SUPPORTING INFORMATION:

The effect of interlayer stacking arrangements in two dimensional NiOOH on water oxidation catalysis

Eitan Yohanan and Maytal Caspary Toroker

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

molecule	E_{tot} [eV]	ZPE [eV]	TS [eV]
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 [eV]	Delta ZPE [eV]	Entropy [eV]
$*OH_2$ to $*OH$	0.04	-0.21	-0.20
$*OH$ to $*'OH_2$	-0.06	0.02	0.47
$*'OH_2$ to $*'OH$	0.04	-0.22	-0.20
$*'OH$ to $*OH_2$	0.04	-0.09	-0.16

Table S3. Total energy differences calculated on reaction $*OH$ to $*O$ with and without vdW corrections.

E_{tot} [eV]	dE (with vdW)	dE (without vdW)	DIFF
Non - displaced	1.11	1.15	0.04
OUT 1	1.13	1.15	0.02
OUT 2	1.06	1.07	0.01
OUT 3	0.48	0.49	0.01
OUT 4	-1.71	-1.72	0.01
OUT 5	4.28	4.27	0.01
ROT 2	1.31	1.33	0.02
ROT 4	1.41	1.44	0.03
ROT 6	1.35	1.37	0.02
ROT 8	1.32	1.35	0.03
ROT 10	1.85	1.51	0.34

Table S4. Free energies for all displaced structures.

Gibbs Free energy [eV]	*OH$_2$ to *OH	*OH to *'OH$_2$	*'OH$_2$ to *'OH	*'OH to *OH$_2$
Non - displaced	1.71	1.58	1.55	-0.33
IN1	1.45	1.57	1.41	0.07
IN2	1.42	1.48	1.42	0.19
IN3	1.63	1.04	1.73	0.10
IN4	2.63	0.69	2.49	-1.30
IN5	1.42	6.11	1.50	-4.52
OUT1	1.46	1.58	1.40	0.07
OUT2	1.45	1.50	1.41	0.15
OUT3	1.68	0.91	1.76	0.15
OUT4	2.79	-1.28	2.80	0.20
OUT5	1.20	4.70	1.83	-3.12
901	1.44	1.60	1.38	0.09
902	1.35	1.65	1.27	0.23
903	1.36	1.70	1.27	0.17
904	1.45	1.75	1.38	-0.07
ROT 2°	1.46	1.76	1.37	-0.08
ROT 4°	1.49	1.87	1.48	-0.32
ROT 6°	1.66	1.80	2.01	-0.96
ROT 8°	1.97	1.78	2.61	-1.85
ROT 10°	2.60	1.94	3.97	-4.00

