

*Supplementary information for:*

**Dual-site OER Mechanism Exploration Through Regulating the  
Asymmetric Multi-site NiOOH**

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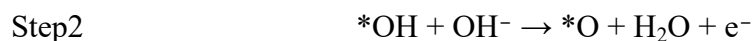
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## Supplementary Methods

Traditional single-site mechanism in OER process in alkaline environment can be described in the following step1~4.<sup>1</sup>



where \* presents an active site on NiOOH surface, and \*OH, \*O, \*OOH indicates intermediates along the OER path.

Reaction free energies ( $\Delta G$ ) for these four elementary steps can be calculated based on the following formula, where  $\Delta G_i$  ( $i = 1 \sim 4$ ) were calculated at  $U = 1.23$  V (vs. RHE) and  $G_{\text{H}} = 1/2 G_{\text{H}_2}$  in this work:

$$\Delta G_1 = \Delta G_{\text{HO}^*} - \Delta G_{*} + G_{\text{H}} - G_{\text{H}_2\text{O}} - eU$$

$$\Delta G_2 = \Delta G_{\text{O}^*} - \Delta G_{\text{HO}^*} + G_{\text{H}} - eU$$

$$\Delta G_3 = \Delta G_{\text{OOH}^*} - \Delta G_{\text{O}^*} - G_{\text{H}_2\text{O}} + G_{\text{H}} - eU$$

$$\Delta G_4 = \Delta G_{*} - \Delta G_{\text{OOH}^*} + G_{\text{H}} + G_{\text{O}_2} - eU$$

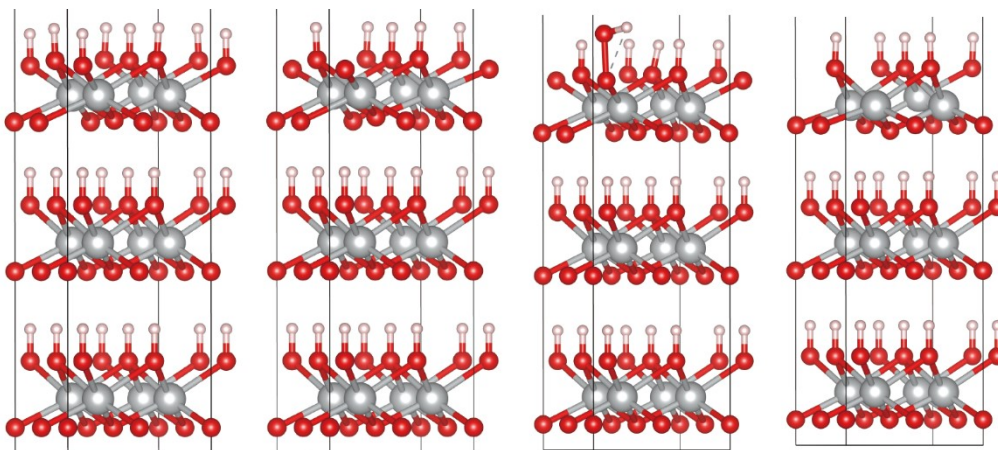
The formation energy ( $E_f$ ) is calculated by the following formula, where  $E_{\text{Fe}(\text{Co})}$  and  $E_{\text{Ni}}$  refers to the calculated energy of the dopant (Fe, Co and Ni) which is obtained from their bulk structures.

$$E_f = E_{\text{NiFe}(\text{Co})\text{OOH}} - E_{\text{NiOOH}} - E_{\text{Fe}(\text{Co})} + E_{\text{Ni}}$$

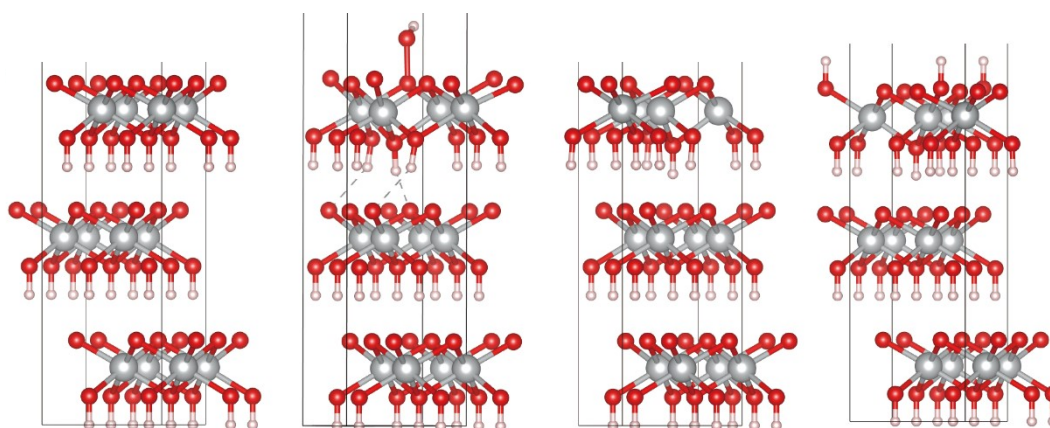
The binding energy ( $E_b$ ) is calculated by the following formula, where A and B refer to NiOOH and FeOOH or CoOOH.

$$E_b = E_{\text{A@B}} - E_{\text{A}} - E_{\text{B}}$$

## Supplementary Figures



**Figure S1** Intermediate Structural Diagrams in the NiOOH (001) OER Reaction under the SSM.



**Figure S2** Intermediate Structural Diagrams in the NiOOH (00 $\bar{1}$ ) OER Reaction under the SSM.

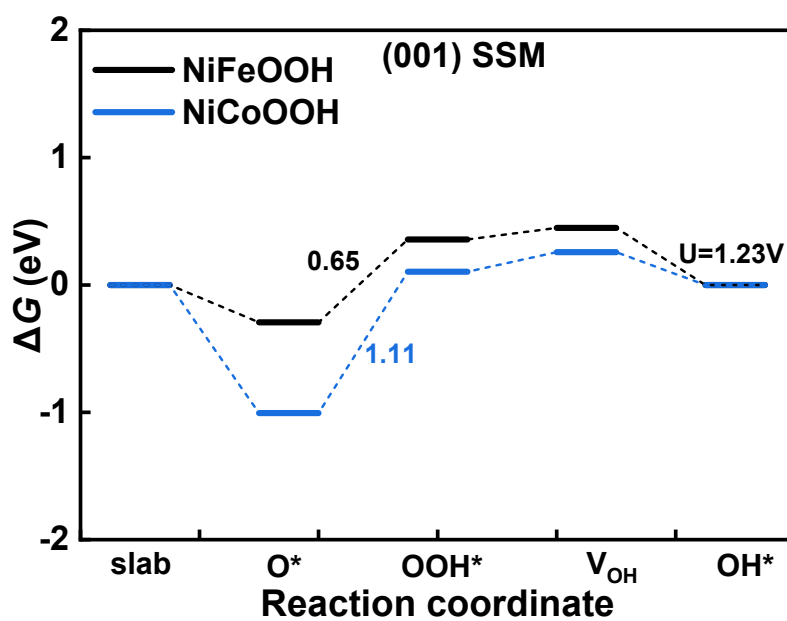


Figure S3 The Gibbs free energy diagrams of NiOOH (001) doped with Fe/Co following SSM

