Electronic Supplementary Information

Dy_2NiRuO_6 perovskite with high activity and durability for the oxygen evolution reaction in acidic electrolyte

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S1. Crystal structure of R_2NiRuO_6

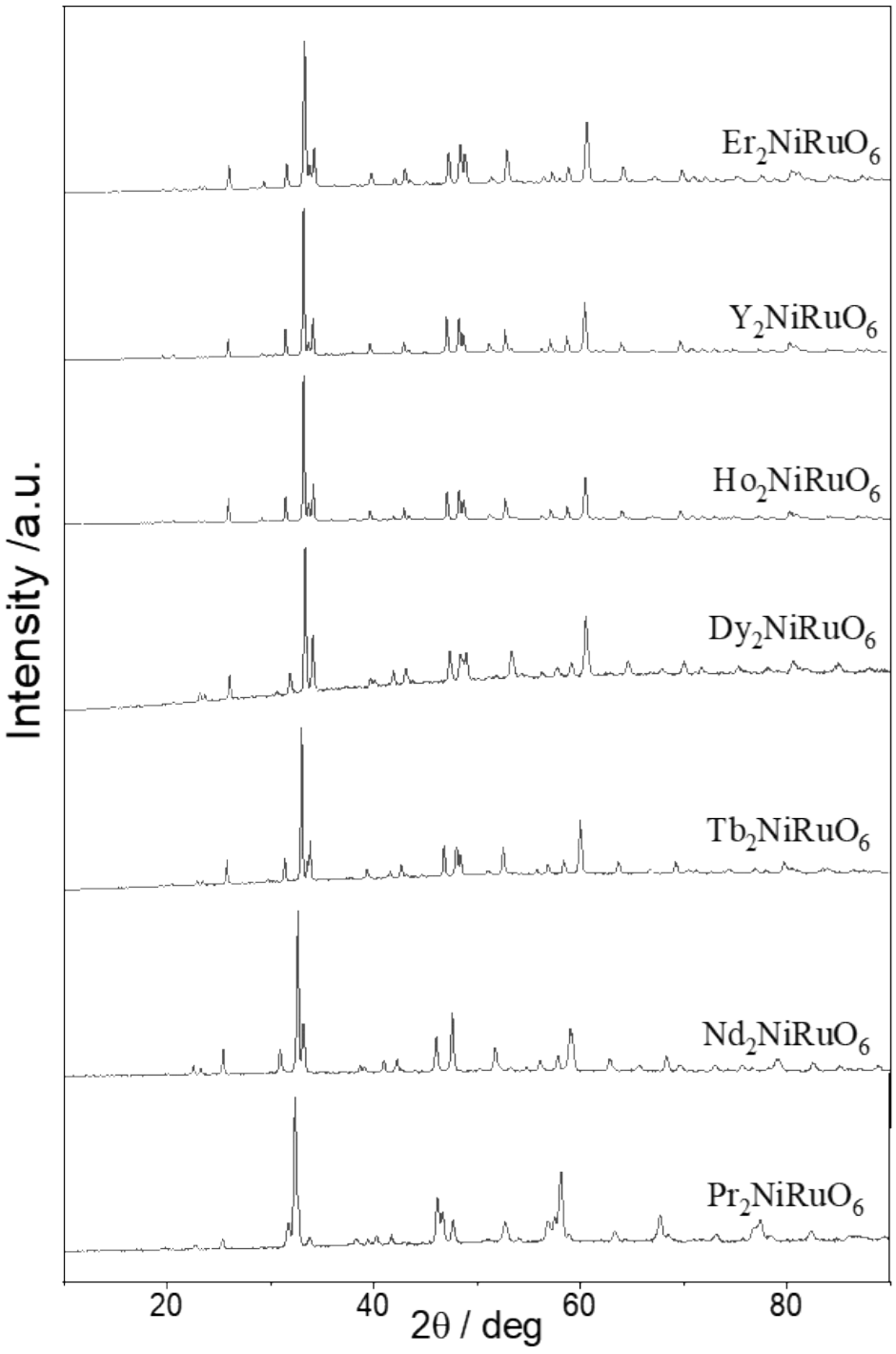


Figure S1. X-ray diffractograms for as prepared R_2NiRuO_6 initial catalysts.

Table S1. Cell parameters and volume for R_2NiRuO_6 from XRD Rietveld refinements.

Oxide	Cell Parameters (Å)	Volume (Å^3)
Dy_2NiRuO_6	a = 5.27718(8) b = 5.6931(1) c = 7.5671(1)	227.343(6)
	β = 89.963(3)	
Er_2NiRuO_6	a = 5.2412(3) b = 5.6718(3) c = 7.5349(4)	223.991(2)
	β = 90.097(6)	
Ho_2NiRuO_6	a = 5.2560(2) b = 5.6872(2) c = 7.5475(3)	225.67(1)
	β = 89.931(5)	
Nd_2NiRuO_6	a = 5.3929(3) b = 5.7826(3) c = 7.6483(5)	238.51(3)
	β = 90.080(9)	
Pr_2NiRuO_6	a = 5.4841(5) b = 5.6462(5) c = 7.7867(7)	241.11(4)
	β = 89.91(1)	
Tb_2NiRuO_6	a = 5.2992(2) b = 5.7047(2) c = 7.5906(3)	229.47(2)
	β = 90.070(5)	
Y_2NiRuO_6	a = 5.2577(2) b = 5.6876(2) c = 7.5457(2)	225.61(1)
	β = 89.921(4)	

S2. Additional electrochemical results

Table S2. Ru-containing oxides (without Ir) reported as electrocatalysts for the OER in acid. The current densities shown are the highest values reported. The values are reported for the initial cycle, after 10 cycles (*) or after 30 cycles (**).

Catalyst	E-iR / V @ 10 mA·cm^{-2}	Tafel slope / mV dec^{-1}	Durability test
Perovskites			
Dy_2NiRuO_6 (this work)	1.507**	55.8	500 cycles (1.1-1.7 V@ 10 mV s^{-1}) decrease 35% activity.
Er_2NiRuO_6 (this work)	1.624**	~170	60 cycles (1.1-1.7 V @ 10 mV s^{-1}) decrease 28% activity
Ho_2NiRuO_6 (this work)	1.647	~138	30 cycles (1.1-1.7 V @ 10 mV s^{-1}) decrease 26% activity
Tb_2NiRuO_6 (this work)	1.591	~128	30 cycles (1.1-1.7 V @ 10 mV s^{-1}) decrease 46% activity
Y_2NiRuO_6 (this work)	1.604**	~159	500 cycles (1.1-1.7 V @ 10 mV s^{-1}) decrease 97% activity
$Sr_{1-x}Na_xRuO_3$ [1]	1.39	40	20 cycles (1.1-1.5 V @ 10 mV s^{-1}) decrease 15% activity
$Sr_{1-x}K_xRuO_3$ [2]	1.38	59	20 cycles (1.1-1.5 V @ 10 mV s^{-1}) decrease 25% activity
$SrRuO_3$ [3]		51.5	Loss of activity after first cycle
$CaCu_3Ru_4O_{12}$ [4]	1.401	40	Stable 24 h @ 10 mAcm^{-2}
Pyrochlores			
Y_2RuMnO_7 [5]	1.49	48	Stable 45 h @ 10 mAcm^{-2}
Dy_2RuMnO_7 [5]	1.51	47	Stable 25 h @ 10 mAcm^{-2}
Tb_2RuMnO_7 [5]	1.54	56	Stable 15 h @ 10 mAcm^{-2}
$Y_{1.7}Sr_{0.3}Ru_2O_7$ [6]	1.494	44.8	-
$Y_{1.85}Zn_{0.15}Ru_2O_{7-\delta}$ [7]	1.521	36.9	-
$Y_2[Ru_{1.6}Y_{0.4}]O_{7-\delta}$ [8]	1.48	37	-
$Y_{1.8}Fe_{0.2}Ru_2O_{7-\delta}$ [9]	1.625*	52-63	-
$Y_{1.8}Cu_{0.2}Ru_2O_{7-\delta}$ [9]	1.58*	52-63	Stable 6 h @ 1 mA cm$^{-2}_{geo}$
$Y_{1.8}Ni_{0.2}Ru_2O_{7-\delta}$ [9]		52-63	-
$Y_{1.8}Co_{0.2}Ru_2O_{7-\delta}$ [9]		52-63	-
$Y_{2x}Ba_xRu_2O_{7-\delta}$ [10]	1.508	40.8	1500 cycles bt. 1.4-1.6 V
$Y_2Ru_2O_7$ [11]	1.561(5) *	40	Stable 1 h @ 1.56 V

$Nd_2Ru_2O_7$ [11]	1.576(9)*	41	Stable 1 h @ 1.56 V
$Gd_2Ru_2O_7$ [11]	1.590(7)	47	Stable 1 h @ 1.56 V
$Bi_2Ru_2O_7$ [11]	1.588(7) *	48	Stable 1 h @ 1.56 V
$Y_2Ru_2O_{7-\delta}$ [12]	1.55	55	Almost stable after 10000 cycles (1.35-1.6 V @ 100 mV s^{-1})
Ru and Ru-based Simple Oxides			
$Cr_{0.6}Ru_{0.4}O_2$ [13]	1.405	58	10 h @10 $mAcm^{-2}$
$W_{0.2}Er_{0.1}Ru_{0.7}O_{2-\delta}$ [14]	1.43	66.8	500 h @10 $mAcm^{-2}$
Ru-MnO_2 [15]	1.391	29.4	Almost stable 200 h @ 10$mAcm^{-2}$
Cu-doped RuO_2 [16]	1.418	43.96	Stable 8 h @ 10$mAcm^{-2}$
Co-doped RuO_2 [17]	1.43		-
Co-RuO_2/Ni-RuO_2 [17]	1.537	58.2	-
RuO_2 [11]	1.626(14)*	77	Stable 1 h @ 1.56 V
RuO_2 NSs [18]	1.429		6 h @ 1 mA cm^{-2} to 10 mA cm^{-2}
Ru–Pt_3Cu [19]	1.45		Almost stable 28 h @ 10 mA cm^{-2}

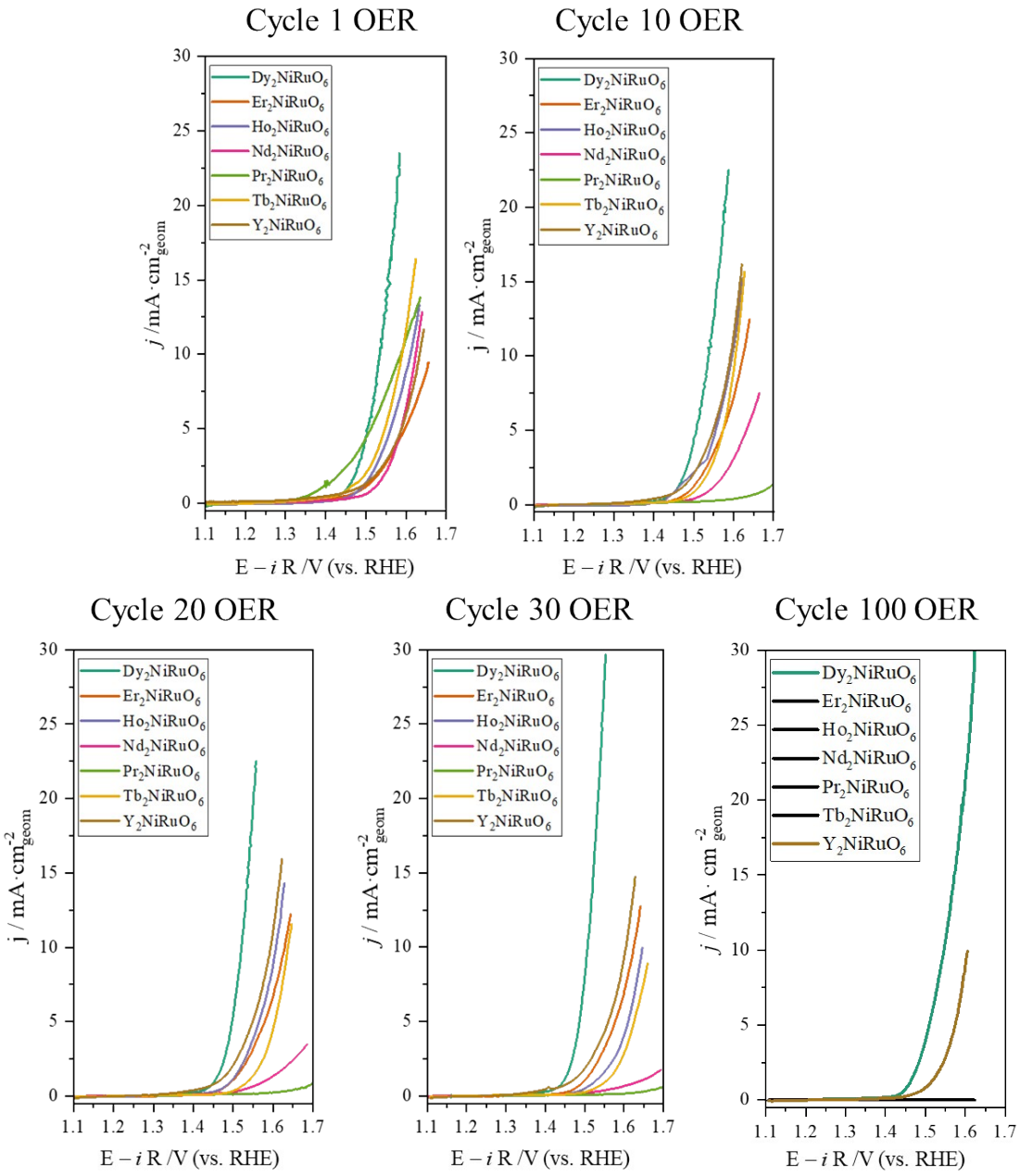


Figure S2. Evolution of the OER activity of R_2NiRuO_6, measured in O_2-saturated 0.1 M $HClO_4$ at 1600 rpm.

