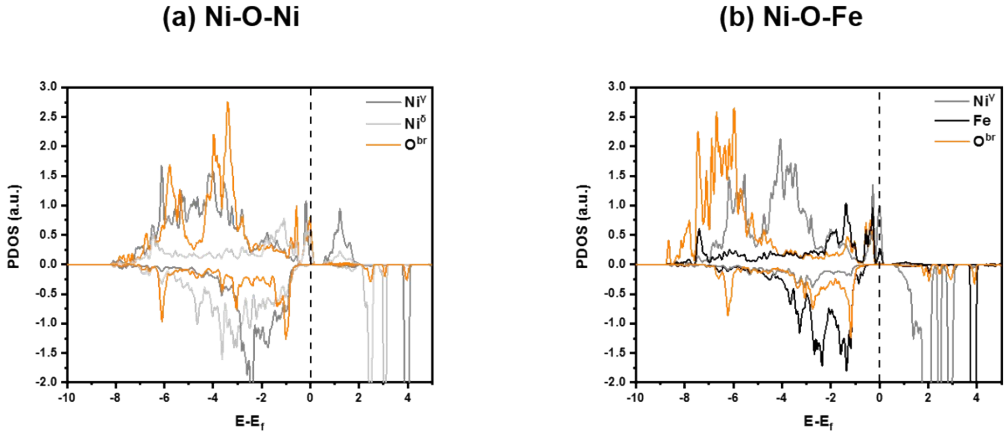



**Fig. S4.** PDOS of O$^{br}$ 2*p* and M 3*d* orbit in state A-1 for NiOOH (a) and NiFeOOH (b) models. The black dash line represents the Fermi level.

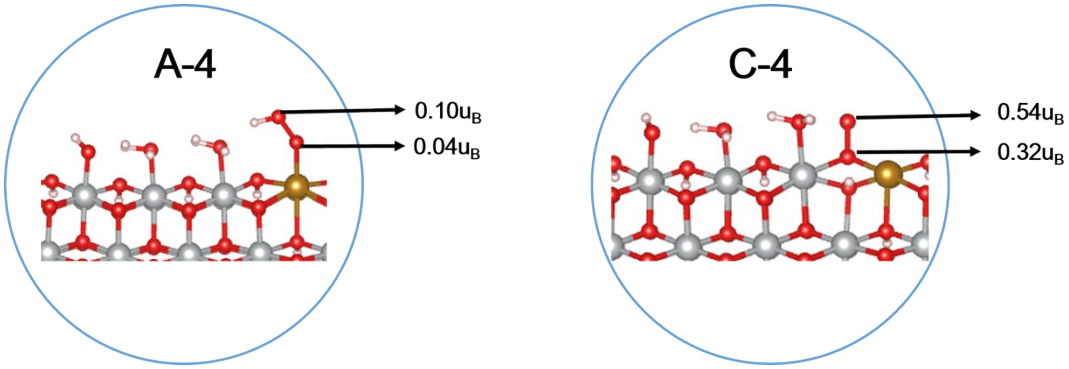



**Fig. S5.** Schematic diagram of magnetic moments ($\mu_B$) of O species.

## 4. Crystal Structure

Crystal Structure for γ-NiOOH in VASP CONTCAR format

1.00000000000000

11.3502998351999995 0.0000000000000000 0.0000000000000000

-0.0012747159000000 4.8056996561999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 33.0000000000000000