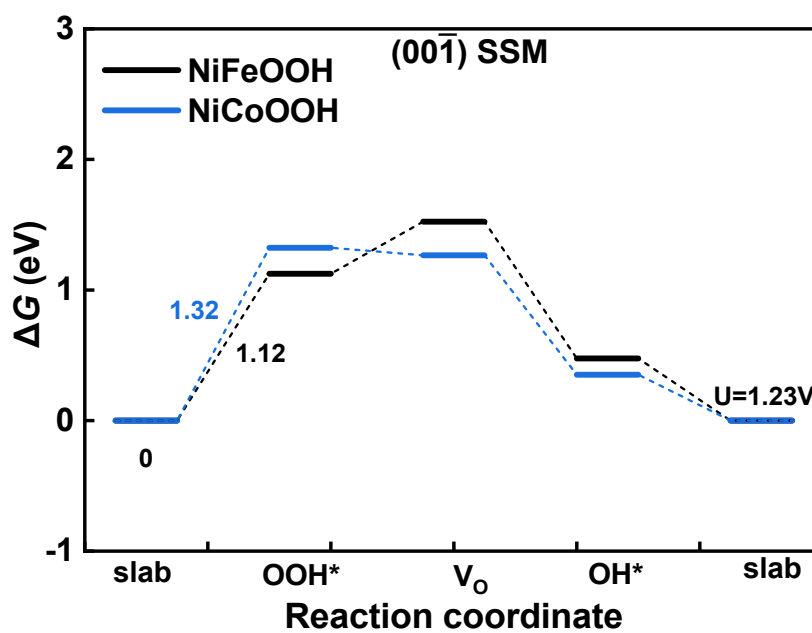
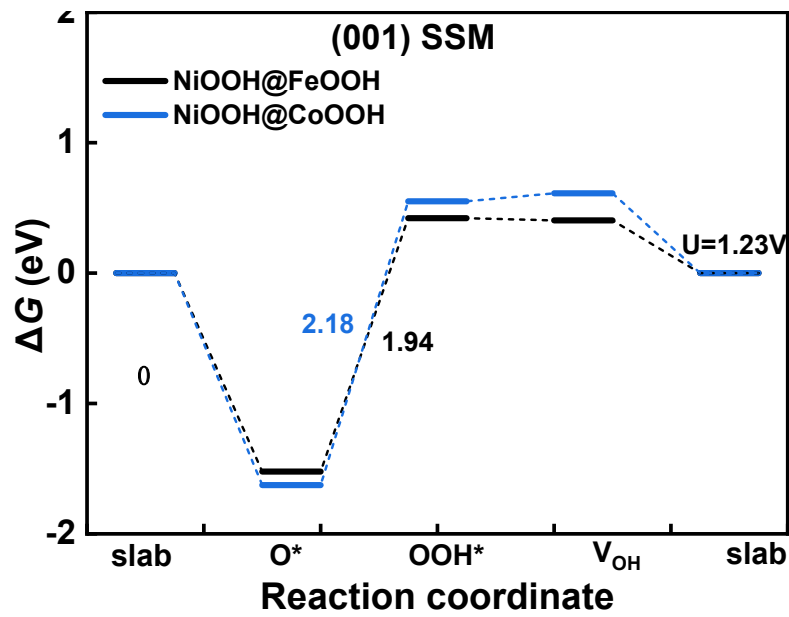
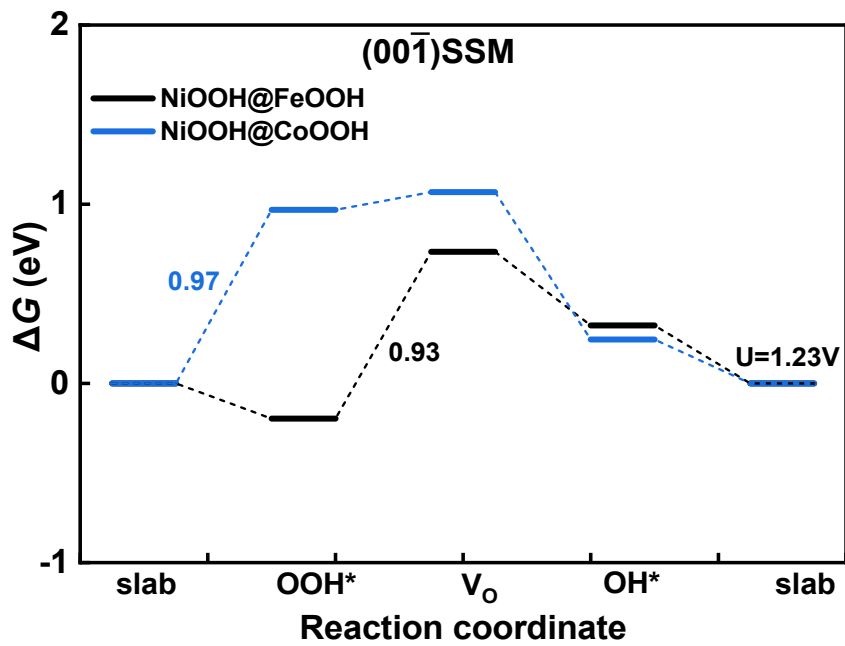


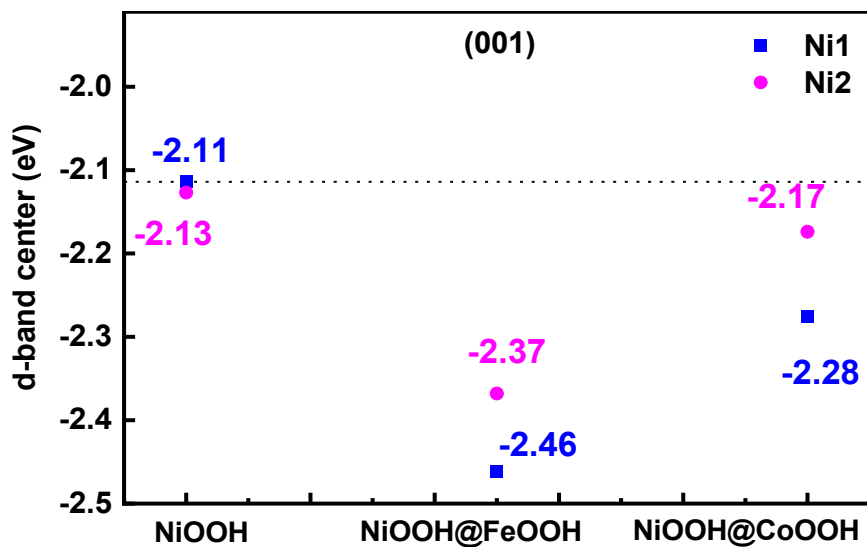
Figure S4 The Gibbs free energy diagrams of NiOOH ( $00\bar{1}$ ) doped with Fe/Co following SSM