Figure S3 shows the Nyquist plot of the values obtained at 1.5 V vs RHE of the initial Dy_2NiRuO_6 and after 50 cycles. We notice the presence of a single semicircle corresponding to a typical equivalent circuit of a solution resistance (R_s) in series to R_{ct} in parallel to CPE_{dl}. As expected from the CVs in Figure 2 and Figure S2, in which the activity increases after the first few cycles, R_{ct} decreases proportionally.

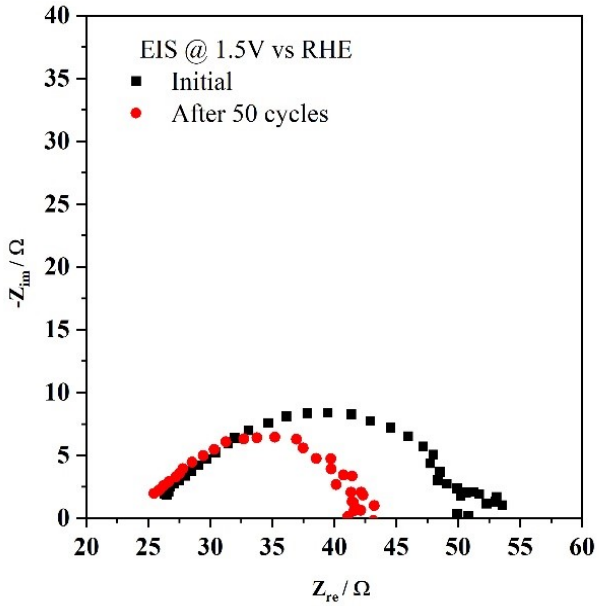
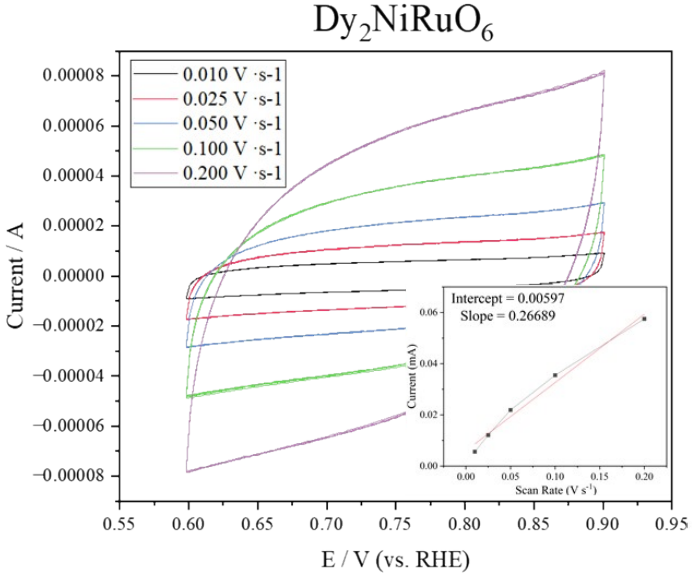
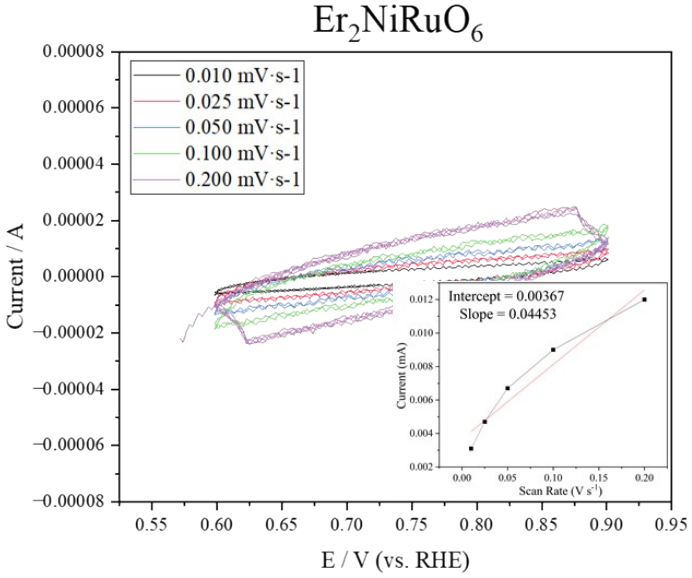
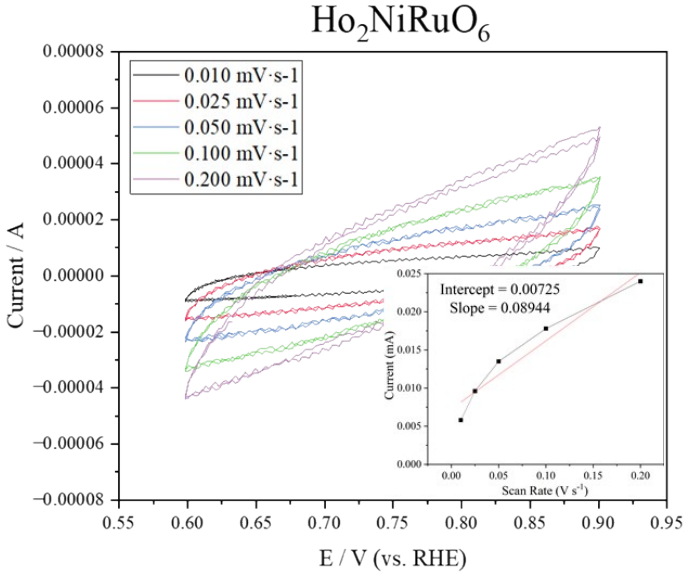


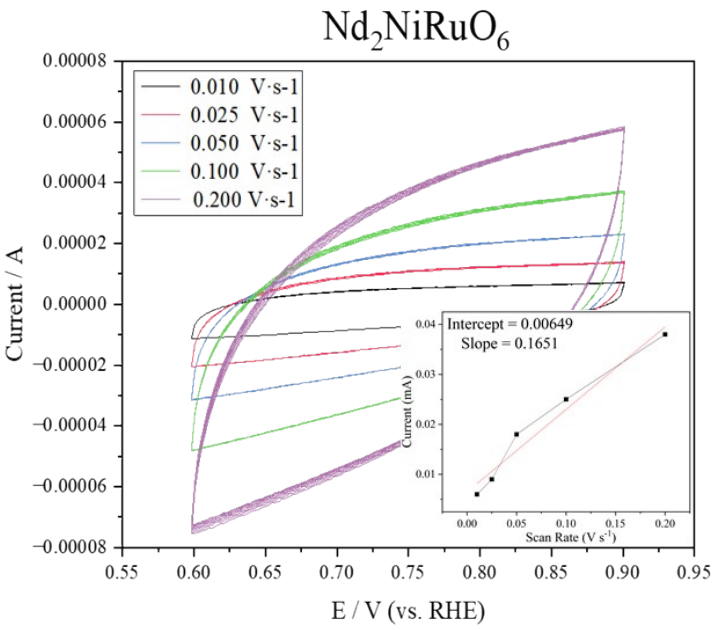
Figure S3. Nyquist plot of the measurements obtained at 1.5 V vs RHE of the initial (black) Dy_2NiRuO_6 and after 50 OER cycles (red).

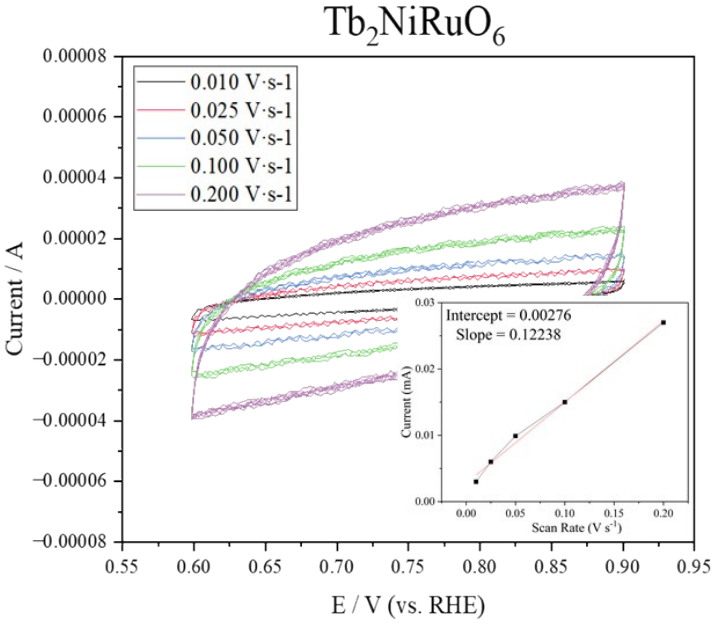
The electrochemically active surface area (ECSA) was calculated by the double-layer capacitance (C_{dl}) of each catalyst. We performed CVs close to the "open circuit potential" in argon-saturated electrolyte (Figure S4) to ensure that the currents obtained are due only to the double-layer capacitance. The cyclic voltammograms are performed at multiple scan rates and the double-layer charging current is equal to the product of the scan rate (ν) and the C_{dl} as shown in the following equation: $i_c = \nu C_{dl}$. Plotting i_c as a function of ν, the slope is the capacitance C_{dl}, and then ECSA= C_{dl}/ C_S, where C_S is the specific capacitance of an atomically flat planar surface of the material per unit area under identical electrolyte conditions. As value of C_S for oxides is ill-defined, we use 0.06 mF/cm^2, in line with previous references.[20,21]


Dy2NiRuO6
0.010 V ·s-1
0.025 V ·s-1
0.050 V ·s-1
0.100 V ·s-1
0.200 V ·s-1
Intercept = 0.00597
Slope = 0.26689
Current (mA)
Scan Rate (V s-1)
Current / A
E / V (vs. RHE)


Er2NiRuO6
0.010 mV·s-1
0.025 mV·s-1
0.050 mV·s-1
0.100 mV·s-1
0.200 mV·s-1
Intercept = 0.00367
Slope = 0.04453
Current (mA)
Scan Rate (V s-1)
Current / A
E / V (vs. RHE)


Ho2NiRuO6
0.010 mV·s-1
0.025 mV·s-1
0.050 mV·s-1
0.100 mV·s-1
0.200 mV·s-1
Intercept = 0.00725
Slope = 0.08944
Current (mA)
Scan Rate (V s-1)
Current / A
E / V (vs. RHE)


Nd2NiRuO6
0.010 V·s-1
0.025 V·s-1
0.050 V·s-1
0.100 V·s-1
0.200 V·s-1
Current / A
E / V (vs. RHE)
Intercept = 0.00649
Slope = 0.1651
Current (mA)
Scan Rate (V s-1)


Tb2NiRuO6
0.010 V·s-1
0.025 V·s-1
0.050 V·s-1
0.100 V·s-1
0.200 V·s-1
Current / A
E / V (vs. RHE)
Intercept = 0.00276
Slope = 0.12238
Current (mA)
Scan Rate (V s-1)