O Ni H

44 20 14

Selective dynamics

Direct

0.0312099997123312 0.5769400000732432 0.0798977239393963

0.0315193642644002 0.8148021333357888 0.2248994326212858

0.0327400006724474 0.0343599989206496 0.1165562141515153

0.0327989929010002 0.2779592961904987 0.2532017272491413

0.1574299931606333 0.4631600081641380 0.0061950255454519

0.1594948606359639 0.6941435549509104 0.1530435418384177

0.1588972346423923 0.9350703138634550 0.2941007029674948

0.1557199954770709 0.9205800294432507 0.0428535186969725

0.1559856850166200 0.1506477193966613 0.1860651566168386

0.1601734558524451 0.4123592382806093 0.3266393233588694

0.2825599909115653 0.5842300057969254 0.0790475814848506

| | | |
|---|---|---|
| 0.2831333308283153 | 0.8223977634061110 | 0.2243960703140418 |
| 0.2807500064147561 | 0.0324099996134919 | 0.1168396047575726 |
| 0.2801240729658755 | 0.2812664358344413 | 0.2570238349279997 |
| 0.4068599939470232 | 0.4575499892431267 | 0.0092256289393902 |
| 0.4067989145803687 | 0.6837142096258001 | 0.1578631323955473 |
| 0.4044570312820680 | 0.9379230070709268 | 0.2936715937624234 |
| 0.4061200023071905 | 0.9425200224812968 | 0.0393033830303011 |
| 0.4056657573900835 | 0.1736611059731006 | 0.1856137536572044 |
| 0.4020138888650315 | 0.4108003246657432 | 0.3262934631807381 |
| 0.5311400294087960 | 0.5850999950386822 | 0.0792365066060583 |
| 0.5312029775723642 | 0.8268804540493923 | 0.2249977196039320 |
| 0.5310599803768028 | 0.0369499997301972 | 0.1166191911515142 |
| 0.5299992082118651 | 0.2873581467027109 | 0.2569207048049417 |
| 0.6571499705423420 | 0.4704400003614992 | 0.0055259313333380 |
| 0.6531525334675955 | 0.7000700454177016 | 0.1524216076019071 |
| 0.6474012110268513 | 0.9433517129251980 | 0.2950585040563996 |
| 0.6576099991900293 | 0.9223399758829061 | 0.0429479783333306 |
| 0.6561229807458345 | 0.1531825095873348 | 0.1872635051830646 |
| 0.6416398826604803 | 0.4237227321566248 | 0.3277717238341493 |
| 0.7815999984875077 | 0.5709099769604506 | 0.0829440730303048 |
| 0.7793267341111277 | 0.8049805573720982 | 0.2297385418810063 |
| 0.7825499772789613 | 0.0557999983736082 | 0.1130139608484839 |
| 0.7824753684598953 | 0.2896574101257122 | 0.2552111424527383 |
| 0.9060299992771945 | 0.4691300094235800 | 0.0053684973030315 |
| 0.9085600012764582 | 0.6946801172968273 | 0.1518429712879420 |
| 0.9135101588453900 | 0.9445207315666351 | 0.2959321714772802 |
| 0.9077100158101103 | 0.9173399805192730 | 0.0431762596666658 |
| 0.9077894325127056 | 0.1431940026457470 | 0.1873066073362598 |
| 0.9175310872726234 | 0.4275542957456041 | 0.3311477984972698 |
| 0.5322699869117811 | 0.0150244105428589 | 0.3614432539681520 |

| | | |
|---|---|---|
| 0.7618854344086066 | 0.0071010114654223 | 0.3731758657501587 |
| 0.0446692523467712 | -0.0324067325481503 | 0.3697881541625547 |
| 0.2810804133848200 | 0.0250957452253714 | 0.3629363443270902 |
| 0.0316199995985542 | 0.6909400223786690 | 0.0243314160909094 |
| 0.0314178145467075 | 0.9192791759409861 | 0.1698865803037748 |
| 0.0330127094556065 | 0.1757388072016315 | 0.3130261031370978 |
| 0.1568900048907977 | 0.8054199814602256 | 0.0980262467575770 |
| 0.1558239444067485 | 0.0468725141699348 | 0.2402130025850815 |
| 0.2794399857903542 | 0.6945599914247111 | 0.0241110083636329 |
| 0.2795176006118543 | 0.9230803004730539 | 0.1699189166341802 |
| 0.2801132626480303 | 0.1702632277962464 | 0.3108666477941464 |
| 0.4060899913397975 | 0.8087000251848977 | 0.0987661823939376 |
| 0.4055497907214431 | 0.0580575576539213 | 0.2408845008590382 |
| 0.5339099764618069 | 0.6965299844907094 | 0.0239535746969679 |
| 0.5336408690212252 | 0.9260771651267016 | 0.1699091832196328 |
| 0.5283457223221710 | 0.1755773435089322 | 0.3114475765133983 |
| 0.6546300053858616 | 0.8103799820231501 | 0.0976562730606076 |
| 0.6544226062402662 | 0.0501711385082768 | 0.2413318710321284 |
| 0.7823799848566608 | 0.6935899853208127 | 0.0250792282727303 |
| 0.7821259891514465 | 0.9194751131419719 | 0.1708198504148063 |
| 0.7806461892650333 | 0.1845427645902067 | 0.3166742033253647 |
| 0.9091299772306840 | 0.8079500199290877 | 0.0978294510000026 |
| 0.9093429858285292 | 0.0445011692563794 | 0.2413938239621788 |
| 0.4059300125083709 | 0.1414300053319266 | 0.0276611440606089 |
| 0.4058587982558996 | 0.3847414542382799 | 0.1759195938687162 |
| 0.4024978066180129 | 0.5842382442021196 | 0.3094192958012408 |
| 0.7827299832966261 | 0.2546100019840836 | 0.1013402275454567 |
| 0.7813524672060207 | 0.4890737234587644 | 0.2430912177444119 |
| 0.1617737397105055 | 0.5848110177442020 | 0.3093099141560228 |
| 0.6354909287838095 | 0.6009768129063335 | 0.3118347838944937 |

0.9167482186668343 0.5970861755767700 0.3135275192316235

0.6735362445396997 0.9960374634027845 0.3756383593635137

0.4493793743080042 0.9690708261316910 0.3678326371198560

0.0116152972538337 0.7799133213347296 0.3668935448031629

0.1325930173170090 0.9473573277226119 0.3713704324042694

0.2880729397487578 0.1943317208859571 0.3793487537071741

0.7890566764820452 0.1408595548318881 0.3932788654312171

Crystal Structure for Fe-doped γ-NiOOH in VASP CONTCAR format

1.00000000000000

11.3502998351999995 0.0000000000000000 0.0000000000000000

-0.0012747159000000 4.8056996561999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 33.0000000000000000

O Ni Fe H

44 19 1 15

Selective dynamics

Direct

0.0312099997123312 0.5769400000732432 0.0798977239393963

0.0301592342866882 0.8195277384269285 0.2247423273314460

0.0327400006724474 0.0343599989206496 0.1165562141515153

0.0339325821456196 0.2866852796542732 0.2568664538536053

0.1574299931606333 0.4631600081641380 0.0061950255454519

0.1585678493151724 0.6945518944980116 0.1530679758173347

0.1558174153498718 0.9396857749009919 0.2937498623849518

0.1557199954770709 0.9205800294432507 0.0428535186969725

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| 0.2788254944727429 | 0.7578642151575102 | 0.3620471537088883 |
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| 0.5478332190679117 | 0.7997466821268684 | 0.3679549476240819 |

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