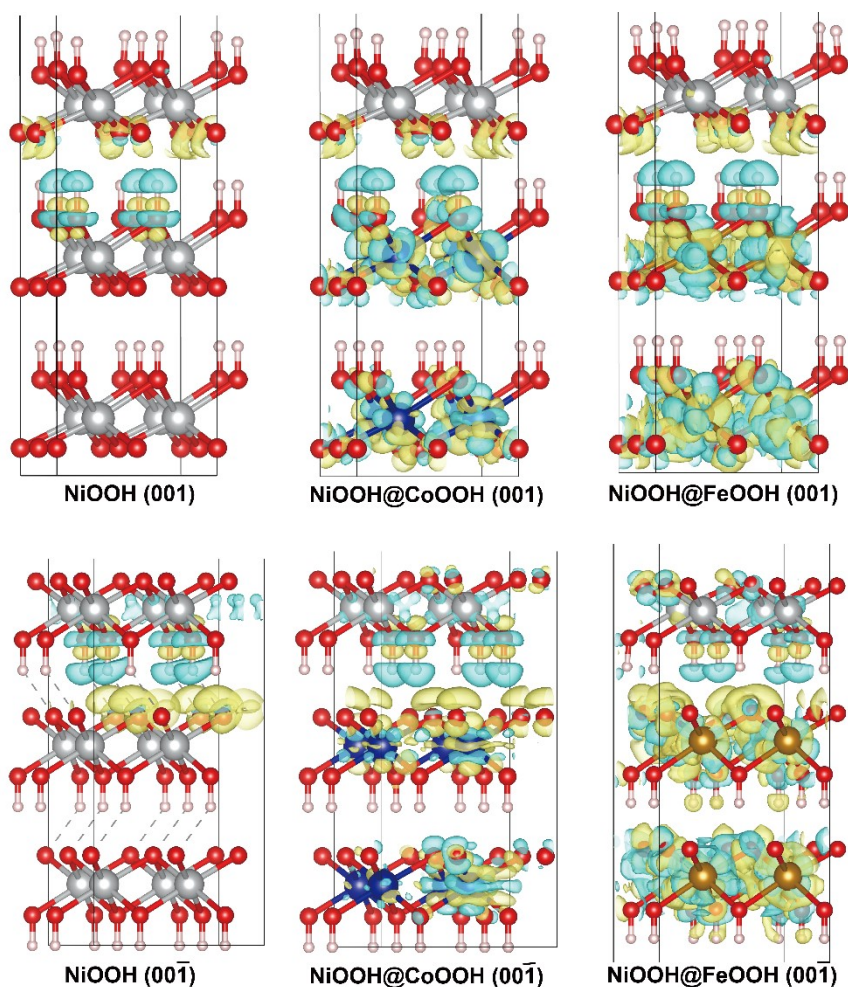
**Figure S5** The Gibbs free energy diagrams for OER under SSM on NiOOH@FeOOH (001) and NiOOH@CoOOH (001).



**Figure S6** The Gibbs free energy diagrams for OER under SSM on NiOOH@FeOOH (00 $\bar{1}$ ) and NiOOH@CoOOH (00 $\bar{1}$ ).

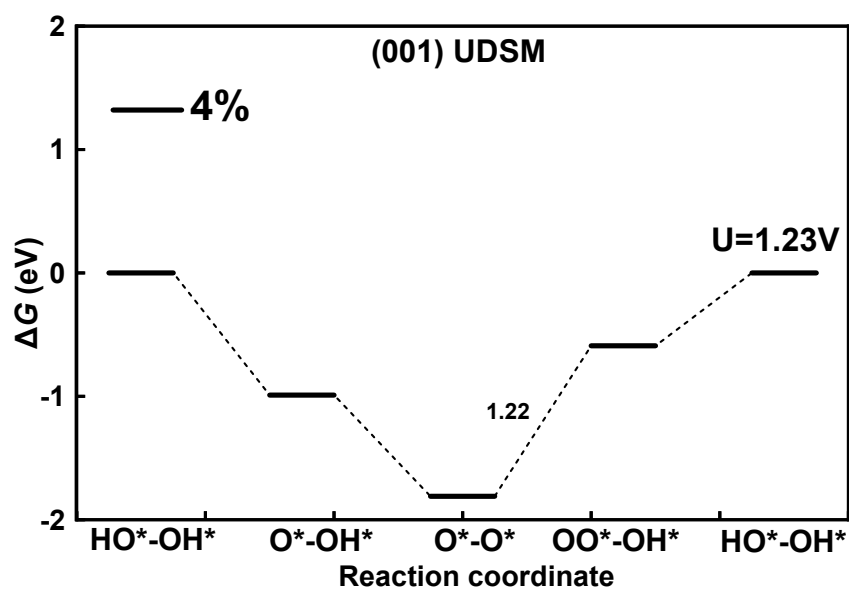


**Figure S7** The change of *d*-band center on heterojunction NiOOH@FeOOH (001) and NiOOH@CoOOH (001).

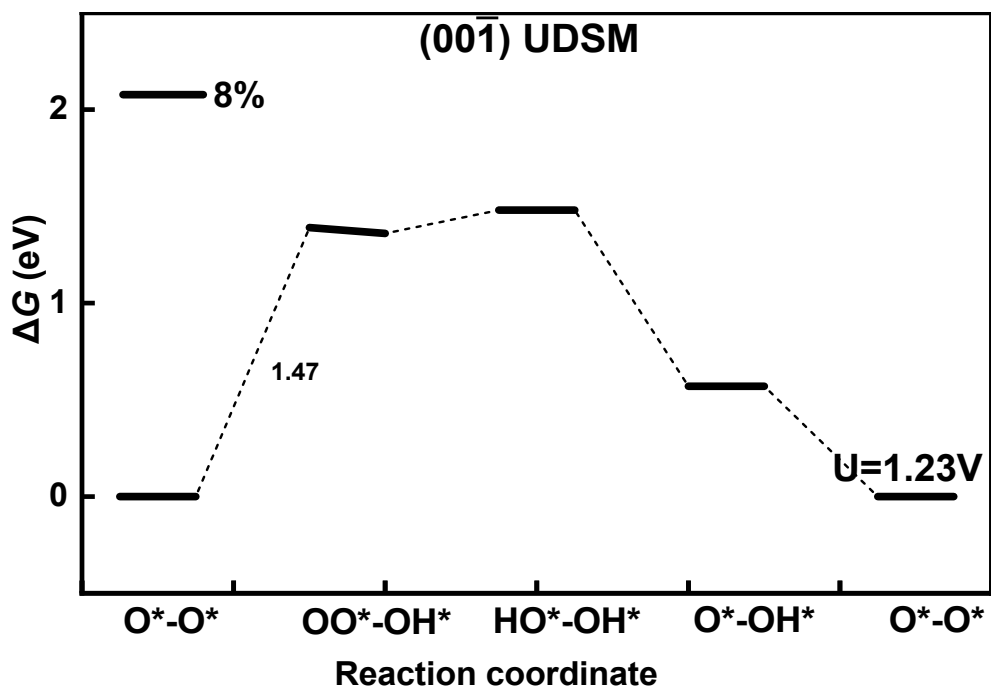


**Figure S8** Charge density difference (EDD) of heterostructures NiOOH@CoOOH and NiOOH@FeOOH, where the isosurface value is set to be  $0.0035\text{e}\text{\AA}^{-3}$ . Positive and negative charges