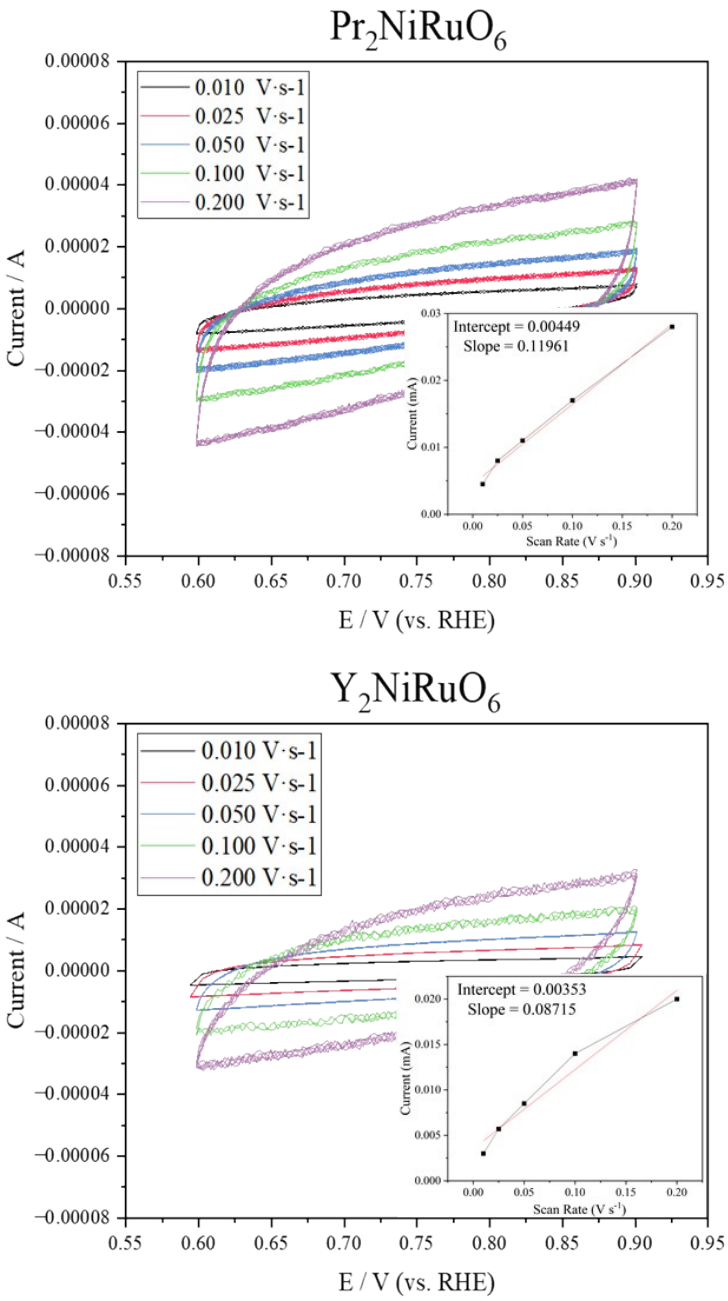


Figure S4. CVs measured at multiple scan rates close to the "open circuit potential" in argon-saturated 0.1 M $HClO_4$ electrolyte for R_2NiRuO_6 samples. Inset: currents obtained at a certain potential vs. scan rate and the corresponding linear fits.

Table S3. ECSA for R_2NiRuO_6.

R_2NiRuO_6	ECSA ($m^2\ g^{-1}$)
R = Dy	8.8
R = Er	1.4
R = Ho	3.0
R = Nd	5.4
R = Pr	4.0
R = Tb	4.0
R = Y	3.0

C_{dl} can be determined either by CV or by electrochemical impedance spectroscopy (EIS). Nevertheless, when measuring C_{dl} by EIS, it is possible to obtain more information by replacing C_{dl} with a constant phase element (CPE_{dl}). The CPE expression is $Z_{CPE} = \frac{1}{(j\omega)^{\varphi} T_{dl}}$, where j is the imaginary unit, ω is the angular frequency, φ is the dimensionless exponent that represents the (non)ideality of the capacitance and T_{dl} is a double-layer capacitance related parameter. As T_{dl} is in units of F $s\varphi^{-1}$, it is not directly proportional to the electrode surface area. To know the exact value of C_{dl}, in F, the following equation is used $C_{dl} = T^{\frac{1}{\varphi}}\left(\frac{1}{R_s}\right)^{1-\frac{1}{\varphi}}$. Additionally, if C_{dl} is measured at a potential in which the OER occurs, information on the kinetics of the reaction can also be obtained since the value of the charge transfer resistance (R_{ct}) can be determined.[22]

To better study the surface changes, $ECSA_{EIS}$ calculated from the T_{dl} has been represented as a function of the cycles for Dy_2NiRuO_6 (Figure S5). During the first 150 cycles, $ECSA_{EIS}$ decreases from approximately 17 to 13 $m^2\ g^{-1}$, and the latter value is maintained during the following cycles. Analogously, φ increases during the first cycles from approximately 0.82 to 0.87, indicating a more homogeneous surface. Note that the ECSA value obtained by EIS is higher, yet in the same order of magnitude, than that obtained by scan-rate dependent CVs. This feature has been previously observed by other authors.[20]

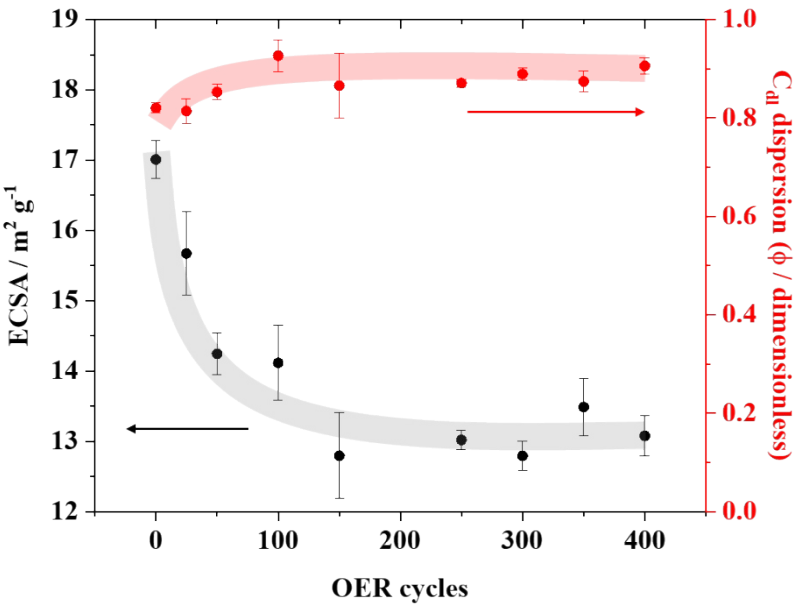


Figure S5. $ECSA_{EIS}$ and Cdl dispersion represented for Dy_2NiRuO_6 OER cycles measured at 10 mV s^{-1}.

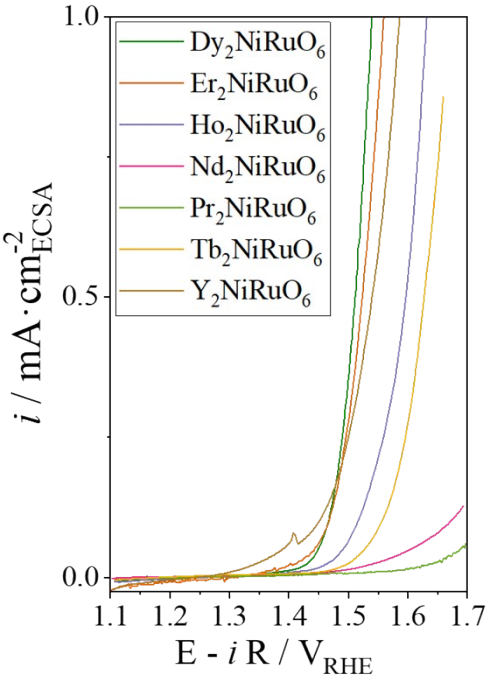


Figure S6. ECSA normalized activity of R_2NiRuO_6 after 30 OER cycles.

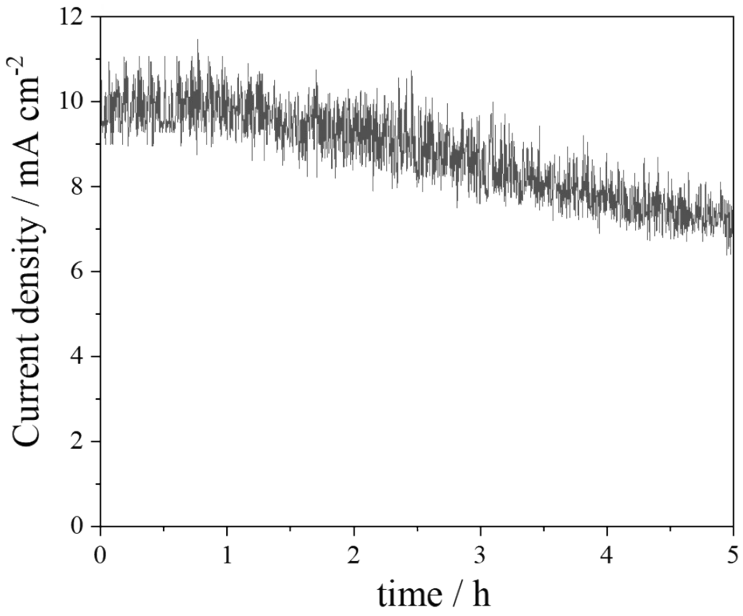


Figure S7. Chronoamperometry for Dy_2NiRuO_6 at the potential where j ~10 mA cm^{-2}, which is ca. 1.55 V.

S3. TEM characterization

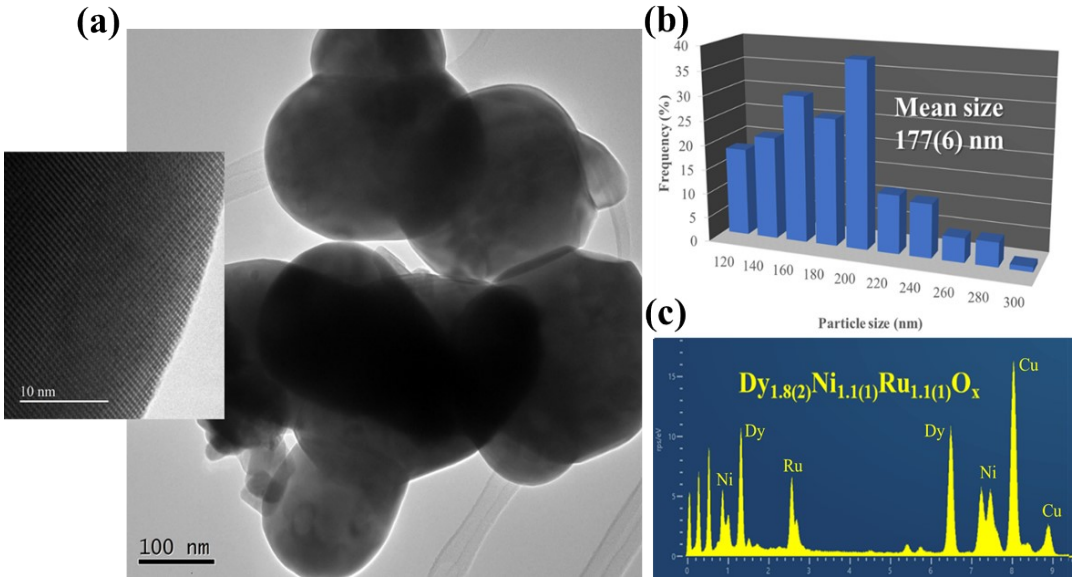


Figure S8. Initial Dy_2NiRuO_6 catalyst. (a) TEM images of groups of particles. Inset: HRTEM. (b) Distribution and mean particle size. (c) EDX corroborating the stoichiometry obtained in the Rietveld analysis of XRD.