Figure S1. Charge density difference calculations between the NiOOH non-displaced supercell and its separated layers.
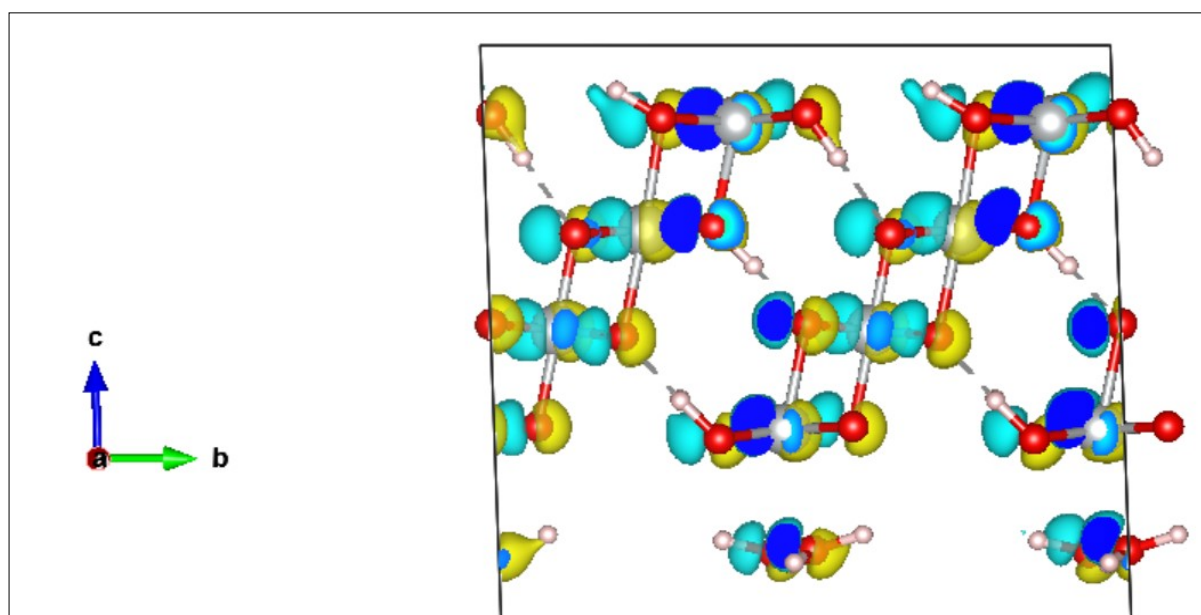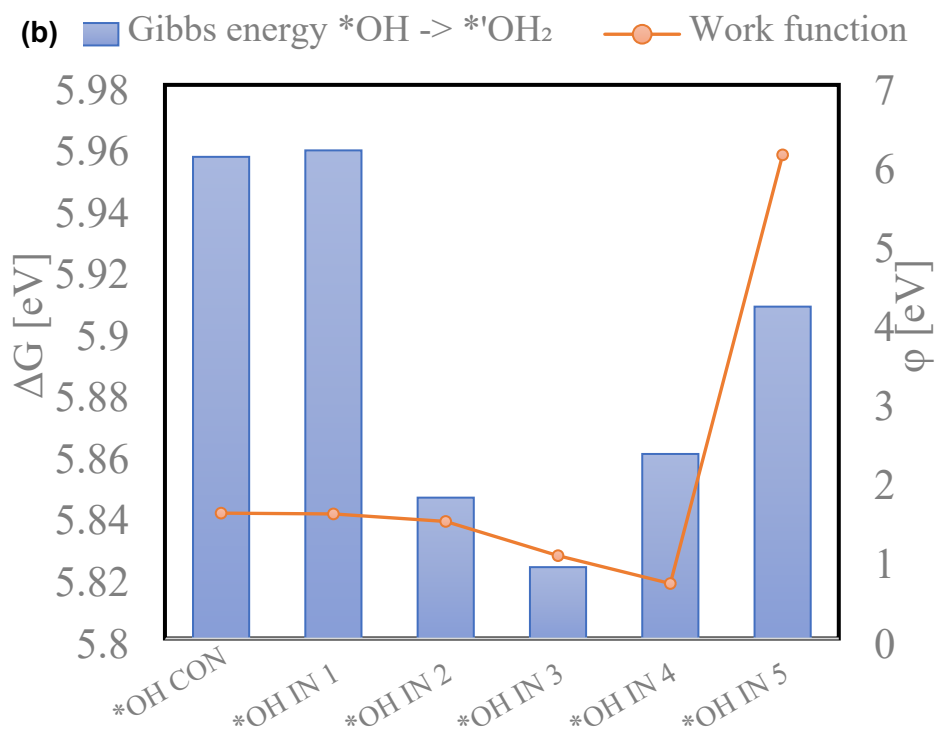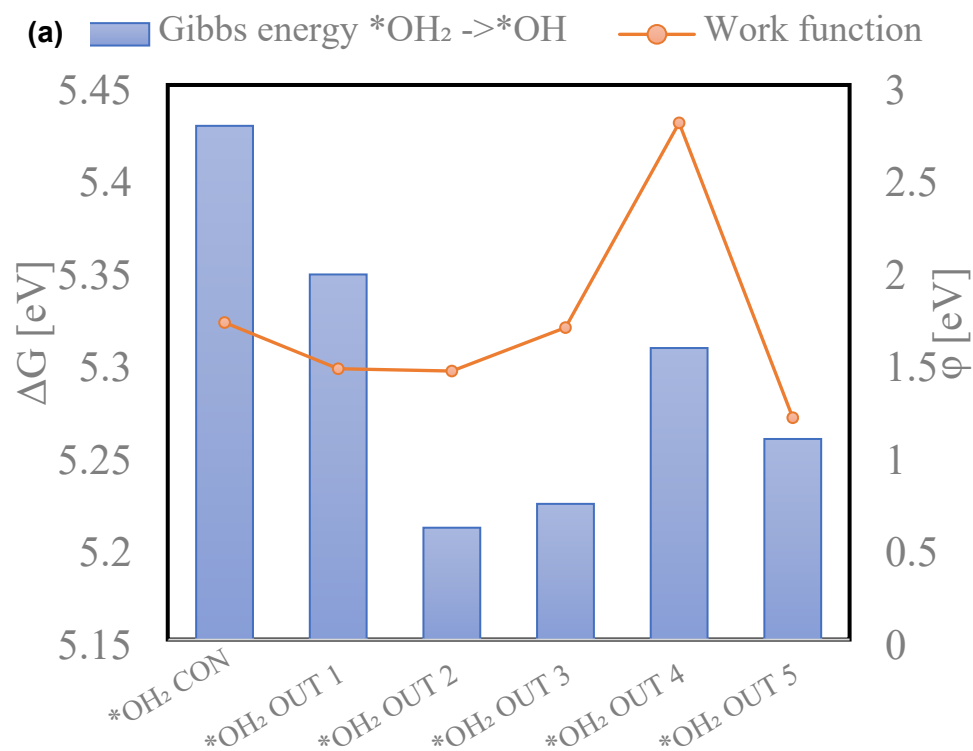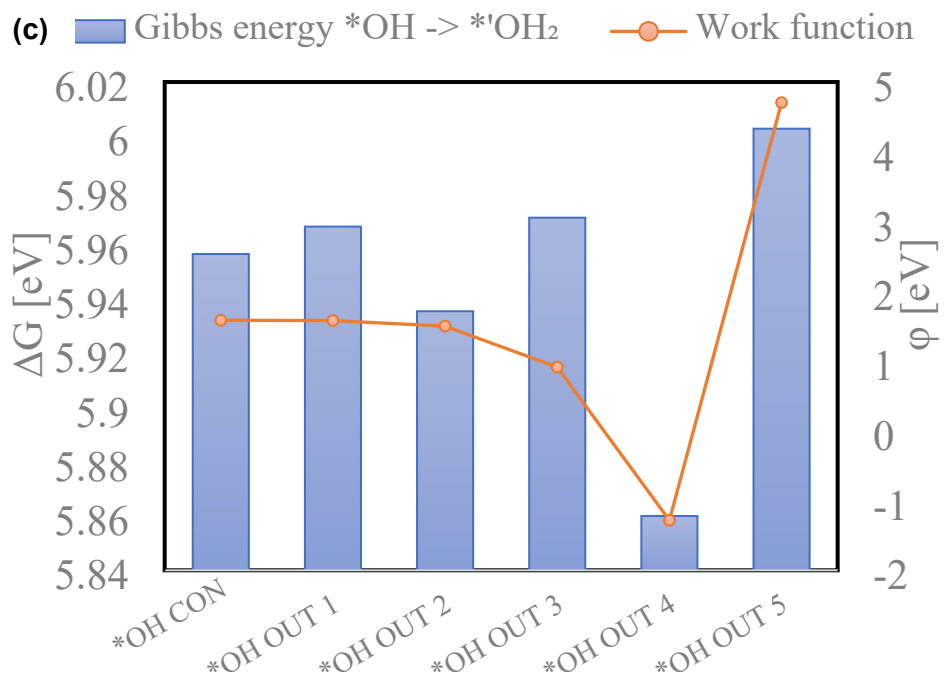
Figure S2. Total Gibbs energy for a reaction to take place and work function for (a) *OH$_2$ OUT (b) *OH IN (C) *OH OUT

**(c)** ▨ Gibbs energy *OH -> *'OH$_2$ ◦— Work function

Magnetism – additional observations

The decreased magnetization means that the charge became more delocalized and as a result a smaller work function is observed since it is easier to extract charge from a delocalized state. As seen in Figure 7, while the layers are sliding relatively to each other, the oxygen (atom number 3) on the left "static" layer is losing its bond with the closest hydrogen adjacent to him from the middle "dynamic" layer. Hence, the oxygen atom detached from the hydrogen atom gains greater localizations of its surrounded electrons. On the other hand, the oxygen atom attached to the hydrogen from the same moving layer (atom number 2) fasten its bond strength so the local magnetization of this oxygen is decreased. Overall, the delocalized bonding at the active site facilitates water oxidation at the transition between IN2 and IN3 that is more reactive.

Table S5. Magnetization of atoms around the active site of NiOOH. The atoms are numbered in Figure S8. The atoms are circled in Figure S8 according to the color representation.

Number	colour representation	atom	A CON	A IN 1	A IN 2	A IN 3	A IN 4
1		Nickel (active site)	1.064	1.056	1.026	1.133	1.148
2		Oxygen (moving layer)	-0.052	-0.052	-0.039	-0.041	-0.027
3		Oxygen (static layer)	0.04	0.043	0.053	-0.058	-0.08
4		Oxygen (static layer)	-0.1	-0.1	-0.088	-0.115	-0.114
5		Oxygen (static layer)	0.073	0.083	0.104	0.099	0.09