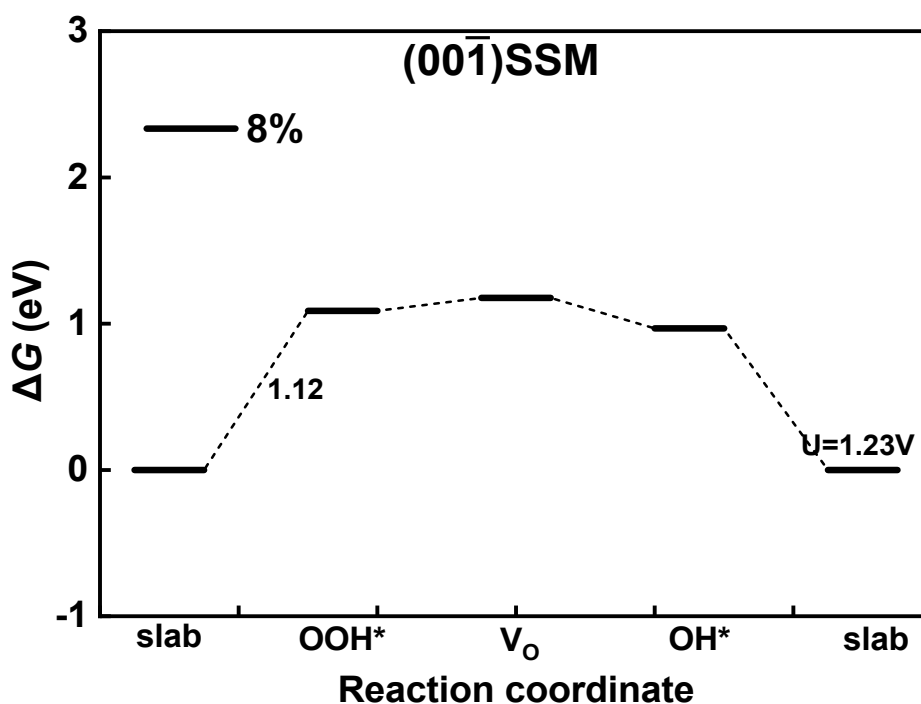
are shown in yellow and cyan.



**Figure S9** The Gibbs free energy diagrams for OER under the UDSM on the NiOOH (001) which compressed to 4%.

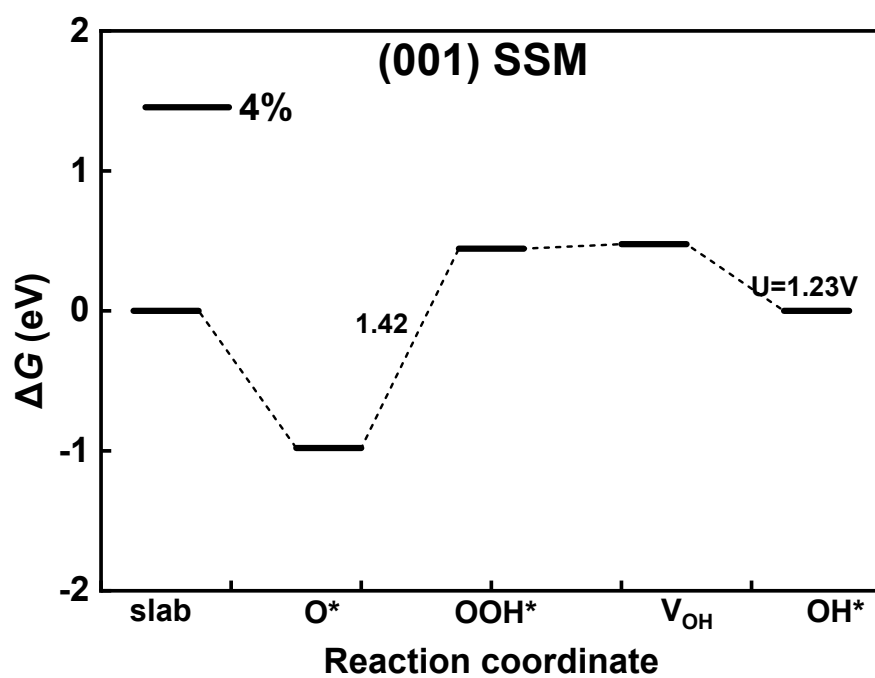


**Figure S10** The Gibbs free energy diagrams for OER under the UDSM on the NiOOH ( $00\bar{1}$ ) which compressed to 7%.

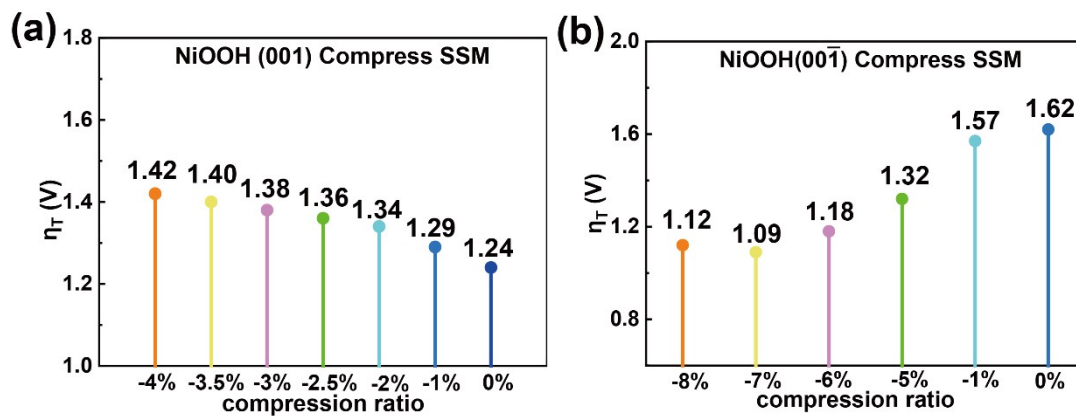


**Figure S11** The Gibbs free energy diagrams for OER under the SSM on the NiOOH ( $00\bar{1}$ ) which compressed to 7%.





**Figure S12** The Gibbs free energy diagrams for OER under the SSM on the NiOOH (001) which compressed to 4%.



**Figure S13** Variation of overpotential with compression ratio for NiOOH (001) and NiOOH (001̄) under the SSM.

## Supplementary Tables

**Table S1** The calculated formation energy ( $E_f$ ) of the structures of NiFeOOH and NiCoOOH. (unit: eV)

	NiFeOOH	NiCoOOH
(001)	-1.93	-0.43
(00 $\bar{1}$ )	-1.83	-0.84

**Table S2** The calculated binding energy ( $E_b$ ) of the structures of NiOOH@FeOOH and NiOOH@CoOOH. (unit: eV)

	NiOOH@FeOOH	NiOOH@CoOOH
(001)	-3.18	-3.18
(00 $\bar{1}$ )	-1.07	-2.70

**Table S3** Ni-O bond length around single Ni atom before and after compression of (001) and (00 $\bar{1}$ ) surfaces. (unit: Å)

	I	II	III	IV	V	VI
(001) 4%	2.14	2.02	2.12	2.04	2.06	1.95
	2.09	2.00	2.08	1.99	1.99	1.92
(00 $\bar{1}$ ) 8%	1.92	1.92	1.92	1.98	1.97	1.97
	1.86	1.86	1.86	1.93	1.92	1.93