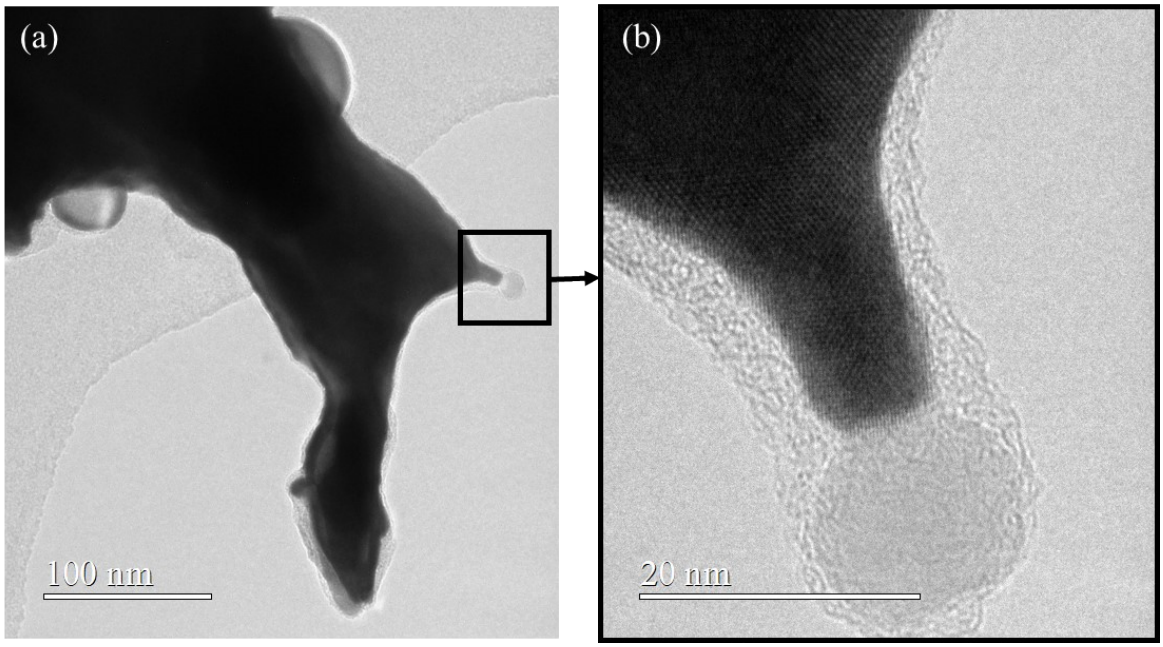


Figure S9. 100-cycles Dy_2NiRuO_6 catalyst. (a) TEM image of a region of 100-Dy_2NiRuO_6 catalyst. (b) One of the isolated Ni-based particles formed during OER reaction.

S4. XPS results of the initial and cycled Dy_2NiRuO_6 catalyst

Table S4. Surface atomic ratios.

	Ru/Dy	***Ru/Ni***	***Ni/Dy***
Dy_2NiRuO_6 ***Initial***	0.65	1.84	0.35
Dy_2NiRuO_6 ***100 CV***	2.03	4.07	0.50
Dy_2NiRuO_6 ***500 CV***	11.41	4.31	2.65
Dy_2NiRuO_6 ***1000 CV***	8.33	2.54	3.28

S5. Full computational details

The DFT calculations were made with the Vienna ab initio simulation package (VASP)[23] and making use of the PBE exchange-correlation functional[24] and the projector augmented-wave (PAW) method.[25] We used a plane-wave cutoff of 400 eV for the plane-wave basis set and the atoms were relaxed until the residual forces were less than 0.05 eV $Å^{-1}$. All calculations were spin unrestricted. To enable a cost-effective localization of the electrons, we used Dudarev et al's GGA+U approach,[26] with U_{eff} = 6.70 eV on the Ru ions, found by Xu et al. for Ru^{4+} by means of a linear-response method;[27] and U_{eff} = 6.01 eV on the Ni ions, which is the average of the values found by Zhou et al. for Ni^{2+}, Ni^{3+} and Ni^{4+}.[28] The k-points for the pristine and dissolved perovskites used to model the OER were chosen as Monkhorst-Pack grids[29] with a sampling of 4×4×1. The Methfessel-Paxton method[29,30] was used to smear the Fermi level with k_BT = 0.01 eV and the energies were extrapolated to 0 K. To avoid spurious electrostatic interactions, a vacuum layer of more than 16 Å separated the periodically repeated images of the slabs, and dipole corrections were also applied in the vertical direction. H_2 and H_2O were calculated in boxes of 15×15×15 $Å^3$, sampling the Γ-point only and with Gaussian smearing and k_BT = 0.001 eV.

The adsorption free energies of *O, *OH and *OOH were evaluated as (see Table S5): $\Delta G_{ads} \approx \Delta E_{ads} + \Delta ZPE - T\Delta S$, where ΔE_{ads} is the DFT-calculated binding energy, ΔZPE is the zero-point energy change calculated with DFT using the harmonic oscillator approximation (the ZPEs of *O, *OH and *OOH are 0.07, 0.36 and 0.43 eV, those of H_2 and H_2O are 0.28 and 0.58 eV), and $T\Delta S$ are entropy corrections, which include all sorts of contributions for H_2 and H_2O (0.40 and 0.67 eV for H_2 and H_2O). The computational hydrogen electrode approach[31] was used to evaluate the energetics of protons and electrons.[31] Water-adsorbate interactions were incorporated in the shape of ad hoc corrections taken from the literature,[32] for *O, *OH and *OOH on Ni/Ru sites: -0.26 ± 0.16/-0.40 ± 0.10, -0.46 ± 0.10/-0.32 ± 0.08, -0.33 ± 0.11/-0.34 eV ± 0.08. These values are averages and the error bars correspond to the standard deviation of the data. Water solvation for adsorbates on Ru sites is assumed to be similar to that of Fe.

To simulate the structures upon Dy dissolution, we first removed the Dy ions from the slabs and relaxed again the structures. To simulate the loss of Ni, we first replaced Ni ions at the top layer by Ru ions (referred to as "less Ni" in Figure 6), and then replaced

all of the Ni ions by Ru ions (referred to as "no Ni" in Figure 6). The most active surface of Dy_2NiRuO_6 upon Dy dissolution is shown in Figure S10. Converged coordinates of all slabs appear at the end of this section.

The OER was assumed to proceed as:[1,5,33,34]

$$* + H_2O \rightarrow *OH + H^+ + e^- \quad \text{(S1)}$$

$$*OH \rightarrow *O + H^+ + e^- \quad \text{(S2)}$$

$$*O + H_2O \rightarrow *OOH + H^+ + e^- \quad \text{(S3)}$$

$$*OOH \rightarrow * + O_2 + H^+ + e^- \quad \text{(S4)}$$

The free energies of those equations are, respectively: $\Delta G_1 = \Delta G_{OH}$, $\Delta G_2 = \Delta G_O - \Delta G_{OH}$, $\Delta G_3 = \Delta G_{OOH} - \Delta G_O$ and $\Delta G_4 = \Delta G_{O_2} - \Delta G_{OOH}$. ΔG_{OH}, ΔG_O and ΔG_{OOH} are defined using protons, electrons, and water as references. The OER overpotential was calculated as: $\eta_{OER} = max(\Delta G_1, \Delta G_2, \Delta G_3, \Delta G_4)/e^- - 1.23$. As shown previously,[1,5] experimental OER data may be added to computational activity plots using Seh *et al*'s[33] semiempirical volcano. The electrochemical-step symmetry index (ESSI) quantifies electrocatalytic symmetry and is defined as (see Table S5): $ESSI = \sum_{i=1}^{n} (\Delta G_i^+ / e^- - U^0)/n$, where ΔG_i^+ are the free energies of the electrochemical steps larger than 1.23 eV.[35–37] The thermodynamically ideal catalyst has $n = 4$, $\Delta G_i^+ = 1.23\ eV$, and $ESSI = 0$. Real catalysts have n between 1 and 3 and highly active OER electrocatalysts are often display $n = 3$.[37]

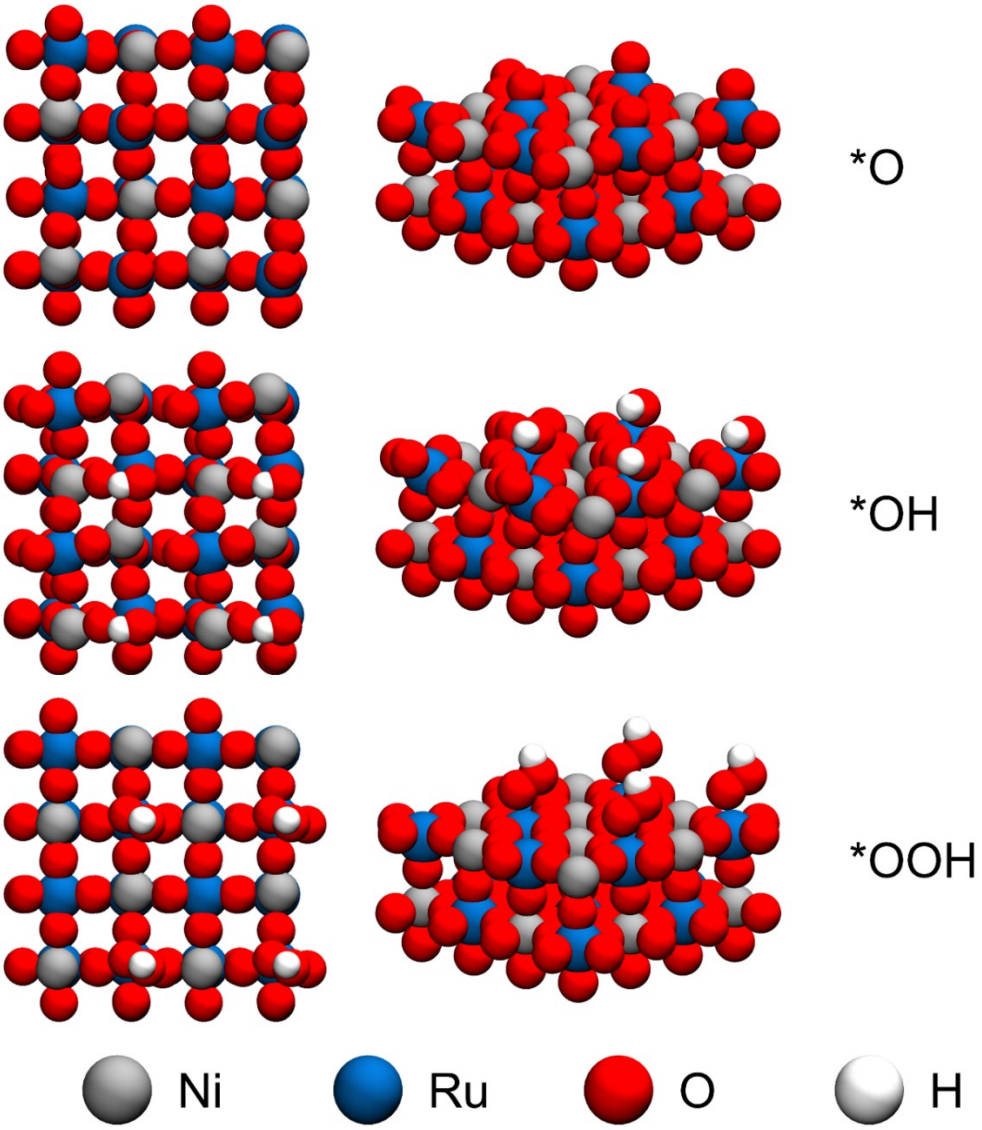


Figure S10. Schematics of $NiRuO_x$ overlayers on Dy_2NiRuO_6 with OER adsorbates on Ru sites. Left: top views. Right: lateral views.

Table S5. Adsorption energies (eV), ESSI (V), OER overpotential (V), and potential-limiting step (abbreviated as PLS) for various sites on pristine and defective Dy_2NiRuO_6.

system	site	ΔG_O	ΔG_{OH}	ΔG_{OOH}	$ESSI$	η_{OER}	PLS
pristine	Ni	3.97	1.50	4.55	0.76	1.24	2
	Ru	2.05	0.44	3.68	0.26	0.40	3
Dy dissolved	Ni	2.75	0.16	2.52	1.26	1.36	2
	Ru	2.70	1.12	3.55	0.24	0.34	2
less Ni	Ru	1.55	0.44	3.82	1.04	1.04	3
no Ni	Ru	1.19	0.76	3.63	0.64	1.22	3
1% strain	Ru	2.93	1.20	4.21	0.28	0.50	2
2% strain	Ru	3.32	1.34	4.20	0.43	0.75	2

In the following, we provide the direct coordinates of the clean slabs and those with *O, *OH and *OOH. Data are provided for Ru sites on pristine Dy_2NiRuO_6; a $NiRuO_x$ overlayer with a Ni:Ru ratio of 1:1; a $NiRuO_x$ overlayer with a Ni:Ru ratio of 1:3; and a RuO_x overlayer.