Figure S3. Unit cell of the NiOOH surface with atom numbering. Atom 1 is Ni and serves as the active site. Atoms 2 - 5 are oxygens that surrounds the active site. Atom 3 is a part of the static layer. Atoms 1,2,4,5 are parts of the moving layer.
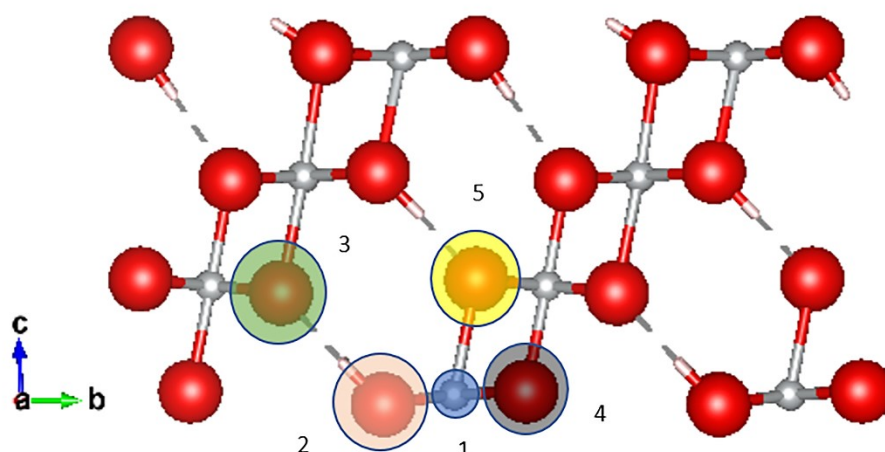
The relaxed geometries of the non-displaced intermediates below are given according to the following order: title, lattice vectors in Cartesian coordinates, atom types and numbers, respectively, and atom locations in fractional coordinates with respect to the lattice vectors. The atom coordinates are given according to the ordering in the atom type row (format of VASP geometrical coordinates files, POSCAR):

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   0.0720454903392915    -0.4803000766864406    27.2717372251130641
  H     O     Ni
  48    72    32
Direct
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  0.1274562390831840    0.7972157131895659    0.7520279191099972
  0.6274562780831837    0.2972157401895646    0.7520279191099972
  0.6274562390831840    0.7972157131895659    0.7520279191099972
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  0.5619153564158026    0.5605879358239358    0.9222265167604859
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    H    O    Ni
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0.7134890420764961    0.4746013781894547    0.7254382123757779
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*'OH$_2$ converged **E$_{tot}$ = -762.49 [eV]**
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0.0000000000            0.0000000000           27.0132007599
H    O    Ni
48    76    32
Direct
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0.131827809           0.802972030           0.763754036
0.631827773           0.302972038           0.763754036
0.631827809           0.802972030           0.763754036
0.216869987           0.426427048           0.849704685
0.216870003           0.926426963           0.849704685
0.716869947           0.426427048           0.849704685
0.716870003           0.926426963           0.849704685
0.053204618           0.076285330           0.897548186
0.053204616           0.576285356           0.897548186
0.553204588           0.076285330           0.897548186
0.553204576           0.576285356           0.897548186
0.135425238           0.223777299           0.968417739
0.135425229           0.723777310           0.968417739
0.635425198           0.223777299           0.968417739
0.635425229           0.723777310           0.968417739
0.382445985           0.314996901           0.753208305
0.382445976           0.814996912           0.753208305
0.882445905           0.314996901           0.753208305
0.882445936           0.814996912           0.753208305
0.462387114           0.413340297           0.842082550
0.462387101           0.913340328           0.842082550
0.962387075           0.413340297           0.842082550
0.962387101           0.913340328           0.842082550
0.317255661           0.089017660           0.903523813
0.317255624           0.589017623           0.903523813
0.817255581           0.089017660           0.903523813
0.817255624           0.589017623           0.903523813
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0.897561957	0.720210075	0.965899857
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0.297023782	0.881888414	0.666772579
0.797023775	0.381888306	0.666772579
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0.776087179	0.987806355	0.635966017
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0.528521875	0.339643129	0.659344968
0.528521831	0.839643121	0.659344968
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0.088357886	0.928531778	0.643313841
0.588357930	0.428531786	0.643313841
0.588357886	0.928531778	0.643313841
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0.563893567	0.574052880	0.736209071
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0.147696927	0.705350016	0.802094756
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0.647696967	0.705350016	0.802094756
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0.232552349	0.862202740	0.873967508
0.732552363	0.362202709	0.873967508
0.732552389	0.862202740	0.873967508
0.073218537	0.493544253	0.941495324
0.073218542	0.993544206	0.941495324
0.573218497	0.493544253	0.941495324
0.573218542	0.993544206	0.941495324
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0.621668108	0.860422906	0.737182120
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0.539734930	0.637406107	0.872157259
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0.900555620	0.709526207	0.801500661
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0.978685253	0.353831328	0.868235266
0.978685279	0.853831359	0.868235266
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0.835527873	0.492876912	0.941832195
0.835527918	0.992876865	0.941832195
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0.364825228	0.876709937	0.729563020
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0.864825228	0.876709937	0.729563020
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0.445447214	0.511829483	0.802046672
0.945447094	0.011829506	0.802046672
0.945447134	0.511829483	0.802046672
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0.295890572	0.648469326	0.877402447
0.795890614	0.148469343	0.877402447
0.795890572	0.648469326	0.877402447
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0.380367165	0.785539762	0.942525919
0.880367209	0.285539770	0.942525919
0.880367165	0.785539762	0.942525919
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0.363570499	0.584435860	0.700761726
0.863570456	0.084435897	0.700761726
0.863570419	0.584435860	0.700761726
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0.235481923	0.937200648	0.650537253
0.735481897	0.437200617	0.650537253
0.735481923	0.937200648	0.650537253
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0.011091956	0.916194734	0.650189367
0.511091881	0.416194742	0.650189367
0.511091917	0.916194734	0.650189367
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0.977909578	0.465617099	0.729506463
0.977909624	0.965617052	0.729506463
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0.049017795	0.606049764	0.803403758
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0.549017795	0.606049764	0.803403758
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0.136167559	0.749364022	0.872379392
0.636167553	0.249363991	0.872379392
0.636167579	0.749364022	0.872379392
0.226043366	0.394706105	0.942931562
0.226043392	0.894706135	0.942931562
0.726043366	0.394706105	0.942931562
0.726043233	0.894706135	0.942931562