## Representative CONTCAR files

NiOOH (001):

```
1.0000000000000000
  6.2588229999999996  0.0000000000000000  0.0000000000000000
 -3.1202581100000000  5.4144727300000000  0.0000000000000000
 -0.0389504600000000 -0.0213445500000000  24.4738197000000000
```

```
Ni  H  O
 12  12  24
```

Selective dynamics

Direct

```
0.1629140000000007  0.3346170000000015  0.0699779999999990  F  F  F
0.6629140000000007  0.3346170000000015  0.0699779999999990  F  F  F
0.16291499999999981  0.8346179999999990  0.0699779999999990  F  F  F
0.66291499999999981  0.8346179999999990  0.0699779999999990  F  F  F
0.1629140000000007  0.3346170000000015  0.2666219999999981  F  F  F
0.6629140000000007  0.3346170000000015  0.2666219999999981  F  F  F
0.16291499999999981  0.8346179999999990  0.2666219999999981  F  F  F
0.66291499999999981  0.8346179999999990  0.2666219999999981  F  F  F
0.1735906518384469  0.3374678334290303  0.4524673467683979  T  T  T
0.6711404148589397  0.3378944561854231  0.4528135517436156  T  T  T
0.1715595778682991  0.8364134380550783  0.4565003989643714  T  T  T
0.6710844653893460  0.8347466592123233  0.4528093582013212  T  T  T
0.3295850000000016  0.1679490000000001  0.1577569999999966  F  F  F
0.8295850000000016  0.1679490000000001  0.1577569999999966  F  F  F
0.32958399999999970  0.6679469999999981  0.1577569999999966  F  F  F
0.82958399999999970  0.6679469999999981  0.1577569999999966  F  F  F
0.3295850000000016  0.1679490000000001  0.3544010000000029  F  F  F
0.8295850000000016  0.1679490000000001  0.3544010000000029  F  F  F
0.32958399999999970  0.6679469999999981  0.3544010000000029  F  F  F
0.82958399999999970  0.6679469999999981  0.3544010000000029  F  F  F
0.3315830612731554  0.1523494586185442  0.5361564976932413  T  T  T
0.3329489084397013  0.6814768952936617  0.5361444168899306  T  T  T
0.8685237053667660  0.6846520855336146  0.5370863024490973  T  T  T
0.8327109937477815  0.1667824328330516  0.5296026782790751  T  T  T
0.9962510000000009  0.0012839999999983  0.0337869999999967  F  F  F
0.3295850000000016  0.1679490000000001  0.1176030000000026  F  F  F
0.4962510000000009  0.0012839999999983  0.0337869999999967  F  F  F
0.8295850000000016  0.1679490000000001  0.1176030000000026  F  F  F
0.9962500000000034  0.5012820000000033  0.0337869999999967  F  F  F
0.32958399999999970  0.6679469999999981  0.1176030000000026  F  F  F
0.4962500000000034  0.5012820000000033  0.0337869999999967  F  F  F
0.82958399999999970  0.6679469999999981  0.1176030000000026  F  F  F
0.9962510000000009  0.0012839999999983  0.2304310000000029  F  F  F
```

0.3295850000000016	0.1679490000000001	0.3142470000000017	F	F	F
0.4962510000000009	0.0012839999999983	0.2304310000000029	F	F	F
0.8295850000000016	0.1679490000000001	0.3142470000000017	F	F	F
0.9962500000000034	0.5012820000000033	0.2304310000000029	F	F	F
0.3295839999999970	0.6679469999999981	0.3142470000000017	F	F	F
0.4962500000000034	0.5012820000000033	0.2304310000000029	F	F	F
0.8295839999999970	0.6679469999999981	0.3142470000000017	F	F	F
0.0132662596589139	0.9914658193260760	0.4188419509606118	T	T	T
0.3343718314356074	0.1594708953121427	0.4963383231203353	T	T	T
0.4808285769132668	0.9911595911760794	0.4183169078539527	T	T	T
0.8354812327984111	0.1682728447791112	0.4897730730830438	T	T	T
0.0138067789351119	0.5231138458203289	0.4188853126407029	T	T	T
0.3348968991713908	0.6765026311904710	0.4963351455165756	T	T	T
0.5093008614129372	0.5054714346148358	0.4211123304420992	T	T	T
0.8546206197145677	0.6778958477804550	0.4973411747692915	T	T	T

NiOOH (00 $\bar{1}$ )

1.0000000000000000		
5.8705040000000004	0.0000000000000000	0.0000000000000000
2.9321272899999999	5.0828586700000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	21.9650217099999985

Ni H O  
12 12 24

Selective dynamics

Direct

0.4991923199999988	0.0001661900000016	0.0906147500000003	F	F	F
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0.5009377866214354	0.5006186553710856	0.4987245481911136	T	T	T
0.9999539700000000	0.4999436200000034	0.2962549900000013	F	F	F
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0.0008985467016638	0.0007034366455879	0.4985259986773540	T	T	T
0.4999539700000000	0.9999436200000034	0.2962549900000013	F	F	F
0.9991923199999988	0.5001661900000016	0.0906147500000003	F	F	F
0.5007912621662973	0.0007529681889623	0.4985714536164297	T	T	T
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0.1675227058520165	0.1671380514287977	0.4525704508907173	T	T	T
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0.1656834300000014	0.1668881900000017	0.0448832399999972	F	F	F
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NiFeOOH (001):

1.0000000000000000

6.2588229999999996 0.0000000000000000 0.0000000000000000

-3.1202581100000000 5.4144727300000000 0.0000000000000000

-0.0389504600000000 -0.0213445500000000 24.4738197000000000

Ni Fe H O

11 1 12 24

Selective dynamics

Direct

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0.6629140000000007	0.3346170000000015	0.0699779999999990	F	F	F
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0.6629149999999981	0.8346179999999990	0.0699779999999990	F	F	F

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0.6629140000000007	0.3346170000000015	0.2666219999999981	F	F	F
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0.8295839999999970	0.6679469999999981	0.1577569999999966	F	F	F
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0.9962510000000009	0.0012839999999983	0.0337869999999967	F	F	F
0.3295850000000016	0.1679490000000001	0.1176030000000026	F	F	F
0.4962510000000009	0.0012839999999983	0.0337869999999967	F	F	F
0.8295850000000016	0.1679490000000001	0.1176030000000026	F	F	F
0.9962500000000034	0.5012820000000033	0.0337869999999967	F	F	F
0.3295839999999970	0.6679469999999981	0.1176030000000026	F	F	F
0.4962500000000034	0.5012820000000033	0.0337869999999967	F	F	F
0.8295839999999970	0.6679469999999981	0.1176030000000026	F	F	F
0.9962510000000009	0.0012839999999983	0.2304310000000029	F	F	F
0.3295850000000016	0.1679490000000001	0.3142470000000017	F	F	F
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0.3295839999999970	0.6679469999999981	0.3142470000000017	F	F	F
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0.8295839999999970	0.6679469999999981	0.3142470000000017	F	F	F
0.0245660420295335	0.9851717914521956	0.4184244778787011	T	T	T
0.3314200976951882	0.1539171148155156	0.4981750556815416	T	T	T
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0.8392921281839136	0.1698565458722051	0.4889555105029671	T	T	T
0.0246747331579245	0.5396522842909672	0.4184587091993707	T	T	T
0.3317196981089831	0.6781944614014765	0.4982032222525962	T	T	T
0.5062863018758851	0.5032395874797352	0.4218743514840434	T	T	T
0.8563802851912549	0.6784334701770679	0.4979797361070033	T	T	T