Pristine clean:

1.00000000000000
7.7508600000000003 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.7508600000000003 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.0000000000000000
Dy Ni Ru O
8 4 4 24
Selective dynamics
Direct
0.0000000000000000 0.0000000000000000 0.0000000000000000 F F F
0.0000000000000000 0.5000000000000000 0.0000000000000000 F F F
0.5000000000000000 0.0000000000000000 0.0000000000000000 F F F
0.5000000000000000 0.5000000000000000 0.0000000000000000 F F F
0.4746725782872709 0.4933576575534972 0.1712129602331113 T T T
0.0290367750738920 0.4924411844268503 0.1717099123446078 T T T
0.5273738182607765 0.9914977632985007 0.1723309534516040 T T T
0.9742366684675194 0.9919425587006694 0.1710428062028278 T T T
0.2500000000000000 0.7500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.2500000000000000 0.0775086000000016 F F F
0.2502083076496453 0.2380622816489859 0.2349321338540636 T T T
0.7502202117351873 0.7376919002184940 0.2350817593307689 T T T
0.2500000000000000 0.2500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.7500000000000000 0.0775086000000016 F F F
0.2498184938377252 0.7477614920082917 0.2386338449868807 T T T
0.7503113512474094 0.2477875112362375 0.2378840118572366 T T T
0.2500000000000000 0.2500000000000000 0.0000000000000000 F F F
0.0000000000000000 0.2500000000000000 0.0775086000000016 F F F
0.2500000000000000 0.0000000000000000 0.0775086000000016 F F F
0.2500000000000000 0.7500000000000000 0.0000000000000000 F F F
0.0000000000000000 0.7500000000000000 0.0775086000000016 F F F
0.2500000000000000 0.5000000000000000 0.0775086000000016 F F F
0.7500000000000000 0.2500000000000000 0.0000000000000000 F F F
0.5000000000000000 0.2500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.0000000000000000 0.0775086000000016 F F F
0.7500000000000000 0.7500000000000000 0.0000000000000000 F F F
0.5000000000000000 0.7500000000000000 0.0775086000000016 F F F
0.2508745171943895 0.2971533315020815 0.1571657291502286 T T T
-0.0002627471029223 0.2392069703160409 0.2280255105058957 T T T
0.2538527795130721 0.9914420592494566 0.2158029949677692 T T T
0.2510151454297779 0.6892944147650515 0.1559308283399345 T T T
0.0000599694157571 0.7494061871712077 0.2283395883991382 T T T
0.2431003059383872 0.4956178056613382 0.2421066985152218 T T T
0.7494877068385648 0.1869879475823013 0.1558307124055184 T T T
0.5004844154843950 0.2500128594737193 0.2286634946106971 T T T
0.7436204707670799 0.9958009767401711 0.2422678101197693 T T T
0.7487203452562644 0.7967230732960939 0.1572217659663604 T T T
0.4996652506008106 0.7391217618670062 0.2292695731143308 T T T
0.7544527313716033 0.4913140054853690 0.2149991833365263 T T T

Pristine with *O @ Ru:

double-perovskite:

1.00000000000000
7.7508600000000003 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.7508600000000003 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.0000000000000000
Dy Ni Ru O
8 4 4 25
Selective dynamics
Direct
0.0000000000000000 0.0000000000000000 0.0000000000000000 F F F
0.0000000000000000 0.5000000000000000 0.0000000000000000 F F F
0.5000000000000000 0.0000000000000000 0.0000000000000000 F F F
0.5000000000000000 0.5000000000000000 0.0000000000000000 F F F
0.5038101297866621 0.4668554668871891 0.1761672177753950 T T T
-0.0045579914609007 0.5211224145816066 0.1754849380923703 T T T
0.5039781176436555 0.0271035680743434 0.1770646000608602 T T T
0.9949292420533249 -0.0245754286164591 0.1762509956368083 T T T
0.2500000000000000 0.7500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.2500000000000000 0.0775086000000016 F F F
0.2386592408319404 0.2479603092274097 0.2386793757747318 T T T
0.7418631881532911 0.7474187722432442 0.2393897334505304 T T T
0.2500000000000000 0.2500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.7500000000000000 0.0775086000000016 F F F
0.2520317920725766 0.7474902605060501 0.2388887540068493 T T T
0.7562468569310663 0.2483826019111446 0.2434447718791712 T T T
0.2500000000000000 0.2500000000000000 0.0000000000000000 F F F
0.0000000000000000 0.2500000000000000 0.0775086000000016 F F F
0.2500000000000000 0.0000000000000000 0.0775086000000016 F F F
0.2500000000000000 0.7500000000000000 0.0000000000000000 F F F
0.0000000000000000 0.7500000000000000 0.0775086000000016 F F F
0.2500000000000000 0.5000000000000000 0.0775086000000016 F F F
0.7500000000000000 0.2500000000000000 0.0000000000000000 F F F
0.5000000000000000 0.2500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.0000000000000000 0.0775086000000016 F F F
0.7500000000000000 0.7500000000000000 0.0000000000000000 F F F
0.5000000000000000 0.7500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.5000000000000000 0.0775086000000016 F F F
0.2587057260875510 0.2476937991294919 0.1545710722295271 T T T
-0.0024586204171723 0.2480038780849323 0.2152977088213077 T T T
0.2482024563035553 -0.0021197728852538 0.2303664186585186 T T T
0.1898388656534346 0.7497513522599489 0.1557424185198108 T T T
-0.0025515415548079 0.7473791980051048 0.2404532353073730 T T T
0.2469712174159824 0.4974428473074963 0.2291250243221948 T T T
0.6964308529526156 0.2468168258609564 0.1578090227440287 T T T
0.4954898117542878 0.2485620984546719 0.2390019244997082 T T T
0.7486342965509792 0.9958219225288092 0.2284639277602254 T T T
0.7863905130849358 0.7506251482953780 0.1545621029256793 T T T
0.4963278180478823 0.7467398220267928 0.2184428975306303 T T T
0.7496035651518123 0.5001402664306926 0.2270181365139937 T T T
0.7979108698516314 0.2503574255697314 0.3129101400571883 T T T

Pristine with *OH @ Ru:

double-perovskite:

1.00000000000000
7.7508600000000003 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.7508600000000003 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.0000000000000000
Dy Ni Ru O H
8 4 4 25 1
Selective dynamics
Direct
0.0000000000000000 0.0000000000000000 0.0000000000000000 F F F
0.0000000000000000 0.5000000000000000 0.0000000000000000 F F F
0.5000000000000000 0.0000000000000000 0.0000000000000000 F F F
0.5000000000000000 0.5000000000000000 0.0000000000000000 F F F
0.4725521647121528 0.4922833874185845 0.1705283353472945 T T T
0.0345284216352560 0.4934933569277395 0.1680787747536370 T T T
0.5172503858558015 0.9927000121909537 0.1757797722034387 T T T
0.9714478580639520 0.9933607696034048 0.1721635579192388 T T T
0.2500000000000000 0.7500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.2500000000000000 0.0775086000000016 F F F
0.2470856850243940 0.2408539793661001 0.2361933573062406 T T T
0.7504289527102338 0.7318941873275351 0.2348269059501375 T T T
0.2500000000000000 0.2500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.7500000000000000 0.0775086000000016 F F F
0.2479953160675301 0.7466259346184304 0.2396151829267836 T T T
0.7505469487517370 0.2509501772975981 0.2361689840616001 T T T
0.2500000000000000 0.2500000000000000 0.0000000000000000 F F F
0.0000000000000000 0.2500000000000000 0.0775086000000016 F F F
0.2500000000000000 0.0000000000000000 0.0775086000000016 F F F
0.2500000000000000 0.7500000000000000 0.0000000000000000 F F F
0.0000000000000000 0.7500000000000000 0.0775086000000016 F F F
0.2500000000000000 0.5000000000000000 0.0775086000000016 F F F
0.7500000000000000 0.2500000000000000 0.0000000000000000 F F F
0.5000000000000000 0.2500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.0000000000000000 0.0775086000000016 F F F
0.7500000000000000 0.7500000000000000 0.0000000000000000 F F F
0.5000000000000000 0.7500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.5000000000000000 0.0775086000000016 F F F
0.2588013646143410 0.2940368798141037 0.1575438823673997 T T T
0.9982662521397624 0.2471074250845493 0.2223789224682746 T T T
0.2445543728748507 0.9929514663172462 0.2190234663864120 T T T
0.2595950750724512 0.6956812266048393 0.1558547839438159 T T T
0.9988631924084057 0.7411279083723347 0.2244172877651217 T T T
0.2484587087896328 0.4957898589925456 0.2410062373806331 T T T
0.7393616024882568 0.1863675998214298 0.1586222426244893 T T T
0.5007904354053572 0.2446060683469739 0.2309288071604669 T T T
0.7540589232829770 0.9946384850686013 0.2391486845766582 T T T
0.7416364562020148 0.7915201413242460 0.1547937742662119 T T T
0.4996843862012129 0.7470490500539643 0.2322714383525396 T T T
0.7496883565191153 0.4901635592230927 0.2085001540276557 T T T
0.7637573285608907 0.3131242656840787 0.3116602835468122 T T T
0.6463927511872820 0.3193053529111636 0.3257572368303099 T T T

Pristine with *OOH @ Ru:

1.00000000000000
7.7508600000000003 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.7508600000000003 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.0000000000000000
Dy Ni Ru O H
8 4 4 26 1
Selective dynamics
Direct
0.0000000000000000 0.0000000000000000 0.0000000000000000 F F F
0.0000000000000000 0.5000000000000000 0.0000000000000000 F F F
0.5000000000000000 0.0000000000000000 0.0000000000000000 F F F
0.5000000000000000 0.5000000000000000 0.0000000000000000 F F F
0.4717505969135134 0.4927700935098521 0.1653443568440028 T T T
0.0327725928688098 0.4944416828562312 0.1664001776544729 T T T
0.5249110288391224 0.9845542928038941 0.1757855070117104 T T T
0.9772601555016772 0.9874962727184831 0.1748545129229345 T T T
0.2500000000000000 0.7500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.2500000000000000 0.0775086000000016 F F F
0.2503063368995175 0.2406349500145905 0.2347976236941113 T T T
0.7519023806301817 0.7144307836441854 0.2375947560529149 T T T
0.2500000000000000 0.2500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.7500000000000000 0.0775086000000016 F F F
0.2511961239409333 0.7423005460170625 0.2397763154913187 T T T
0.7493738406543782 0.2522996059417237 0.2332689971297591 T T T
0.2500000000000000 0.2500000000000000 0.0000000000000000 F F F
0.0000000000000000 0.2500000000000000 0.0775086000000016 F F F
0.2500000000000000 0.0000000000000000 0.0775086000000016 F F F
0.2500000000000000 0.7500000000000000 0.0000000000000000 F F F
0.0000000000000000 0.7500000000000000 0.0775086000000016 F F F
0.2500000000000000 0.5000000000000000 0.0775086000000016 F F F
0.7500000000000000 0.2500000000000000 0.0000000000000000 F F F
0.5000000000000000 0.2500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.0000000000000000 0.0775086000000016 F F F
0.7500000000000000 0.7500000000000000 0.0000000000000000 F F F
0.5000000000000000 0.7500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.5000000000000000 0.0775086000000016 F F F
0.2491364211133211 0.2973720710249265 0.1567961673901344 T T T
0.9987966406444092 0.2437032609059385 0.2243133679489022 T T T
0.2543615816589820 0.9901777688352886 0.2199084942205968 T T T
0.2523942876138978 0.6955525020005696 0.1557646742550008 T T T
-0.0001393156312245 0.7444028983711505 0.2279216328702604 T T T
0.2353614581395813 0.4937633541395151 0.2429708669709366 T T T
0.7496624807707098 0.1742122595136713 0.1574476594184861 T T T
0.5001754020817847 0.2501098394434853 0.2233015746184705 T T T
0.7451837559235462 0.9976039921044860 0.2418354007862069 T T T
0.7507137371701388 0.7918332202974480 0.1556265213783523 T T T
0.5019036712856417 0.7309949291993592 0.2282162828144236 T T T
0.7523222155370197 0.4844055472872871 0.2009800316768024 T T T
0.7522782702802119 0.3563440166547251 0.3072784843544926 T T T
0.8217085888217169 0.5311441225275669 0.3082694609560591 T T T
0.9456411550681125 0.5118625904202503 0.3011740595592356 T T T

Dy-dissolved clean:

1.00000000000000
7.7508600000000003 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.7508600000000003 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.0000000000000000
Ni Ru O
4 4 24
Selective dynamics
Direct
0.2500000000000000 0.7500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.2500000000000000 0.0775086000000016 F F F
0.2500000000000000 0.2500000000000000 0.2291639694781763 T T T
0.7500000000000000 0.7500000000000000 0.2291639694781763 T T T
0.2500000000000000 0.2500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.7500000000000000 0.0775086000000016 F F F
0.2500000000000000 0.7500000000000000 0.2271579383410472 T T T
0.7500000000000000 0.2500000000000000 0.2271579383410472 T T T
0.2500000000000000 0.2500000000000000 0.0000000000000000 F F F
0.0000000000000000 0.2500000000000000 0.0775086000000016 F F F
0.2500000000000000 0.0000000000000000 0.0775086000000016 F F F
0.2500000000000000 0.7500000000000000 0.0000000000000000 F F F
0.0000000000000000 0.7500000000000000 0.0775086000000016 F F F
0.2500000000000000 0.5000000000000000 0.0775086000000016 F F F
0.7500000000000000 0.2500000000000000 0.0000000000000000 F F F
0.5000000000000000 0.2500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.0000000000000000 0.0775086000000016 F F F
0.7500000000000000 0.7500000000000000 0.0000000000000000 F F F
0.5000000000000000 0.7500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.5000000000000000 0.0775086000000016 F F F
0.2500000000000000 0.2500000000000000 0.1523498454851587 T T T
0.9806760280726584 0.2500000000000000 0.2420933151427298 T T T
0.2500000000000000 0.9806760280726584 0.2420933151427298 T T T
0.2500000000000000 0.7500000000000000 0.1588447346602159 T T T
0.0193239719273415 0.7500000000000000 0.2420933151427298 T T T
0.2500000000000000 0.5193239719273416 0.2420933151427298 T T T
0.7500000000000000 0.2500000000000000 0.1588447346602159 T T T
0.5193239719273416 0.2500000000000000 0.2420933151427298 T T T
0.7500000000000000 0.0193239719273415 0.2420933151427298 T T T
0.7500000000000000 0.7500000000000000 0.1523498454851587 T T T
0.4806760280726585 0.7500000000000000 0.2420933151427298 T T T
0.7500000000000000 0.4806760280726585 0.2420933151427298 T T T