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0.388076688          0.749553157          0.871180186
0.888076638          0.249553223          0.871180186
0.888076608          0.749553157          0.871180186
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0.476924923          0.891182071          0.943712557
0.976924976          0.391182040          0.943712557
0.976925003          0.891182071          0.943712557
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0.209393893          0.969393734          0.737024452
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*'OH converged E_{tot} = -741.21 [eV]
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H    O    Ni
44   76   32
Direct
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0.128401624          0.806002983          0.766200463
0.628401593          0.306002972          0.766200463
0.628401624          0.806002983          0.766200463
0.222247441          0.412088946          0.843960229
0.222247408          0.912088976          0.843960229
0.722247381          0.412088946          0.843960229
0.722247408          0.912088976          0.843960229
0.054598279          0.070200255          0.895845262
0.054598311          0.570200242          0.895845262
0.554598274          0.070200255          0.895845262
0.554598391          0.570200242          0.895845262
0.138456126          0.220139475          0.967203916
0.138456137          0.720139487          0.967203916
0.638456106          0.220139475          0.967203916
0.638456137          0.720139487          0.967203916
0.383087733          0.325197137          0.756960627
0.383087719          0.825197168          0.756960627
0.883087693          0.325197137          0.756960627
0.883087719          0.825197168          0.756960627
0.472577153          0.405910692          0.840211225
0.472577189          0.905910685          0.840211225
0.972577153          0.405910692          0.840211225
0.972577269          0.905910685          0.840211225
0.317535009          0.082105832          0.901298884
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0.817535168          0.082105832          0.901298884
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0.769353455	0.888072034	0.659913010
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0.602202131	0.939592372	0.657512972
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0.465384829	0.992273934	0.638918350
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0.965384829	0.992273934	0.638918350
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0.066995994	0.572009809	0.732074548
0.566995908	0.072009778	0.732074548
0.566995974	0.572009809	0.732074548
0.146123663	0.204725352	0.801006899
0.146123709	0.704725383	0.801006899
0.646123663	0.204725352	0.801006899
0.646123689	0.704725383	0.801006899
0.237551460	0.353401314	0.869535654
0.237551445	0.853401267	0.869535654
0.737551400	0.353401314	0.869535654
0.737551445	0.853401267	0.869535654
0.071045691	0.491401826	0.942137645
0.071045657	0.991401780	0.942137645
0.571045691	0.491401826	0.942137645
0.571045657	0.991401780	0.942137645
0.119792335	0.362641296	0.739208923
0.119792361	0.862641327	0.739208923
0.619792335	0.362641296	0.739208923
0.619792361	0.862641327	0.739208923
0.200573690	0.006277300	0.800594830
0.200573696	0.506277331	0.800594830
0.700573690	0.006277300	0.800594830
0.700573636	0.506277331	0.800594830
0.044252057	0.130556234	0.869847247
0.044252053	0.630556226	0.869847247
0.544252037	0.130556234	0.869847247
0.544252073	0.630556226	0.869847247
0.124468370	0.284371556	0.943255441
0.124468376	0.784371510	0.943255441
0.624468410	0.284371556	0.943255441
0.624468376	0.784371510	0.943255441
0.269862388	0.109288773	0.725896205
0.269862392	0.609288736	0.725896205
0.769862548	0.109288773	0.725896205
0.769862431	0.609288736	0.725896205
0.407186182	0.207289298	0.798881809
0.407186187	0.707289252	0.798881809
0.907186142	0.207289298	0.798881809

0.907186267	0.707289252	0.798881809
0.485588936	0.350908999	0.867414801
0.485588892	0.850908991	0.867414801
0.985588856	0.350908999	0.867414801
0.985588892	0.850908991	0.867414801
0.335666652	0.490130936	0.942745580
0.335666678	0.990130966	0.942745580
0.835666652	0.490130936	0.942745580
0.835666678	0.990130966	0.942745580
0.364790719	0.385260962	0.732170080
0.364790675	0.885260954	0.732170080
0.864790719	0.385260962	0.732170080
0.864790675	0.885260954	0.732170080
0.452269046	0.007626294	0.795577212
0.452268999	0.507626300	0.795577212
0.952269006	0.007626294	0.795577212
0.952268959	0.507626300	0.795577212
0.298461710	0.140225739	0.874550306
0.298461719	0.640225760	0.874550306
0.798461650	0.140225739	0.874550306
0.798461679	0.640225760	0.874550306
0.387118139	0.281813827	0.941658640
0.387118095	0.781813819	0.941658640
0.887118059	0.281813827	0.941658640
0.887118095	0.781813819	0.941658640
0.364028552	0.093946068	0.700804444
0.364028576	0.593946108	0.700804444
0.864028631	0.093946068	0.700804444
0.864028576	0.593946108	0.700804444
0.210094620	0.454927478	0.664690207
0.210094636	0.954927392	0.664690207
0.710094620	0.454927478	0.664690207
0.710094596	0.954927392	0.664690207
0.011138000	0.434619990	0.659394111
0.011138016	0.934620020	0.659394111
0.511137990	0.434619990	0.659394111
0.511138016	0.934620020	0.659394111
0.478689382	0.468855568	0.729093124
0.478689368	0.968855598	0.729093124
0.978689422	0.468855568	0.729093124
0.978689448	0.968855598	0.729093124
0.052141051	0.104524237	0.800239601
0.052141082	0.604524248	0.800239601
0.552141051	0.104524237	0.800239601
0.552141082	0.604524248	0.800239601
0.140248163	0.244074245	0.871374146
0.140248174	0.744074179	0.871374146
0.640248163	0.244074245	0.871374146
0.640248293	0.744074179	0.871374146
0.229191269	0.389428619	0.942586924
0.229191275	0.889428572	0.942586924
0.729191229	0.389428619	0.942586924
0.729191275	0.889428572	0.942586924
0.299830242	0.109842586	0.801361775
0.299830256	0.609842588	0.801361775
0.799830142	0.109842586	0.801361775

```
0.799830176            0.609842588            0.801361775
0.392232402            0.245452465            0.869685626
0.392232428            0.745452496            0.869685626
0.892232482            0.245452465            0.869685626
0.892232428            0.745452496            0.869685626
0.479213066            0.388410308            0.943740659
0.479213081            0.888410223            0.943740659
0.979213106            0.388410308            0.943740659
0.979213161            0.888410223            0.943740659
0.209530547            0.471201186            0.733540582
0.209530513            0.971201139            0.733540582
0.709530547            0.471201186            0.733540582
0.709530513            0.971201139            0.733540582
```

Each displacement type was calculated with specific approach:

IN-X: In a specific layer, calculate the vector between two adjacent Ni atoms with different Z values, divide the result into 5 steps (each step describes specific sliding vector, layer is moving in) where at the last step, first Ni atom (closer to the surface) is located in the second Ni atom initial coordinates. all the atoms coordinate from the moving layer are shifted according to the sliding vector of each specific step.

OUT-X: In a specific layer, calculate the vector between two adjacent Ni atoms with different Z values, divide the result into 5 steps (each step describes specific sliding vector, layer is moving out) where at the last step, second Ni atom (farther from surface) is located in the first Ni atom initial coordinates. all the atoms coordinate from the moving layer are shifted according to the sliding vector of each specific step.

90-X: In a specific layer, calculate the vector between two adjacent Ni atoms with same Z values, divide the result into 4 steps (each step describes specific sliding vector, fifth step is identical to first step because of periodicity of the system in VASP calculations). all the atoms coordinate from the moving layer are shifted according to the sliding vector of each specific step.

ROT X°: In a specific layer, calculate the rotation matrix according to the facet axis. all the atoms coordinate from the moving layer are shifted according to the calculations of each specific step.