NiFeOOH (00 $\bar{1}$ ):

1.0000000000000000		
5.8705040000000004	0.0000000000000000	0.0000000000000000
2.9321276100000002	5.0828587599999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	21.9650210000000001

Ni	Fe	H	O
11	1	12	24

Selective dynamics

Direct

0.4991920000000007	0.0001660000000001	0.0906149999999997	F	F	F
0.0037978975520066	0.4994950177505791	0.4982838554532995	T	T	T
0.4999540000000025	0.4999439999999993	0.2962550000000022	F	F	F
0.9991920000000007	0.0001660000000001	0.0906149999999997	F	F	F
0.4993022268504036	0.4996411807776985	0.4984227317482513	T	T	T
0.9999540000000025	0.4999439999999993	0.2962550000000022	F	F	F
0.4991920000000007	0.5001660000000001	0.0906149999999997	F	F	F
0.4999540000000025	0.9999439999999993	0.2962550000000022	F	F	F
0.9991920000000007	0.5001660000000001	0.0906149999999997	F	F	F
0.4991413906502145	0.0041410980068585	0.4983238601096928	T	T	T
0.9999540000000025	0.9999439999999993	0.2962550000000022	F	F	F
0.0008179834104032	0.0010489534907241	0.5029952696891161	T	T	T
0.1555139212379681	0.1571372449438553	0.4070885414034454	T	T	T
0.1661509999999993	0.1668239999999983	0.2056400000000025	F	F	F
0.1653889999999976	0.1670459999999991	0.0000000000000000	F	F	F
0.6891399678923403	0.1569492408341723	0.4072068056641140	T	T	T
0.6661509999999993	0.1668239999999983	0.2056400000000025	F	F	F
0.6653889999999976	0.1670459999999991	0.0000000000000000	F	F	F
0.1551425157385955	0.6896237310306091	0.4071667567602713	T	T	T
0.1661509999999993	0.6668239999999983	0.2056400000000025	F	F	F
0.1653889999999976	0.6670459999999991	0.0000000000000000	F	F	F
0.6672191339108392	0.6679334405351188	0.4103042074302599	T	T	T
0.6661509999999993	0.6668239999999983	0.2056400000000025	F	F	F
0.6653889999999976	0.6670459999999991	0.0000000000000000	F	F	F
0.3339154457448834	0.3344084658259750	0.5384611086536287	T	T	T
0.3332839968698623	0.3332902806586696	0.3383837447136180	T	T	T
0.3326950000000011	0.3334529999999987	0.1334500000000034	F	F	F
0.1619364406405849	0.1626331348576008	0.4518869351846361	T	T	T
0.1664450000000031	0.1666659999999993	0.2505230000000012	F	F	F
0.1656830000000014	0.1668880000000001	0.0448829999999987	F	F	F
0.8434469514734850	0.3168624125260592	0.5408057673220398	T	T	T
0.8338725200997747	0.3323067145691097	0.3391076068862019	T	T	T
0.8326950000000011	0.3334529999999987	0.1334500000000034	F	F	F

0.6775206803710278	0.1627218286812864	0.4519901751968423	T	T	T
0.6664450000000031	0.1666659999999993	0.2505230000000012	F	F	F
0.6656830000000014	0.1668880000000001	0.0448829999999987	F	F	F
0.3165755694128792	0.8432381237035784	0.5407746346274633	T	T	T
0.3324738170127813	0.8336803878334567	0.3390961103829980	T	T	T
0.3326950000000011	0.8334529999999987	0.1334500000000034	F	F	F
0.1619641278857496	0.6778341692965620	0.4519489115257511	T	T	T
0.1664450000000031	0.6666659999999993	0.2505230000000012	F	F	F
0.1656830000000014	0.6668880000000001	0.0448829999999987	F	F	F
0.8431828762185322	0.8430544434576552	0.5407750098150829	T	T	T
0.8338925665762932	0.8335180515476960	0.3391160639266101	T	T	T
0.8326950000000011	0.8334529999999987	0.1334500000000034	F	F	F
0.6673981542466920	0.6677456303212098	0.4552730010492769	T	T	T
0.6664450000000031	0.6666659999999993	0.2505230000000012	F	F	F
0.6656830000000014	0.6668880000000001	0.0448829999999987	F	F	F

NiOOH@FeOOH (001):

1.0000000000000000

6.2588229999999996	0.0000000000000000	0.0000000000000000
-3.1202581100000000	5.4144727300000000	0.0000000000000000
-0.0389504600000000	-0.0213445500000000	24.4738197000000000

Fe Ni H O  
8 4 12 24

Selective dynamics

Direct

0.1629140000000007	0.3346170000000015	0.0699779999999990	F	F	F
0.6629140000000007	0.3346170000000015	0.0699779999999990	F	F	F
0.1629149999999981	0.8346179999999990	0.0699779999999990	F	F	F
0.6629149999999981	0.8346179999999990	0.0699779999999990	F	F	F
0.1629140000000007	0.3346170000000015	0.2666219999999981	F	F	F
0.6629140000000007	0.3346170000000015	0.2666219999999981	F	F	F
0.1629149999999981	0.8346179999999990	0.2666219999999981	F	F	F
0.6629149999999981	0.8346179999999990	0.2666219999999981	F	F	F
0.1759609043402627	0.3409084374078335	0.4524903294999231	T	T	T
0.6737662723022062	0.3411808946016623	0.4525424184971951	T	T	T
0.1719827060588812	0.8350590152790132	0.4561129518535412	T	T	T
0.6718486949413441	0.8354762382808253	0.4537602323960114	T	T	T
0.3295850000000016	0.1679490000000001	0.1577569999999966	F	F	F
0.8295850000000016	0.1679490000000001	0.1577569999999966	F	F	F
0.3295839999999970	0.6679469999999981	0.1577569999999966	F	F	F
0.8295839999999970	0.6679469999999981	0.1577569999999966	F	F	F
0.3295850000000016	0.1679490000000001	0.3544010000000029	F	F	F
0.8295850000000016	0.1679490000000001	0.3544010000000029	F	F	F
0.3295839999999970	0.6679469999999981	0.3544010000000029	F	F	F