Dy-dissolved with *O @ Ru:

1.00000000000000
7.7508600000000003 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.7508600000000003 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.0000000000000000
Ni Ru O
4 4 25
Selective dynamics
Direct
0.2500000000000000 0.7500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.2500000000000000 0.0775086000000016 F F F

0.2306200882990875 0.2880178003868754 0.2251571060780266 T T T
0.7785180012136576 0.7250467393818910 0.2254512921806080 T T T
0.2500000000000000 0.2500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.7500000000000000 0.0775086000000016 F F F
0.2785368834810113 0.7319840420699457 0.2289384481931239 T T T
0.7117039170327002 0.2106048851093764 0.2467545262955736 T T T
0.2500000000000000 0.2500000000000000 0.0000000000000000 F F F
0.0000000000000000 0.2500000000000000 0.0775086000000016 F F F
0.2500000000000000 0.0000000000000000 0.0775086000000016 F F F
0.2500000000000000 0.7500000000000000 0.0000000000000000 F F F
0.0000000000000000 0.7500000000000000 0.0775086000000016 F F F
0.2500000000000000 0.5000000000000000 0.0775086000000016 F F F
0.7500000000000000 0.2500000000000000 0.0000000000000000 F F F
0.5000000000000000 0.2500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.0000000000000000 0.0775086000000016 F F F
0.7500000000000000 0.7500000000000000 0.0000000000000000 F F F
0.5000000000000000 0.7500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.5000000000000000 0.0775086000000016 F F F
0.2500314599099575 0.2499472462172503 0.1510795876890785 T T T
-0.0164827008931361 0.2504192732438870 0.2358446478261557 T T T
0.2625308042736657 0.9205081738744539 0.2639284933337032 T T T
0.2206650294945708 0.7581157849954745 0.1628248512333789 T T T
0.0019015296316762 0.7362408018750777 0.2501828985116976 T T T
0.2330656012859142 0.5224810299985717 0.2547523272519306 T T T
0.7811114539190573 0.2716121081515687 0.1751509364149069 T T T
0.4823369870970334 0.2344818740417075 0.2387210490503580 T T T
0.7260265613263498 -0.0163785051600219 0.2383447761341066 T T T
0.7573170003300771 0.7499583941386746 0.1502638326773864 T T T
0.5026953150913029 0.7108117442613726 0.2244695828862398 T T T
0.7639819434191188 0.4718632226433515 0.2350302847372383 T T T
0.7464718069963274 0.2483090348495669 0.3126914658423696 T T T

Dy-dissolved with *OH @ Ru:

1.00000000000000
7.7508600000000003 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.7508600000000003 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.0000000000000000
Ni Ru O H
4 4 25 1
Selective dynamics
Direct
0.2500000000000000 0.7500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.2500000000000000 0.0775086000000016 F F F
0.3332658845113549 0.1854083690270979 0.2175536245021642 T T T
0.6964545827300974 0.8173981434606498 0.2180099143600128 T T T
0.2500000000000000 0.2500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.7500000000000000 0.0775086000000016 F F F
0.2739227811228253 0.7086568598417219 0.2289473466045806 T T T
0.7821943778561877 0.2862648233544943 0.2299390392184534 T T T
0.2500000000000000 0.2500000000000000 0.0000000000000000 F F F
0.0000000000000000 0.2500000000000000 0.0775086000000016 F F F
0.2500000000000000 0.0000000000000000 0.0775086000000016 F F F
0.2500000000000000 0.7500000000000000 0.0000000000000000 F F F
0.0000000000000000 0.7500000000000000 0.0775086000000016 F F F
0.2500000000000000 0.5000000000000000 0.0775086000000016 F F F
0.7500000000000000 0.2500000000000000 0.0000000000000000 F F F
0.5000000000000000 0.2500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.0000000000000000 0.0775086000000016 F F F
0.7500000000000000 0.7500000000000000 0.0000000000000000 F F F
0.5000000000000000 0.7500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.5000000000000000 0.0775086000000016 F F F
0.2552208164634228 0.2508044391330352 0.1539819897373324 T T T
0.0021807547020191 0.2695018589320823 0.2340085178589533 T T T
0.2731529281086337 0.9820441788552379 0.2455434646421120 T T T
0.2252640250172112 0.7579575207128788 0.1640009268626802 T T T
0.0978148117724154 0.7107783178490499 0.2685904715426800 T T T
0.3233379516981134 0.4925033593887546 0.2259288857069510 T T T
0.7439786974085673 0.2638231642552932 0.1622018802876548 T T T
0.5460021363213030 0.2184409592757360 0.2499901348555077 T T T
0.7663238112548857 0.0193498409137919 0.2419340694877476 T T T
0.7485752139384437 0.7371584575489925 0.1563955047018647 T T T
0.4805582554093706 0.7756606951768612 0.2534910833064488 T T T
0.7426054980818299 0.4984471704504753 0.2442670555138998 T T T
0.8042693030172589 0.2023394459913936 0.3092020980893195 T T T
0.6817516280853061 0.1816570900220143 0.3179729861861633 T T T

Dy-dissolved with *OOH @ Ru:

1.00000000000000
7.7508600000000003 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.7508600000000003 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.0000000000000000
Ni Ru O H
4 4 26 1
Selective dynamics
Direct
0.2500000000000000 0.7500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.2500000000000000 0.0775086000000016 F F F
0.2360586212090220 0.2367405615822741 0.2305518387705541 T T T
0.7606224635288070 0.7661950004110543 0.2300530826521222 T T T
0.2500000000000000 0.2500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.7500000000000000 0.0775086000000016 F F F
0.2528066731580887 0.7401649242180046 0.2268748267600774 T T T
0.7439344929828721 0.2709725036840400 0.2291308793766607 T T T
0.2500000000000000 0.2500000000000000 0.0000000000000000 F F F
0.0000000000000000 0.2500000000000000 0.0775086000000016 F F F
0.2500000000000000 0.0000000000000000 0.0775086000000016 F F F
0.2500000000000000 0.7500000000000000 0.0000000000000000 F F F
0.0000000000000000 0.7500000000000000 0.0775086000000016 F F F
0.2500000000000000 0.5000000000000000 0.0775086000000016 F F F
0.7500000000000000 0.2500000000000000 0.0000000000000000 F F F
0.5000000000000000 0.2500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.7500000000000000 0.0775086000000016 F F F
0.2500000000000000 0.2500000000000000 0.0000000000000000 F F F
0.0000000000000000 0.2500000000000000 0.0775086000000016 F F F
0.2500000000000000 0.0000000000000000 0.0775086000000016 F F F
0.2500000000000000 0.7500000000000000 0.0000000000000000 F F F
0.0000000000000000 0.7500000000000000 0.0775086000000016 F F F
0.2500000000000000 0.5000000000000000 0.0775086000000016 F F F
0.7500000000000000 0.2500000000000000 0.0000000000000000 F F F
0.5000000000000000 0.2500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.0000000000000000 0.0775086000000016 F F F
0.7500000000000000 0.7500000000000000 0.0000000000000000 F F F
0.5000000000000000 0.7500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.5000000000000000 0.0775086000000016 F F F
0.2500000000000000 0.2500000000000000 0.1594207312242809 T T T
0.0006723454707970 0.2500000000000000 0.2459173011889324 T T T
0.2500000000000000 0.0006723454707970 0.2459173011889324 T T T
0.2500000000000000 0.7500000000000000 0.1605444257475392 T T T
-0.0006723454707970 0.7500000000000000 0.2459173011889324 T T T
0.2500000000000000 0.4993276545292029 0.2459173011889324 T T T
0.7500000000000000 0.2500000000000000 0.1605444257475392 T T T
0.4993276545292029 0.2500000000000000 0.2459173011889324 T T T
0.7500000000000000 -0.0006723454707970 0.2459173011889324 T T T
0.7500000000000000 0.7500000000000000 0.1594207312242809 T T T
0.5006723454707971 0.7500000000000000 0.2459173011889324 T T T
0.7500000000000000 0.5006723454707970 0.2459173011889324 T T T

Less Ni with *O @ Ru:

1.00000000000000
7.7508600000000003 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.7508600000000003 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.0000000000000000
Ni Ru O
2 6 25
Selective dynamics
Direct
0.2500000000000000 0.7500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.2500000000000000 0.0775086000000016 F F F
0.2472608922825169 0.2775374863648631 0.2327063590222150 T T T
0.7644375241253855 0.7580561782665062 0.2303903091134374 T T T
0.2500000000000000 0.2500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.7500000000000000 0.0775086000000016 F F F
0.2555040709912025 0.7127100675077847 0.2242656874937638 T T T
0.6909445213336692 0.1856018283062865 0.2553030977757311 T T T
0.2500000000000000 0.2500000000000000 0.0000000000000000 F F F
0.0000000000000000 0.2500000000000000 0.0775086000000016 F F F
0.2500000000000000 0.0000000000000000 0.0775086000000016 F F F
0.2500000000000000 0.7500000000000000 0.0000000000000000 F F F
0.0000000000000000 0.7500000000000000 0.0775086000000016 F F F
0.2500000000000000 0.5000000000000000 0.0775086000000016 F F F
0.7500000000000000 0.2500000000000000 0.0000000000000000 F F F
0.5000000000000000 0.2500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.0000000000000000 0.0775086000000016 F F F
0.7500000000000000 0.7500000000000000 0.0000000000000000 F F F
0.5000000000000000 0.7500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.5000000000000000 0.0775086000000016 F F F
0.2569430673373203 0.2209095213619017 0.1650456143850570 T T T
0.1162759560912438 0.1469815836224567 0.2683143807175914 T T T
0.2937773972554358 0.8379285315900257 0.2781458626779935 T T T
0.2028925731934958 0.7992814931161668 0.1632142542051574 T T T
-0.0302678328715241 0.8423502458660782 0.2432342652382771 T T T
0.1503096180533320 0.5021569667879490 0.2406961538557929 T T T
0.7876631571321659 0.2473619773081385 0.1973965792392119 T T T
0.4693712211331120 0.2945945769962303 0.2594923212136504 T T T
0.6193105991325667 0.9570084530955696 0.2434135924746127 T T T
0.7501686162571224 0.7315467136690222 0.1598088389554589 T T T
0.4541504788976721 0.6226925671130120 0.2102928071007185 T T T
0.7363569027709387 0.5799109789330960 0.2697221394347559 T T T
0.7812318132803786 0.1844541043124966 0.3164300540181982 T T T

Less Ni with *OH @ Ru:

double-perovskite:
1.00000000000000
7.7508600000000003 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.7508600000000003 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.0000000000000000
Ni Ru O H
2 6 25 1
Selective dynamics
Direct
0.2500000000000000 0.7500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.2500000000000000 0.0775086000000016 F F F
0.2642944617582924 0.2392514633758294 0.2320044250614383 T T T
0.7380331872725184 0.7849886634320772 0.2298033454919609 T T T
0.2500000000000000 0.2500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.7500000000000000 0.0775086000000016 F F F
0.2965315930157397 0.7318837283970826 0.2272758168670942 T T T
0.8283006849813278 0.3502901439764955 0.2455741845349479 T T T
0.2500000000000000 0.2500000000000000 0.0000000000000000 F F F
0.0000000000000000 0.2500000000000000 0.0775086000000016 F F F
0.2500000000000000 0.0000000000000000 0.0775086000000016 F F F
0.2500000000000000 0.7500000000000000 0.0000000000000000 F F F
0.0000000000000000 0.7500000000000000 0.0775086000000016 F F F
0.2500000000000000 0.5000000000000000 0.0775086000000016 F F F
0.7500000000000000 0.2500000000000000 0.0000000000000000 F F F
0.5000000000000000 0.2500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.0000000000000000 0.0775086000000016 F F F
0.7500000000000000 0.7500000000000000 0.0000000000000000 F F F
0.5000000000000000 0.7500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.5000000000000000 0.0775086000000016 F F F
0.2902068777149969 0.2607475505757099 0.1616752222336389 T T T
0.0619462143984487 0.3884850415222065 0.2482650860524845 T T T
0.1603136948140878 0.0420354007235908 0.2383874335604567 T T T
0.1992084452130099 0.7649159289421480 0.1663096603771863 T T T
0.1780430484009341 0.7241688827111777 0.2840264053299054 T T T
0.3869331642651984 0.5281724564261236 0.2218270282636598 T T T
0.7619267532506541 0.2545545281129260 0.1880819371643249 T T T
0.4482179831271925 0.2342300834037990 0.2709600133006383 T T T
0.8584849388529341 0.9142568965934464 0.2681907877536981 T T T
0.7582114982000632 0.7290563610357648 0.1612625618439709 T T T
0.4954059112346761 0.8562407178984657 0.2339731626880058 T T T
0.7167536469909878 0.5508810188988894 0.2604147913027984 T T T
0.7809686606372838 0.2351769094003139 0.3091633681444715 T T T
0.6529830002510226 0.2248435526826026 0.3114424036493664 T T T