Examples of each displacement type POSCAR is presented referring to intermediate $*OH_2$:

```
*OH₂ IN 1 Etot = -742.15 [eV]
1.0
11.383055687       0.0000000000        0.0000000000
2.8146468734      11.6314701430        0.0000000000
0.1444123649      -0.9612483604       27.2587363156
H    O    Ni
48    72   32
Direct
```

0.138674746	0.766859307	0.757078840
0.638530403	0.767462526	0.756534318
0.229970948	0.386166617	0.848429891
0.729826537	0.386769775	0.847885369
0.076362522	0.522928956	0.925495526
0.576218085	0.523532134	0.924951004
0.161291913	0.174200752	0.969173176
0.661147591	0.174803894	0.968628584
0.388461055	0.766807365	0.758100222
0.888316609	0.767410496	0.757555630
0.488094976	0.386709849	0.848176173
0.987950651	0.387313001	0.847631581
0.323275222	0.523159864	0.924531452
0.823130777	0.523762995	0.923986860
0.411304209	0.175087553	0.968319308
0.911159756	0.175690711	0.967774785
0.269859976	0.830445804	0.660028079
0.769715467	0.831049023	0.659483557
0.307217616	0.940359749	0.644620732
0.807073252	0.940962887	0.644076210
0.556546650	0.943470905	0.645041544
0.467007655	0.053122995	0.665298791
0.966863222	0.053726075	0.664754199
0.056402248	0.944073949	0.644496881
0.107252162	0.294591830	0.767506490
0.607107882	0.295194968	0.766961967
0.196960027	0.914662981	0.866117487
0.696815624	0.915266113	0.865572895
0.128280967	0.702696967	0.986860701
0.628136520	0.703300186	0.986316179
0.357038480	0.294539684	0.768527871
0.856893951	0.295142815	0.767983279
0.455083997	0.915206111	0.865863768
0.954939779	0.915809166	0.865319246
0.378293176	0.703583861	0.986006973
0.878148689	0.704186993	0.985462381
0.238437361	0.358178204	0.670455728
0.738292966	0.358781383	0.669911206
0.275794968	0.468092027	0.655048381
0.775650677	0.468695205	0.654503859
0.525124097	0.471203306	0.655469193
0.435585034	0.580855278	0.675726440
0.935440702	0.581458456	0.675181918
0.024979602	0.471806432	0.654924531
0.043351516	0.051425340	0.943183122
0.290264341	0.051656125	0.942218977
0.543207170	0.052028533	0.942638529
0.790119795	0.052259324	0.941674455
0.162163118	0.177092609	0.796795794
0.662018712	0.177695751	0.796251202
0.245481797	0.325191585	0.875265977
0.745337449	0.325794743	0.874721455
0.086839782	0.475684358	0.955285621
0.586695408	0.476287536	0.954741099
0.123533670	0.827395534	0.730815335
0.623389287	0.827998583	0.730270743

0.059696267	0.104123705	0.868846325
0.559551954	0.104726852	0.868301733
0.144152311	0.244416862	0.950707002
0.644007965	0.245020010	0.950162480
0.411892854	0.177011153	0.797555410
0.911748490	0.177614295	0.797010818
0.503551492	0.325357554	0.875003792
0.003407008	0.325960712	0.874459270
0.336652273	0.475193954	0.954108272
0.836507817	0.475797126	0.953563680
0.373616923	0.826225674	0.731272533
0.873472517	0.826828811	0.730728010
0.299589889	0.104417365	0.868586449
0.799445460	0.105020513	0.868041927
0.394082892	0.245084550	0.949746077
0.893938523	0.245687708	0.949201554
0.235707041	0.910653289	0.652158607
0.735562467	0.911256426	0.651614085
0.470692632	0.973959273	0.653996212
0.970548164	0.974562493	0.653451690
0.320828022	0.040040012	0.740869264
0.462482322	0.969572279	0.811926052
0.569426378	0.040958404	0.740568804
0.820683580	0.040643213	0.740324742
0.962337875	0.970175417	0.811381530
0.069570790	0.040355203	0.741113326
0.212107532	0.968603582	0.811230880
0.711963042	0.969206720	0.810686358
0.038148162	0.568087637	0.751541045
0.538003957	0.568690728	0.750996453
0.129152221	0.705588963	0.814483390
0.629007878	0.706192100	0.813938867
0.212470810	0.853687791	0.892953643
0.712326491	0.854290923	0.892409050
0.092111074	0.355127771	0.741242985
0.591966702	0.355730943	0.740698392
0.180684958	0.496335983	0.821658530
0.680540448	0.496939121	0.821114007
0.026685390	0.632620023	0.886533920
0.526540923	0.633223155	0.885989328
0.111141378	0.772913022	0.968394597
0.610996997	0.773516235	0.967850005
0.289405379	0.567772464	0.751296983
0.789261070	0.568375555	0.750752391
0.378881986	0.705507476	0.815243006
0.878737676	0.706110567	0.814698414
0.470540623	0.853853877	0.892691388
0.970396176	0.854457014	0.892146865
0.342194303	0.353958177	0.741700182
0.842049819	0.354561294	0.741155659
0.431059832	0.497304598	0.822353702
0.930915458	0.497907777	0.821809179
0.266578866	0.632913720	0.886274044
0.766434557	0.633516810	0.885729452
0.361072002	0.773580792	0.967433672
0.860927450	0.774184011	0.966889150

```
0.204284403          0.438385608          0.662586256
0.704139883          0.438988786          0.662041734
0.439270047          0.501691633          0.664423861
0.939125442          0.502294730          0.663879339
0.053828913          0.004180671          0.972973216
0.303641250          0.003690364          0.971795867
0.553684509          0.004783869          0.972428624
0.803496923          0.004293440          0.971251275
0.471984897          0.932833241          0.738027980
0.971840198          0.933436378          0.737483458
0.063481458          0.072660446          0.801243635
0.563337110          0.073263604          0.800699113
0.152267158          0.214064868          0.871340198
0.652122766          0.214668036          0.870795676
0.239341011          0.363144630          0.948689919
0.739196616          0.363747809          0.948145397
0.312489281          0.072641566          0.801056040
0.812344852          0.073244713          0.800511518
0.402286135          0.213970987          0.871875554
0.902141899          0.214574118          0.871330961
0.489904972          0.363790814          0.948280093
0.989760479          0.364393966          0.947735501
0.221962843          0.933503699          0.737976621
0.721818210          0.934106913          0.737432029
0.440562177          0.460565641          0.748455630
0.940417761          0.461168820          0.747911107
0.030470581          0.601156718          0.818931230
0.530326143          0.601759814          0.818386708
0.119256187          0.742561181          0.889027793
0.619111868          0.743164313          0.888483201
0.206330016          0.891640872          0.966377514
0.706185820          0.892244009          0.965832992
0.279478408          0.601137818          0.818743705
0.779334141          0.601740909          0.818199113
0.369275184          0.742467474          0.889563149
0.869130948          0.743070606          0.889018557
0.456893984          0.892286947          0.965967618
0.956749452          0.892890085          0.965423096
0.190540123          0.461236182          0.748404270
0.690395688          0.461839354          0.747859678
```