0.8295839999999970	0.6679469999999981	0.3544010000000029	F	F	F
0.3326595168558683	0.1579728615351171	0.5343409792889026	T	T	T
0.3329713294513583	0.6842693771627935	0.5372042317620965	T	T	T
0.8667897152677226	0.6835466179796410	0.5374642129668511	T	T	T
0.8270227543998182	0.1488315080016382	0.5306951425075986	T	T	T
0.9962510000000009	0.0012839999999983	0.0337869999999967	F	F	F
0.3295850000000016	0.1679490000000001	0.1176030000000026	F	F	F
0.4962510000000009	0.0012839999999983	0.0337869999999967	F	F	F
0.8295850000000016	0.1679490000000001	0.1176030000000026	F	F	F
0.9962500000000034	0.5012820000000033	0.0337869999999967	F	F	F
0.3295839999999970	0.6679469999999981	0.1176030000000026	F	F	F
0.4962500000000034	0.5012820000000033	0.0337869999999967	F	F	F
0.8295839999999970	0.6679469999999981	0.1176030000000026	F	F	F
0.9962510000000009	0.0012839999999983	0.2304310000000029	F	F	F
0.3295850000000016	0.1679490000000001	0.3142470000000017	F	F	F
0.4962510000000009	0.0012839999999983	0.2304310000000029	F	F	F
0.8295850000000016	0.1679490000000001	0.3142470000000017	F	F	F
0.9962500000000034	0.5012820000000033	0.2304310000000029	F	F	F
0.3295839999999970	0.6679469999999981	0.3142470000000017	F	F	F
0.4962500000000034	0.5012820000000033	0.2304310000000029	F	F	F
0.8295839999999970	0.6679469999999981	0.3142470000000017	F	F	F
0.0074477909082438	0.9828354446758739	0.4185720499153630	T	T	T
0.3359684578811815	0.1632046391148900	0.4944875515210067	T	T	T
0.4823872398394283	0.9831056319854173	0.4183695208400587	T	T	T
0.8340341157670401	0.1608284657450770	0.4909607477071479	T	T	T
0.0136502629038620	0.5177086924987979	0.4196481918921672	T	T	T
0.3372564174198527	0.6795822380264882	0.4973994832998110	T	T	T
0.5131203985576338	0.5159073198014531	0.4207646370604879	T	T	T
0.8542187655355427	0.6794783238299027	0.4977034884554708	T	T	T

NiOOH@FeOOH (00 $\bar{1}$ ):

1.0000000000000000		
6.0730339999999998	0.0000000000000000	0.0000000000000000
3.0334377600000000	5.2576238999999996	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.4215449999999983

Ni Fe H O  
4 8 12 24

Selective dynamics

Direct

0.9715562289953940	0.2634643292030773	0.4843092074234954	T	T	T
0.4696817942900947	0.7652209833173038	0.4843260587126293	T	T	T
0.4713310439800953	0.2645617503605179	0.4873329603867711	T	T	T
0.9715958490801774	0.7653376601413618	0.4843415728627450	T	T	T

0.9683250000000001	0.2658369999999977	0.1511720000000025	F	F	F
0.4683259999999976	0.7658380000000022	0.1511730000000000	F	F	F
0.4683259999999976	0.2658360000000002	0.1511739999999975	F	F	F
0.9683250000000001	0.7658369999999977	0.1511730000000000	F	F	F
0.9683199999999985	0.2658399999999972	0.3215149999999980	F	F	F
0.4683229999999980	0.7658380000000022	0.3215149999999980	F	F	F
0.4683179999999965	0.2658399999999972	0.3215160000000026	F	F	F
0.9683149999999969	0.7658399999999972	0.3215149999999980	F	F	F
0.6505943711029650	0.4443588428296288	0.4141549183319133	T	T	T
0.6349749999999972	0.4325120000000027	0.0729350000000011	F	F	F
0.1382424629190268	0.9315067188271987	0.4114016524439314	T	T	T
0.1349889999999974	0.9325040000000016	0.0729359999999986	F	F	F
0.1103060755182991	0.4444804486863013	0.4143549522401307	T	T	T
0.1349889999999974	0.4325059999999965	0.0729359999999986	F	F	F
0.6503522137567187	0.9045412081418066	0.4143252256156837	T	T	T
0.6349799999999988	0.9325109999999981	0.0729359999999986	F	F	F
0.6349790000000013	0.4325100000000006	0.2432889999999972	F	F	F
0.1349820000000008	0.9325120000000027	0.2432879999999997	F	F	F
0.1349799999999988	0.4325070000000011	0.2432879999999997	F	F	F
0.6349700000000027	0.9325159999999997	0.2432879999999997	F	F	F
0.8203283321867945	0.0901932138550330	0.5156889333660754	T	T	T
0.8015979999999985	0.0991959999999992	0.1852370000000008	F	F	F
0.6437075883685259	0.4373772846579361	0.4500455531834640	T	T	T
0.6349390000000028	0.4325309999999973	0.1087149999999966	F	F	F
0.2964751113210644	0.6139177637626558	0.5156894902771257	T	T	T
0.3016009999999980	0.5991969999999966	0.1852370000000008	F	F	F
0.1378530122601576	0.9316267565682993	0.4474492887452180	T	T	T
0.1349510000000009	0.9325240000000008	0.1087160000000011	F	F	F
0.2964706423761200	0.0901895250817184	0.5157027948072718	T	T	T
0.3016069999999971	0.0991980000000012	0.1852379999999982	F	F	F
0.1248701833469597	0.4377042590766675	0.4502092468481170	T	T	T
0.1349519999999984	0.4325260000000029	0.1087160000000011	F	F	F
0.8038044879991459	0.5975267291683861	0.5176272145666508	T	T	T
0.8016000000000005	0.5992040000000003	0.1852370000000008	F	F	F
0.6437855772479161	0.9190878110447963	0.4501965919927988	T	T	T
0.6349489999999989	0.9325299999999999	0.1087160000000011	F	F	F
0.8018575389596773	0.0991058675259527	0.3556834737716972	T	T	T
0.6349400000000003	0.4325219999999987	0.2790639999999982	F	F	F
0.3009908809806718	0.6001448337566880	0.3556933157160397	T	T	T
0.1349469999999968	0.9325210000000013	0.2790650000000028	F	F	F
0.3009735360085981	0.0989422812805851	0.3557060592884572	T	T	T
0.1349469999999968	0.4325270000000003	0.2790639999999982	F	F	F
0.8011306287068347	0.5994599198179057	0.3563191111585433	T	T	T
0.6349289999999996	0.9325419999999980	0.2790630000000007	F	F	F

NiOOH@CoOOH (001):