Less Ni with *OOH @ Ru:

1.00000000000000
7.7508600000000003 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.7508600000000003 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.0000000000000000
Ni Ru O H
2 6 26 1
Selective dynamics
Direct
0.2500000000000000 0.7500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.2500000000000000 0.0775086000000016 F F F
0.2418817502404019 0.2672972522455079 0.2301267017100499 T T T
0.7709090032679033 0.7485929252266654 0.2299982286745774 T T T
0.2500000000000000 0.2500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.7500000000000000 0.0775086000000016 F F F
0.2717317026616335 0.7639537733428653 0.2302641566771817 T T T
0.7436597717731002 0.2478371355846463 0.2340081229400851 T T T
0.2500000000000000 0.2500000000000000 0.0000000000000000 F F F
0.0000000000000000 0.2500000000000000 0.0775086000000016 F F F
0.2500000000000000 0.0000000000000000 0.0775086000000016 F F F
0.2500000000000000 0.7500000000000000 0.0000000000000000 F F F
0.0000000000000000 0.7500000000000000 0.0775086000000016 F F F
0.2500000000000000 0.5000000000000000 0.0775086000000016 F F F
0.7500000000000000 0.2500000000000000 0.0000000000000000 F F F
0.5000000000000000 0.2500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.0000000000000000 0.0775086000000016 F F F
0.7500000000000000 0.7500000000000000 0.0000000000000000 F F F
0.5000000000000000 0.7500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.5000000000000000 0.0775086000000016 F F F
0.2479359576788709 0.2390613875653831 0.1594350542577549 T T T
0.9947342729932518 0.2375773212433019 0.2463603113508905 T T T
0.2385032318926606 -0.0086566679608689 0.2468920097106979 T T T
0.2583181353492980 0.7452616064313202 0.1603305297129885 T T T
0.0001247910318471 0.7388167244740964 0.2437088471714578 T T T
0.2333410935001259 0.5023514035358041 0.2456890484225154 T T T
0.7414089110453030 0.2441968803190351 0.1629478726393517 T T T
0.4820451558963034 0.2371650323201960 0.2477685004036800 T T T
0.7371252230969758 -0.0152203649085144 0.2487304289130605 T T T
0.7327372281117653 0.7587535434903178 0.1599306911095312 T T T
0.4958650222621780 0.7421684807627120 0.2492377594492022 T T T
0.7320870311548829 0.5068397348472149 0.2445567786614299 T T T
0.7202009708707483 0.2802513813134166 0.3229393824492329 T T T
0.8532044458426791 0.2188393424686125 0.3528003370118052 T T T
0.8207175717018363 0.2545341657426712 0.3894934523146847 T T T

No Ni clean:

1.00000000000000
7.7508600000000003 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.7508600000000003 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.0000000000000000
Ru O

Less Ni clean:

1.00000000000000
7.7508600000000003 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.7508600000000003 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.0000000000000000
Ni Ru O
2 6 24
Selective dynamics
Direct
0.2500000000000000 0.7500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.2500000000000000 0.0775086000000016 F F F
0.2500000000000000 0.2500000000000000 0.2308368143171349 T T T
0.7500000000000000 0.7500000000000000 0.2308368143171349 T T T
0.2500000000000000 0.2500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.7500000000000000 0.0775086000000016 F F F
0.2500000000000000 0.7500000000000000 0.2308821176112478 T T T
0.7500000000000000 0.2500000000000000 0.2308821176112478 T T T
0.2500000000000000 0.2500000000000000 0.0000000000000000 F F F
0.0000000000000000 0.2500000000000000 0.0775086000000016 F F F
0.2500000000000000 0.0000000000000000 0.0775086000000016 F F F
0.2500000000000000 0.7500000000000000 0.0000000000000000 F F F
0.0000000000000000 0.7500000000000000 0.0775086000000016 F F F
0.2500000000000000 0.5000000000000000 0.0775086000000016 F F F
0.7500000000000000 0.2500000000000000 0.0000000000000000 F F F
0.5000000000000000 0.2500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.0000000000000000 0.0775086000000016 F F F
0.7500000000000000 0.7500000000000000 0.0000000000000000 F F F
0.5000000000000000 0.7500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.5000000000000000 0.0775086000000016 F F F
0.2500000000000000 0.2500000000000000 0.1594207312242809 T T T
0.0006723454707970 0.2500000000000000 0.2459173011889324 T T T
0.2500000000000000 0.0006723454707970 0.2459173011889324 T T T
0.2500000000000000 0.7500000000000000 0.1605444257475392 T T T
-0.0006723454707970 0.7500000000000000 0.2459173011889324 T T T
0.2500000000000000 0.4993276545292029 0.2459173011889324 T T T
0.7500000000000000 0.2500000000000000 0.1605444257475392 T T T
0.4993276545292029 0.2500000000000000 0.2459173011889324 T T T
0.7500000000000000 -0.0006723454707970 0.2459173011889324 T T T
0.7500000000000000 0.7500000000000000 0.1594207312242809 T T T
0.5006723454707971 0.7500000000000000 0.2459173011889324 T T T
0.7500000000000000 0.5006723454707970 0.2459173011889324 T T T

Less Ni with *O @ Ru:

1.00000000000000
7.7508600000000003 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.7508600000000003 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.0000000000000000
Ni Ru O
2 6 25
Selective dynamics
Direct
0.2500000000000000 0.7500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.2500000000000000 0.0775086000000016 F F F
0.2472608922825169 0.2775374863648631 0.2327063590222150 T T T
0.7644375241253855 0.7580561782665062 0.2303903091134374 T T T
0.2500000000000000 0.2500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.7500000000000000 0.0775086000000016 F F F
0.2555040709912025 0.7127100675077847 0.2242656874937638 T T T
0.6909445213336692 0.1856018283062865 0.2553030977757311 T T T
0.2500000000000000 0.2500000000000000 0.0000000000000000 F F F
0.0000000000000000 0.2500000000000000 0.0775086000000016 F F F
0.2500000000000000 0.0000000000000000 0.0775086000000016 F F F
0.2500000000000000 0.7500000000000000 0.0000000000000000 F F F
0.0000000000000000 0.7500000000000000 0.0775086000000016 F F F
0.2500000000000000 0.5000000000000000 0.0775086000000016 F F F
0.7500000000000000 0.2500000000000000 0.0000000000000000 F F F
0.5000000000000000 0.2500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.0000000000000000 0.0775086000000016 F F F
0.7500000000000000 0.7500000000000000 0.0000000000000000 F F F
0.5000000000000000 0.7500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.5000000000000000 0.0775086000000016 F F F
0.2569430673373203 0.2209095213619017 0.1650456143850570 T T T
0.1162759560912438 0.1469815836224567 0.2683143807175914 T T T
0.2937773972554358 0.8379285315900257 0.2781458626779935 T T T
0.2028925731934958 0.7992814931161668 0.1632142542051574 T T T
-0.0302678328715241 0.8423502458660782 0.2432342652382771 T T T
0.1503096180533320 0.5021569667879490 0.2406961538557929 T T T
0.7876631571321659 0.2473619773081385 0.1973965792392119 T T T
0.4693712211331120 0.2945945769962303 0.2594923212136504 T T T
0.6193105991325667 0.9570084530955696 0.2434135924746127 T T T
0.7501686162571224 0.7315467136690222 0.1598088389554589 T T T

8 24

Selective dynamics

Direct

0.2500000000000000 0.7500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.2500000000000000 0.0775086000000016 F F F
0.2500000000000000 0.2500000000000000 0.2299041483037148 T T T
0.7500000000000000 0.7500000000000000 0.2299041483037148 T T T
0.2500000000000000 0.2500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.7500000000000000 0.0775086000000016 F F F
0.2500000000000000 0.7500000000000000 0.2318664258141746 T T T
0.7500000000000000 0.2500000000000000 0.2318664258141746 T T T
0.2500000000000000 0.2500000000000000 0.0000000000000000 F F F
0.0000000000000000 0.2500000000000000 0.0775086000000016 F F F
0.2500000000000000 0.0000000000000000 0.0775086000000016 F F F
0.2500000000000000 0.7500000000000000 0.0000000000000000 F F F
0.0000000000000000 0.7500000000000000 0.0775086000000016 F F F
0.2500000000000000 0.5000000000000000 0.0775086000000016 F F F
0.7500000000000000 0.2500000000000000 0.0000000000000000 F F F
0.5000000000000000 0.2500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.0000000000000000 0.0775086000000016 F F F
0.7500000000000000 0.7500000000000000 0.0000000000000000 F F F
0.5000000000000000 0.7500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.5000000000000000 0.0775086000000016 F F F
0.2500000000000000 0.2500000000000000 0.1581844454853021 T T T
0.9986801324734600 0.2500000000000000 0.2454152670577331 T T T
0.2500000000000000 0.9986801324734600 0.2454152670577331 T T T
0.2500000000000000 0.7500000000000000 0.1605466604908865 T T T
0.0013198675265399 0.7500000000000000 0.2454152670577331 T T T
0.2500000000000000 0.5013198675265400 0.2454152670577331 T T T
0.7500000000000000 0.2500000000000000 0.1605466604908865 T T T
0.5013198675265400 0.2500000000000000 0.2454152670577331 T T T
0.7500000000000000 0.0013198675265399 0.2454152670577331 T T T
0.7500000000000000 0.7500000000000000 0.1581844454853021 T T T
0.4986801324734602 0.7500000000000000 0.2454152670577331 T T T
0.7500000000000000 0.4986801324734602 0.2454152670577331 T T T

No Ni with *O:

1.00000000000000

7.7508600000000003 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.7508600000000003 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.0000000000000000

Ru O

8 25

Selective dynamics

Direct

0.2500000000000000 0.7500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.2500000000000000 0.0775086000000016 F F F
0.2677570536012171 0.1718870618974822 0.2221841281532649 T T T
0.7746095683084877 0.7475565849366725 0.2350597982766950 T T T
0.2500000000000000 0.2500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.7500000000000000 0.0775086000000016 F F F
0.2894234470154968 0.7188105417706003 0.2225011852682148 T T T
0.7797751524646619 0.1896010619814193 0.2263746787282795 T T T
0.2500000000000000 0.2500000000000000 0.0000000000000000 F F F
0.0000000000000000 0.2500000000000000 0.0775086000000016 F F F
0.2500000000000000 0.0000000000000000 0.0775086000000016 F F F
0.2500000000000000 0.7500000000000000 0.0000000000000000 F F F
0.0000000000000000 0.7500000000000000 0.0775086000000016 F F F
0.2500000000000000 0.5000000000000000 0.0775086000000016 F F F
0.7500000000000000 0.2500000000000000 0.0000000000000000 F F F
0.5000000000000000 0.2500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.0000000000000000 0.0775086000000016 F F F
0.7500000000000000 0.7500000000000000 0.0000000000000000 F F F
0.5000000000000000 0.7500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.5000000000000000 0.0775086000000016 F F F
0.2508238560775186 0.2775523679062485 0.1555312845571021 T T T
0.0082862417966739 0.1127778666962337 0.2241899908492140 T T T
0.2976772206641136 0.9171860968500255 0.2573743661772711 T T T
0.1809515406602684 0.7492877414182636 0.1613045249297134 T T T
-0.0165199779756278 0.7670444630266813 0.2583575788584754 T T T
0.2428440737049697 0.5286845955564463 0.2534916938697359 T T T
0.7483118198154357 0.2827479549641113 0.1622169453130896 T T T
0.4926468060622265 0.2245085485746278 0.2389661074047222 T T T
0.6886610021940809 0.9658370452657749 0.2437215305885038 T T T
0.8009074251542172 0.7169338643080603 0.1663807251930891 T T T
0.4943166097597346 0.6960687854933558 0.1962900224416733 T T T
0.6769554942551155 0.6272427455293293 0.2826177891010791 T T T
0.8085088506512320 0.3396059584592948 0.2753306438615551 T T T