*OH₂ out 1 Eₜₒₜ = -742.24 [eV]

```
1.0
11.3830556870       0.0000000000          0.0000000000
2.8146468734       11.6314701430          0.0000000000
0.1444123649-       0.9612483604         27.2587363156
H    O    Ni
48   72   32
Direct
0.138674746          0.766859307          0.757078840
0.638530403          0.767462526          0.756534318
0.229970948          0.386166617          0.848429891
0.729826537          0.386769775          0.847885369
0.076362522          0.522928956          0.925495526
```

0.576218085	0.523532134	0.924951004
0.161291913	0.174200752	0.969173176
0.661147591	0.174803894	0.968628584
0.388461055	0.766807365	0.758100222
0.888316609	0.767410496	0.757555630
0.488094976	0.386709849	0.848176173
0.987950651	0.387313001	0.847631581
0.323275222	0.523159864	0.924531452
0.823130777	0.523762995	0.923986860
0.411304209	0.175087553	0.968319308
0.911159756	0.175690711	0.967774785
0.269859976	0.830445804	0.660028079
0.769715467	0.831049023	0.659483557
0.307217616	0.940359749	0.644620732
0.807073252	0.940962887	0.644076210
0.556546650	0.943470905	0.645041544
0.467007655	0.053122995	0.665298791
0.966863222	0.053726075	0.664754199
0.056402248	0.944073949	0.644496881
0.171685688	0.238363106	0.739391245
0.671541466	0.238966264	0.738846723
0.261393532	0.858434257	0.838002242
0.761249274	0.859037476	0.837457720
0.192714491	0.646468249	0.958745527
0.692570109	0.647071462	0.958200935
0.421471948	0.238310939	0.740412627
0.921327456	0.238914091	0.739868034
0.519517564	0.858977304	0.837748524
0.019373308	0.859580518	0.837203932
0.442726757	0.647355172	0.957891658
0.942582435	0.647958310	0.957347136
0.302870929	0.301949480	0.642340484
0.802726478	0.302552632	0.641795892
0.340228504	0.411863344	0.626933137
0.840084099	0.412466481	0.626388614
0.589557604	0.414974576	0.627353878
0.500018571	0.524626595	0.647611196
0.999874293	0.525229726	0.647066604
0.089413178	0.415577713	0.626809356
0.107785076	0.995196637	0.915067877
0.354697879	0.995427381	0.914103803
0.607640670	0.995799774	0.914523355
0.854553371	0.996030595	0.913559211
0.162163118	0.177092609	0.796795794
0.662018712	0.177695751	0.796251202
0.245481797	0.325191585	0.875265977
0.745337449	0.325794743	0.874721455
0.086839782	0.475684358	0.955285621
0.586695408	0.476287536	0.954741099
0.123533670	0.827395534	0.730815335
0.623389287	0.827998583	0.730270743
0.059696267	0.104123705	0.868846325
0.559551954	0.104726852	0.868301733
0.144152311	0.244416862	0.950707002
0.644007965	0.245020010	0.950162480
0.411892854	0.177011153	0.797555410

0.911748490	0.177614295	0.797010818
0.503551492	0.325357554	0.875003792
0.003407008	0.325960712	0.874459270
0.336652273	0.475193954	0.954108272
0.836507817	0.475797126	0.953563680
0.373616923	0.826225674	0.731272533
0.873472517	0.826828811	0.730728010
0.299589889	0.104417365	0.868586449
0.799445460	0.105020513	0.868041927
0.394082892	0.245084550	0.949746077
0.893938523	0.245687708	0.949201554
0.235707041	0.910653289	0.652158607
0.735562467	0.911256426	0.651614085
0.470692632	0.973959273	0.653996212
0.970548164	0.974562493	0.653451690
0.320828022	0.040040012	0.740869264
0.462482322	0.969572279	0.811926052
0.569426378	0.040958404	0.740568804
0.820683580	0.040643213	0.740324742
0.962337875	0.970175417	0.811381530
0.069570790	0.040355203	0.741113326
0.212107532	0.968603582	0.811230880
0.711963042	0.969206720	0.810686358
0.102581698	0.511858872	0.723425801
0.602437410	0.512462045	0.722881209
0.193585757	0.649360198	0.786368145
0.693441302	0.649963370	0.785823553
0.276904359	0.797459061	0.864838328
0.776759996	0.798062199	0.864293806
0.156544590	0.298899087	0.713127740
0.656400286	0.299502240	0.712583148
0.245118484	0.440107259	0.793543285
0.744974029	0.440710432	0.792998693
0.091118908	0.576391334	0.858418606
0.590974470	0.576994431	0.857874084
0.175574863	0.716684380	0.940279353
0.675430502	0.717287511	0.939734761
0.353838884	0.511543740	0.723181739
0.853694649	0.512146872	0.722637147
0.443315449	0.649278752	0.787127761
0.943171087	0.649881884	0.786583169
0.534974045	0.797625153	0.864576143
0.034829618	0.798228290	0.864031621
0.406627850	0.297729453	0.713584937
0.906483402	0.298332591	0.713040415
0.495493347	0.441075833	0.794238457
0.995349140	0.441679011	0.793693935
0.331012413	0.576684995	0.858158800
0.830868049	0.577288133	0.857614278
0.425505559	0.717352027	0.939318427
0.925360965	0.717955246	0.938773905
0.268717940	0.382156843	0.634471012
0.768573482	0.382760021	0.633926489
0.503703552	0.445462909	0.636308617
0.003559117	0.446066000	0.635764024
0.118262450	0.947951998	0.944857972

0.368074763	0.947461635	0.943680623
0.618118002	0.948555135	0.944313450
0.867930486	0.948064767	0.943136031
0.471984897	0.932833241	0.738027980
0.971840198	0.933436378	0.737483458
0.063481458	0.072660446	0.801243635
0.563337110	0.073263604	0.800699113
0.152267158	0.214064868	0.871340198
0.652122766	0.214668036	0.870795676
0.239341011	0.363144630	0.948689919
0.739196616	0.363747809	0.948145397
0.312489281	0.072641566	0.801056040
0.812344852	0.073244713	0.800511518
0.402286135	0.213970987	0.871875554
0.902141899	0.214574118	0.871330961
0.489904972	0.363790814	0.948280093
0.989760479	0.364393966	0.947735501
0.221962843	0.933503699	0.737976621
0.721818210	0.934106913	0.737432029
0.504995766	0.404336917	0.720340385
0.004851352	0.404940090	0.719795793
0.094904107	0.544927994	0.790815986
0.594759722	0.545531131	0.790271464
0.183689682	0.686332498	0.860912549
0.683545360	0.686935635	0.860368026
0.270763563	0.835412147	0.938262270
0.770619221	0.836015367	0.937717748
0.343911999	0.544909088	0.790628391
0.843767541	0.545512266	0.790083869
0.433708835	0.686238668	0.861447904
0.933564463	0.686841841	0.860903312
0.521327550	0.836058311	0.937852444
0.021183042	0.836661442	0.937307852
0.254973681	0.405007499	0.720289026
0.754829277	0.405610630	0.719744434