1.0000000000000000

6.2588229999999996 0.0000000000000000 0.0000000000000000

-3.1202581100000000 5.4144727300000000 0.0000000000000000

-0.0389504600000000 -0.0213445500000000 24.4738197000000000

Co Ni H O

8 4 12 24

Selective dynamics

Direct

0.1629140000000007	0.3346170000000015	0.0699779999999990	F	F	F
0.6629140000000007	0.3346170000000015	0.0699779999999990	F	F	F
0.1629149999999981	0.8346179999999990	0.0699779999999990	F	F	F
0.6629149999999981	0.8346179999999990	0.0699779999999990	F	F	F
0.1629140000000007	0.3346170000000015	0.2666219999999981	F	F	F
0.6629140000000007	0.3346170000000015	0.2666219999999981	F	F	F
0.1629149999999981	0.8346179999999990	0.2666219999999981	F	F	F
0.6629149999999981	0.8346179999999990	0.2666219999999981	F	F	F
0.1736192003271145	0.3376241629133740	0.4524963428586254	T	T	T
0.6711554306895628	0.3379614067985766	0.4527955383715525	T	T	T
0.1716616043292734	0.8362902243255269	0.4564623841428705	T	T	T
0.6709295087189979	0.8346446288217798	0.4528211360251911	T	T	T
0.3295850000000016	0.1679490000000001	0.1577569999999966	F	F	F
0.8295850000000016	0.1679490000000001	0.1577569999999966	F	F	F
0.3295839999999970	0.6679469999999981	0.1577569999999966	F	F	F
0.8295839999999970	0.6679469999999981	0.1577569999999966	F	F	F
0.3295850000000016	0.1679490000000001	0.3544010000000029	F	F	F
0.8295850000000016	0.1679490000000001	0.3544010000000029	F	F	F
0.3295839999999970	0.6679469999999981	0.3544010000000029	F	F	F
0.8295839999999970	0.6679469999999981	0.3544010000000029	F	F	F
0.3315096228587452	0.1523080330004957	0.5361532694246219	T	T	T
0.3328527270721232	0.6814357428247290	0.5361732206410349	T	T	T
0.8683217583892582	0.6845419513189984	0.5370882884463454	T	T	T
0.8327692097299382	0.1667993907586520	0.5296396929866061	T	T	T
0.9962510000000009	0.0012839999999983	0.0337869999999967	F	F	F
0.3295850000000016	0.1679490000000001	0.1176030000000026	F	F	F
0.4962510000000009	0.0012839999999983	0.0337869999999967	F	F	F
0.8295850000000016	0.1679490000000001	0.1176030000000026	F	F	F
0.9962500000000034	0.5012820000000033	0.0337869999999967	F	F	F
0.3295839999999970	0.6679469999999981	0.1176030000000026	F	F	F
0.4962500000000034	0.5012820000000033	0.0337869999999967	F	F	F
0.8295839999999970	0.6679469999999981	0.1176030000000026	F	F	F
0.9962510000000009	0.0012839999999983	0.2304310000000029	F	F	F
0.3295850000000016	0.1679490000000001	0.3142470000000017	F	F	F

0.4962510000000009	0.0012839999999983	0.2304310000000029	F	F	F
0.8295850000000016	0.1679490000000001	0.3142470000000017	F	F	F
0.9962500000000034	0.5012820000000033	0.2304310000000029	F	F	F
0.3295839999999970	0.6679469999999981	0.3142470000000017	F	F	F
0.4962500000000034	0.5012820000000033	0.2304310000000029	F	F	F
0.8295839999999970	0.6679469999999981	0.3142470000000017	F	F	F
0.0134915121992848	0.9914731535747989	0.4186906730175709	T	T	T
0.3342800436657961	0.1593527551965518	0.4963416916631081	T	T	T
0.4810207534869388	0.9911954939755766	0.4182248713582565	T	T	T
0.8357520710829461	0.1683930553946295	0.4898290519621460	T	T	T
0.0139467740900628	0.5231723282787498	0.4187865871490664	T	T	T
0.3348378096882140	0.6765724964815301	0.4963709712417545	T	T	T
0.5091175692695054	0.5053181950477238	0.4211205886296474	T	T	T
0.8545617880885359	0.6779355744859371	0.4973573483482310	T	T	T

NiOOH@CoOOH (00 $\bar{1}$ ):

1.0000000000000000		
5.8705040000000004	0.0000000000000000	0.0000000000000000
2.9321276100000002	5.0828587599999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	21.9650210000000001

Co Ni H O  
8 4 12 24

Selective dynamics

Direct

0.4991920000000007	0.0001660000000001	0.0906149999999997	F	F	F
0.4999540000000025	0.4999439999999993	0.2962550000000022	F	F	F
0.9991920000000007	0.0001660000000001	0.0906149999999997	F	F	F
0.9999540000000025	0.4999439999999993	0.2962550000000022	F	F	F
0.4991920000000007	0.5001660000000001	0.0906149999999997	F	F	F
0.4999540000000025	0.9999439999999993	0.2962550000000022	F	F	F
0.9991920000000007	0.5001660000000001	0.0906149999999997	F	F	F
0.9999540000000025	0.9999439999999993	0.2962550000000022	F	F	F
0.0006668639133344	0.5004326629834471	0.4988165854295103	T	T	T
0.5006254879790694	0.5006395030332368	0.4988653639682827	T	T	T
0.0007153386411837	0.0005486967834193	0.4988290077751136	T	T	T
0.5005383327642019	0.0006370643806572	0.4988795594212007	T	T	T
0.1668703038092816	0.1674328849216459	0.4076750914396304	T	T	T
0.1661509999999993	0.1668239999999983	0.2056400000000025	F	F	F
0.1653889999999976	0.1670459999999991	0.0000000000000000	F	F	F
0.6669897355652494	0.1674374203643357	0.4077330555084608	T	T	T
0.6661509999999993	0.1668239999999983	0.2056400000000025	F	F	F
0.6653889999999976	0.1670459999999991	0.0000000000000000	F	F	F
0.1660723208552980	0.6674706310520470	0.4077038125027610	T	T	T

0.1661509999999993	0.6668239999999983	0.2056400000000025	F	F	F
0.1653889999999976	0.6670459999999991	0.0000000000000000	F	F	F
0.6672236478748164	0.6675844013854588	0.4077195105113792	T	T	T
0.6661509999999993	0.6668239999999983	0.2056400000000025	F	F	F
0.6653889999999976	0.6670459999999991	0.0000000000000000	F	F	F
0.3337567915186748	0.3341132932453247	0.5393714910489450	T	T	T
0.3335016428075377	0.3333722546803287	0.3375267559892156	T	T	T
0.3326950000000011	0.3334529999999987	0.1334500000000034	F	F	F
0.1672442389218293	0.1672701410791853	0.4525069719772286	T	T	T
0.1664450000000031	0.1666659999999993	0.2505230000000012	F	F	F
0.1656830000000014	0.1668880000000001	0.0448829999999987	F	F	F
0.8343244088575218	0.3340411215249614	0.5393586539214837	T	T	T
0.8328368444977772	0.3335119845493191	0.3375296522756236	T	T	T
0.8326950000000011	0.3334529999999987	0.1334500000000034	F	F	F
0.6672193076413382	0.1673905698317308	0.4525825507255004	T	T	T
0.6664450000000031	0.1666659999999993	0.2505230000000012	F	F	F
0.6656830000000014	0.1668880000000001	0.0448829999999987	F	F	F
0.3339263210695820	0.8338550785955172	0.5393762553148637	T	T	T
0.3335473032477420	0.8329464513139819	0.3375248111118769	T	T	T
0.3326950000000011	0.8334529999999987	0.1334500000000034	F	F	F
0.1669993483372318	0.6672362127250036	0.4525488516232729	T	T	T
0.1664450000000031	0.6666659999999993	0.2505230000000012	F	F	F
0.1656830000000014	0.6668880000000001	0.0448829999999987	F	F	F
0.8342078671133774	0.8338624890773744	0.5393518184326909	T	T	T
0.8331670309382966	0.8333099209503515	0.3375878427251383	T	T	T
0.8326950000000011	0.8334529999999987	0.1334500000000034	F	F	F
0.6672868466868835	0.6672944041822344	0.4525683224257661	T	T	T
0.6664450000000031	0.6666659999999993	0.2505230000000012	F	F	F
0.6656830000000014	0.6668880000000001	0.0448829999999987	F	F	F

**Reference:**

1. H. Dau, C. Limberg, T. Reier, M. Risch, S. Roggan and P. Strasser, *ChemCatChem*, 2010, **2**, 724–761.