*OH₂ 901 **E_tot = -742.36 [eV]**
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11.3830556870	0.0000000000	0.0000000000
2.8146468734	11.6314701430	0.0000000000
0.1444123649	-0.9612483604	27.2587363156

H   O   Ni
48   72   32
Direct
0.138674746	0.766859307	0.757078840
0.638530403	0.767462526	0.756534318
0.229970948	0.386166617	0.848429891
0.729826537	0.386769775	0.847885369
0.076362522	0.522928956	0.925495526
0.576218085	0.523532134	0.924951004
0.161291913	0.174200752	0.969173176
0.661147591	0.174803894	0.968628584
0.388461055	0.766807365	0.758100222
0.888316609	0.767410496	0.757555630

0.488094976	0.386709849	0.848176173
0.987950651	0.387313001	0.847631581
0.323275222	0.523159864	0.924531452
0.823130777	0.523762995	0.923986860
0.411304209	0.175087553	0.968319308
0.911159756	0.175690711	0.967774785
0.269859976	0.830445804	0.660028079
0.769715467	0.831049023	0.659483557
0.307217616	0.940359749	0.644620732
0.807073252	0.940962887	0.644076210
0.556546650	0.943470905	0.645041544
0.467007655	0.053122995	0.665298791
0.966863222	0.053726075	0.664754199
0.056402248	0.944073949	0.644496881
0.089667351	0.266481355	0.753486477
0.589523084	0.267084528	0.752941885
0.179375187	0.886552542	0.852097405
0.679230761	0.887155761	0.851552882
0.110696135	0.674586492	0.972840689
0.610551698	0.675189670	0.972296167
0.339453650	0.266429203	0.754507789
0.839309202	0.267032340	0.753963267
0.437499217	0.887095595	0.851843756
0.937354939	0.887698726	0.851299164
0.360708459	0.675473427	0.971986961
0.860563932	0.676076553	0.971442298
0.220852528	0.330067729	0.656435716
0.720708225	0.330670881	0.655891124
0.258210115	0.439981634	0.641028369
0.758065741	0.440584812	0.640483847
0.507539215	0.443092866	0.641449111
0.418000191	0.552744844	0.661706428
0.917855872	0.553347975	0.661161836
0.007394801	0.443695998	0.640904518
0.025766693	0.023314952	0.929163109
0.272679486	0.023545742	0.928198965
0.525622302	0.023918033	0.928618517
0.772534940	0.024148941	0.927654443
0.162163118	0.177092609	0.796795794
0.662018712	0.177695751	0.796251202
0.245481797	0.325191585	0.875265977
0.745337449	0.325794743	0.874721455
0.086839782	0.475684358	0.955285621
0.586695408	0.476287536	0.954741099
0.123533670	0.827395534	0.730815335
0.623389287	0.827998583	0.730270743
0.059696267	0.104123705	0.868846325
0.559551954	0.104726852	0.868301733
0.144152311	0.244416862	0.950707002
0.644007965	0.245020010	0.950162480
0.411892854	0.177011153	0.797555410
0.911748490	0.177614295	0.797010818
0.503551492	0.325357554	0.875003792
0.003407008	0.325960712	0.874459270
0.336652273	0.475193954	0.954108272
0.836507817	0.475797126	0.953563680

0.373616923	0.826225674	0.731272533
0.873472517	0.826828811	0.730728010
0.299589889	0.104417365	0.868586449
0.799445460	0.105020513	0.868041927
0.394082892	0.245084550	0.949746077
0.893938523	0.245687708	0.949201554
0.235707041	0.910653289	0.652158607
0.735562467	0.911256426	0.651614085
0.470692632	0.973959273	0.653996212
0.970548164	0.974562493	0.653451690
0.320828022	0.040040012	0.740869264
0.462482322	0.969572279	0.811926052
0.569426378	0.040958404	0.740568804
0.820683580	0.040643213	0.740324742
0.962337875	0.970175417	0.811381530
0.069570790	0.040355203	0.741113326
0.212107532	0.968603582	0.811230880
0.711963042	0.969206720	0.810686358
0.020563363	0.539977157	0.737520963
0.520419114	0.540580294	0.736976441
0.111567389	0.677478488	0.800463377
0.611423048	0.678081620	0.799918785
0.194886054	0.825577351	0.878933560
0.694741734	0.826180483	0.878388968
0.074526276	0.327017331	0.727222902
0.574381860	0.327620509	0.726678380
0.163100178	0.468225467	0.807638517
0.662955628	0.468828599	0.807093925
0.009100560	0.604509543	0.872513838
0.508956081	0.605112721	0.871969316
0.093556518	0.744802664	0.954374515
0.593412134	0.745405883	0.953829993
0.271820549	0.539661984	0.737276901
0.771676227	0.540265121	0.736732379
0.361297153	0.677397001	0.801222993
0.861152750	0.678000133	0.800678401
0.452955781	0.825743443	0.878671375
0.952811336	0.826346575	0.878126783
0.324609466	0.325847723	0.727680169
0.824465065	0.326450840	0.727135647
0.413475041	0.469194123	0.808333689
0.913330544	0.469797296	0.807789097
0.248994036	0.604803239	0.872253962
0.748849714	0.605406376	0.871709440
0.343487191	0.745470399	0.953413660
0.843342630	0.746073489	0.952869067
0.186699603	0.410275174	0.648566244
0.686555053	0.410878305	0.648021652
0.421685215	0.473581158	0.650403849
0.921540686	0.474184290	0.649859257
0.036244081	0.976070288	0.958953204
0.286056460	0.975579919	0.957775785
0.536099573	0.976673420	0.958408612
0.785912075	0.976182975	0.957231263
0.471984897	0.932833241	0.738027980
0.971840198	0.933436378	0.737483458

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0.063481458          0.072660446          0.801243635
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0.152267158          0.214064868          0.871340198
0.652122766          0.214668036          0.870795676
0.239341011          0.363144630          0.948689919
0.739196616          0.363747809          0.948145397
0.312489281          0.072641566          0.801056040
0.812344852          0.073244713          0.800511518
0.402286135          0.213970987          0.871875554
0.902141899          0.214574118          0.871330961
0.489904972          0.363790814          0.948280093
0.989760479          0.364393966          0.947735501
0.221962843          0.933503699          0.737976621
0.721818210          0.934106913          0.737432029
0.422977428          0.432455166          0.734435617
0.922832941          0.433058298          0.733891025
0.012885779          0.573046161          0.804911218
0.512741345          0.573649375          0.804366626
0.101671337          0.714450782          0.875007711
0.601527015          0.715053920          0.874463189
0.188745237          0.863530520          0.952357502
0.688600792          0.864133651          0.951812910
0.261893576          0.573027343          0.804723693
0.761749300          0.573630469          0.804179031
0.351690458          0.714356911          0.875543067
0.851546210          0.714960090          0.874998544
0.439309246          0.864176595          0.951947606
0.939164589          0.864779733          0.951403084
0.172955315          0.433125783          0.734384188
0.672810678          0.433728920          0.733839666
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*OH₂ 2 degrees E_tot = -741.82 [eV]

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1.0
  11.383055687          0.0000000000          0.0000000000
   2.8146468734         11.6314701430          0.0000000000
   0.1444123649         -0.9612483604         27.2587363156
  H    O    Ni
  48   72   32
Direct
0.138674746          0.766859307          0.757078840
0.638530403          0.767462526          0.756534318
0.229970948          0.386166617          0.848429891
0.729826537          0.386769775          0.847885369
0.076362522          0.522928956          0.925495526
0.576218085          0.523532134          0.924951004
0.161291913          0.174200752          0.969173176
0.661147591          0.174803894          0.968628584
0.388461055          0.766807365          0.758100222
0.888316609          0.767410496          0.757555630
0.488094976          0.386709849          0.848176173
0.987950651          0.387313001          0.847631581
0.323275222          0.523159864          0.924531452
0.823130777          0.523762995          0.923986860
0.411304209          0.175087553          0.968319308
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0.911159756	0.175690711	0.967774785
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0.769715467	0.831049023	0.659483557
0.307217616	0.940359749	0.644620732
0.807073252	0.940962887	0.644076210
0.556546650	0.943470905	0.645041544
0.467007655	0.053122995	0.665298791
0.966863222	0.053726075	0.664754199
0.056402248	0.944073949	0.644496881
0.157583973	0.254393319	0.748271393
0.654045596	0.267289727	0.752969874
0.224610285	0.880190810	0.849358420
0.721071741	0.893087218	0.854056901
0.154996747	0.665235691	0.968829683
0.651458243	0.678132018	0.973528164
0.405608542	0.260481424	0.751911687
0.902069940	0.273377894	0.756610168
0.480973903	0.887083358	0.851812758
0.977435421	0.899979849	0.856511239
0.403329645	0.672274952	0.970599835
0.899790967	0.685171396	0.975298246
0.291818899	0.321633331	0.652772331
0.788280436	0.334529745	0.657470882
0.326914799	0.433110516	0.638034686
0.823376307	0.446006883	0.642733167
0.574436561	0.442369507	0.641077629
0.481442321	0.550440727	0.660667064
0.977904050	0.563337048	0.665365474
0.070897952	0.455265834	0.645776110
0.063977525	0.013918401	0.925142308
0.309255719	0.020221711	0.926768037
0.560439072	0.026814815	0.929840858
0.805717138	0.033118012	0.931466518
0.162163118	0.177092609	0.796795794
0.662018712	0.177695751	0.796251202
0.245481797	0.325191585	0.875265977
0.745337449	0.325794743	0.874721455
0.086839782	0.475684358	0.955285621
0.586695408	0.476287536	0.954741099
0.123533670	0.827395534	0.730815335
0.623389287	0.827998583	0.730270743
0.059696267	0.104123705	0.868846325
0.559551954	0.104726852	0.868301733
0.144152311	0.244416862	0.950707002
0.644007965	0.245020010	0.950162480
0.411892854	0.177011153	0.797555410
0.911748490	0.177614295	0.797010818
0.503551492	0.325357554	0.875003792
0.003407008	0.325960712	0.874459270
0.336652273	0.475193954	0.954108272
0.836507817	0.475797126	0.953563680
0.373616923	0.826225674	0.731272533
0.873472517	0.826828811	0.730728010
0.299589889	0.104417365	0.868586449
0.799445460	0.105020513	0.868041927
0.394082892	0.245084550	0.949746077

0.893938523	0.245687708	0.949201554
0.235707041	0.910653289	0.652158607
0.735562467	0.911256426	0.651614085
0.470692632	0.973959273	0.653996212
0.970548164	0.974562493	0.653451690
0.320828022	0.040040012	0.740869264
0.462482322	0.969572279	0.811926052
0.569426378	0.040958404	0.740568804
0.820683580	0.040643213	0.740324742
0.962337875	0.970175417	0.811381530
0.069570790	0.040355203	0.741113326
0.212107532	0.968603582	0.811230880
0.711963042	0.969206720	0.810686358
0.082661518	0.527780339	0.732268934
0.579123163	0.540676660	0.736967345
0.165771408	0.668274027	0.796498833
0.662232823	0.681170348	0.801197244
0.240069191	0.819227784	0.876199894
0.736530754	0.832124269	0.880898305
0.142470667	0.314923177	0.722005229
0.638932165	0.327819668	0.726703710
0.222056952	0.459074401	0.803689087
0.718518386	0.471970892	0.808387568
0.061754559	0.592319032	0.867279582
0.558215974	0.605215435	0.871977993
0.137191495	0.735447583	0.950362810
0.633652930	0.748343991	0.955061291
0.332227258	0.533640902	0.734658688
0.828688879	0.546537316	0.739357239
0.413755776	0.674331408	0.799876732
0.910217231	0.687227816	0.804575213
0.496389314	0.825739888	0.878644226
0.992850771	0.838636290	0.883342637
0.390852287	0.319895141	0.725081759
0.887313752	0.332791509	0.729780239
0.470658149	0.466203859	0.807011988
0.967119616	0.479100391	0.811710469
0.300018970	0.598512442	0.869535969
0.796480603	0.611408810	0.874234450
0.385455299	0.742264622	0.952024505
0.881916744	0.755161072	0.956722986
0.256239025	0.401469474	0.644747031
0.752700522	0.414365883	0.649445512
0.487845182	0.470917473	0.649206768
0.984306595	0.483813881	0.653905248
0.073904098	0.966639500	0.954918828
0.322093389	0.972288960	0.956359901
0.570365469	0.979535909	0.959617308
0.818554888	0.985185532	0.961058382
0.471984897	0.932833241	0.738027980
0.971840198	0.933436378	0.737483458
0.063481458	0.072660446	0.801243635
0.563337110	0.073263604	0.800699113
0.152267158	0.214064868	0.871340198
0.652122766	0.214668036	0.870795676
0.239341011	0.363144630	0.948689919

0.739196616	0.363747809	0.948145397
0.312489281	0.072641566	0.801056040
0.812344852	0.073244713	0.800511518
0.402286135	0.213970987	0.871875554
0.902141899	0.214574118	0.871330961
0.489904972	0.363790814	0.948280093
0.989760479	0.364393966	0.947735501
0.221962843	0.933503699	0.737976621
0.721818210	0.934106913	0.737432029
0.485345659	0.429532763	0.733134418
0.981807072	0.442429172	0.737832899
0.070260132	0.560809360	0.799649603
0.566721544	0.573705856	0.804348153
0.150649288	0.705169750	0.871018956
0.647110869	0.718066158	0.875717437
0.228715762	0.857202995	0.949641538
0.725177281	0.870099485	0.954340019
0.317580775	0.566912568	0.802073013
0.814042322	0.579808942	0.806771564
0.398934237	0.711222052	0.874175674
0.895396040	0.724118414	0.878874084
0.477577229	0.864013636	0.951860771
0.974038537	0.876909963	0.956559251
0.237014306	0.424060321	0.730463096
0.733475845	0.436956729	0.735161577

[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.