No Ni with *OH:

1.00000000000000

7.7508600000000003 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.7508600000000003 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.0000000000000000

Ru O H

8 25 1

Selective dynamics

Direct

0.2500000000000000 0.7500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.2500000000000000 0.0775086000000016 F F F
0.2731979519425569 0.2341687331907749 0.2282099157997380 T T T
0.7224059596210757 0.7767044786713340 0.2246843940123297 T T T
0.2500000000000000 0.2500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.7500000000000000 0.0775086000000016 F F F
0.2755622254929933 0.7385613384987280 0.2320563756962620 T T T
0.7779112840836405 0.3005017236528973 0.2336716523997793 T T T
0.2500000000000000 0.2500000000000000 0.0000000000000000 F F F
0.0000000000000000 0.2500000000000000 0.0775086000000016 F F F
0.2500000000000000 0.0000000000000000 0.0775086000000016 F F F
0.2500000000000000 0.7500000000000000 0.0000000000000000 F F F
0.0000000000000000 0.7500000000000000 0.0775086000000016 F F F
0.2500000000000000 0.5000000000000000 0.0775086000000016 F F F
0.7500000000000000 0.2500000000000000 0.0000000000000000 F F F
0.5000000000000000 0.2500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.0000000000000000 0.0775086000000016 F F F
0.7500000000000000 0.7500000000000000 0.0000000000000000 F F F
0.5000000000000000 0.7500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.5000000000000000 0.0775086000000016 F F F
0.2500000000000000 0.2500000000000000 0.0000000000000000 F F F
0.0000000000000000 0.2500000000000000 0.0775086000000016 F F F
0.2500000000000000 0.0000000000000000 0.0775086000000016 F F F
0.2500000000000000 0.7500000000000000 0.0000000000000000 F F F
0.0000000000000000 0.7500000000000000 0.0775086000000016 F F F
0.2500000000000000 0.5000000000000000 0.0775086000000016 F F F
0.7500000000000000 0.2500000000000000 0.0000000000000000 F F F
0.5000000000000000 0.2500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.5000000000000000 0.0775086000000016 F F F
0.2500000000000000 0.2500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.7500000000000000 0.0775086000000016 F F F
0.2500000000000000 0.5000000000000000 0.0775086000000016 F F F
0.7500000000000000 0.2500000000000000 0.0000000000000000 F F F
0.2500000000000000 0.7500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.2500000000000000 0.0775086000000016 F F F
0.2452011383992727 0.2668389451875369 0.2300256252440290 T T T
0.7669256234835203 0.7476515656820413 0.2300068782348549 T T T
0.2500000000000000 0.2500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.7500000000000000 0.0775086000000016 F F F
0.2634591226695700 0.7599648273980925 0.2301833746730237 T T T
0.7497533502804505 0.2488788434565253 0.2350158076223121 T T T
0.2500000000000000 0.2500000000000000 0.0000000000000000 F F F
0.0000000000000000 0.2500000000000000 0.0775086000000016 F F F
0.2500000000000000 0.0000000000000000 0.0775086000000016 F F F
0.2500000000000000 0.7500000000000000 0.0000000000000000 F F F
0.0000000000000000 0.7500000000000000 0.0775086000000016 F F F
0.2500000000000000 0.5000000000000000 0.0775086000000016 F F F
0.7500000000000000 0.2500000000000000 0.0000000000000000 F F F
0.5000000000000000 0.2500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.0000000000000000 0.0775086000000016 F F F
0.7500000000000000 0.7500000000000000 0.0000000000000000 F F F
0.5000000000000000 0.7500000000000000 0.0775086000000016 F F F
0.7500000000000000 0.5000000000000000 0.0775086000000016 F F F
0.2500000000000000 0.2500000000000000 0.0000000000000000 F F F
0.2168734254295300 0.2362140723473874 0.1596128067950228 T T T
-0.0104874624615634 0.2442290770019777 0.2496705667296560 T T T
0.2261147841720011 -0.0140124104013851 0.2454141744577411 T T T
0.2183875798779621 0.7423498961941781 0.1603602578352585 T T T
-0.0106958222311959 0.7367666025954583 0.2474852240730788 T T T
0.2352043074778262 0.5020916748980020 0.2454683420830419 T T T
0.7422102086918572 0.2433641691236432 0.1627708358262971 T T T
0.4772233664841307 0.2299103046920501 0.2461880277451244 T T T
0.7349731000044304 -0.0183286716733072 0.2473337035446806 T T T
0.7241417618976800 0.7531749882404148 0.1606797265059786 T T T
0.4859089973377936 0.7483267463952411 0.2461813256643933 T T T
0.7232138311726242 0.5086400320940910 0.2438558483823557 T T T
0.7162502191044431 0.2811553392489349 0.3206535216578250 T T T
0.8353840374321488 0.1965631226439289 0.3513798984310291 T T T
0.8059392692331396 0.2364902706237421 0.3878245319154042 T T T

1% strain clean:

1.00000000000000

7.8283686000000001 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.8283686000000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.0000000000000000

Ni Ru O

4 4 24

Selective dynamics

Direct

0.2500000000000000 0.7500000000000000 0.0782836859999989 F F F
0.7500000000000000 0.2500000000000000 0.0782836859999989 F F F
0.2500000000000000 0.2500000000000000 0.2307241866652885 T T T
0.7500000000000000 0.7500000000000000 0.2307241866652885 T T T
0.2500000000000000 0.2500000000000000 0.0782836859999989 F F F
0.7500000000000000 0.7500000000000000 0.0782836859999989 F F F
0.2500000000000000 0.7500000000000000 0.2279585550270335 T T T
0.7500000000000000 0.2500000000000000 0.2279585550270335 T T T
0.2500000000000000 0.2500000000000000 0.0000000000000000 F F F
0.0000000000000000 0.2500000000000000 0.0782836859999989 F F F
0.2500000000000000 0.0000000000000000 0.0782836859999989 F F F
0.2500000000000000 0.7500000000000000 0.0000000000000000 F F F
0.0000000000000000 0.7500000000000000 0.0782836859999989 F F F
0.2500000000000000 0.5000000000000000 0.0782836859999989 F F F
0.7500000000000000 0.2500000000000000 0.0000000000000000 F F F
0.5000000000000000 0.2500000000000000 0.0782836859999989 F F F
0.7500000000000000 0.0000000000000000 0.0782836859999989 F F F
0.7500000000000000 0.7500000000000000 0.0000000000000000 F F F
0.5000000000000000 0.7500000000000000 0.0782836859999989 F F F
0.7500000000000000 0.5000000000000000 0.0782836859999989 F F F
0.2500000000000000 0.2500000000000000 0.1560740355258542 T T T
-0.0212564790616447 0.2500000000000000 0.2434626647278146 T T T
0.2500000000000000 -0.0212564790616447 0.2434626647278146 T T T
0.2500000000000000 0.7500000000000000 0.1594764640483806 T T T
0.0212564790616447 0.7500000000000000 0.2434626647278146 T T T
0.2500000000000000 0.5212564790616444 0.2434626647278146 T T T
0.7500000000000000 0.2500000000000000 0.1594764640483806 T T T
0.5212564790616444 0.2500000000000000 0.2434626647278146 T T T
0.7500000000000000 0.0212564790616447 0.2434626647278146 T T T
0.7500000000000000 0.7500000000000000 0.1560740355258542 T T T
0.4787435209383553 0.7500000000000000 0.2434626647278146 T T T
0.7500000000000000 0.4787435209383553 0.2434626647278146 T T T

1% strain with *O:

1.00000000000000

7.8283686000000001 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.8283686000000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.0000000000000000

Ni Ru O

4 4 25

Selective dynamics

Direct

0.2500000000000000 0.7500000000000000 0.0782836859999989 F F F
0.7500000000000000 0.2500000000000000 0.0782836859999989 F F F
0.2227283163978600 0.2910310315270397 0.2268925996780449 T T T
0.7767020276167836 0.7293459086451024 0.2257659732610048 T T T
0.2500000000000000 0.2500000000000000 0.0782836859999989 F F F
0.7500000000000000 0.7500000000000000 0.0782836859999989 F F F
0.2799987960042991 0.7265775449269543 0.2330380599712000 T T T
0.7043745409310964 0.2134715899181641 0.2473838287336154 T T T
0.2500000000000000 0.2500000000000000 0.0000000000000000 F F F
0.0000000000000000 0.2500000000000000 0.0782836859999989 F F F
0.2500000000000000 0.0000000000000000 0.0782836859999989 F F F
0.2500000000000000 0.7500000000000000 0.0000000000000000 F F F
0.0000000000000000 0.7500000000000000 0.0782836859999989 F F F
0.2500000000000000 0.5000000000000000 0.0782836859999989 F F F
0.7500000000000000 0.0000000000000000 0.0782836859999989 F F F
0.7500000000000000 0.7500000000000000 0.0000000000000000 F F F
0.5000000000000000 0.7500000000000000 0.0782836859999989 F F F
0.7500000000000000 0.5000000000000000 0.0782836859999989 F F F
0.2365836105217018 0.2436614678966540 0.1559019708739714 T T T
0.9793188830220921 0.2582147756606379 0.2390144519183142 T T T
0.2528638101579503 0.9002902116105865 0.2726933795041882 T T T
0.2172086101546312 0.7590579137360909 0.1686876252251086 T T T
0.9925038571104206 0.7307582460794041 0.2515072758346150 T T T
0.2388914865063370 0.5223694504898273 0.2591350832674622 T T T
0.7789816159677388 0.2757046626686037 0.1775948976642758 T T T
0.4770455413989853 0.2369742595034030 0.2399646398809828 T T T
0.7192763595154623 0.9878069578342846 0.2385071135994769 T T T
0.7507873565631362 0.7464506034779899 0.1512595006405150 T T T
0.4992991783362430 0.7166087686032816 0.2278808317523991 T T T
0.7548980574586959 0.4768706430692135 0.2377781844872499 T T T
0.7406217854651891 0.2460700450049076 0.3135065166006953 T T T

1% strain with *OH:

1.00000000000000

7.8283686000000001 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.8283686000000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.0000000000000000

Ni Ru O H

4 4 25 1

Selective dynamics

Direct

0.2500000000000000 0.7500000000000000 0.0782836859999989 F F F
0.7500000000000000 0.2500000000000000 0.0782836859999989 F F F
0.1537022631602758 0.1936643365861272 0.2213438505817443 T T T
0.7199983056710464 0.7901647055078865 0.2228373060508851 T T T
0.2500000000000000 0.2500000000000000 0.0782836859999989 F F F
0.7500000000000000 0.7500000000000000 0.0782836859999989 F F F
0.2814522908485725 0.7738236873244501 0.2329980998586587 T T T
0.6526890384897469 0.2519676074953890 0.2287415895078090 T T T
0.2500000000000000 0.2500000000000000 0.0000000000000000 F F F
0.0000000000000000 0.2500000000000000 0.0782836859999989 F F F
0.2500000000000000 0.0000000000000000 0.0782836859999989 F F F
0.2500000000000000 0.7500000000000000 0.0000000000000000 F F F
0.0000000000000000 0.7500000000000000 0.0782836859999989 F F F
0.2500000000000000 0.5000000000000000 0.0782836859999989 F F F
0.7500000000000000 0.2500000000000000 0.0000000000000000 F F F
0.5000000000000000 0.2500000000000000 0.0782836859999989 F F F
0.7500000000000000 0.0000000000000000 0.0782836859999989 F F F
0.7500000000000000 0.7500000000000000 0.0000000000000000 F F F
0.5000000000000000 0.7500000000000000 0.0782836859999989 F F F
0.7500000000000000 0.5000000000000000 0.0782836859999989 F F F
0.2025816591424255 0.2605909724568719 0.1542516426310815 T T T
0.9359619299158852 0.2504773050825561 0.2411490434063061 T T T
0.1575527254499327 0.9545588192983051 0.2476099822646264 T T T
0.2774264976807210 0.7483745104138330 0.1646039173975090 T T T
0.8566102429722315 0.7183256559456310 0.2693052721118504 T T T
0.2160683503280109 0.5905752757580977 0.2623311353567677 T T T
0.6844494575631903 0.2721051125613581 0.1595483658215210 T T T
0.4324838403551418 0.2023207072275696 0.2307389677982545 T T T
0.7589170681182896 0.0279957456437548 0.2264567017708905 T T T
0.7329319812090521 0.7360122912810975 0.1562135005269345 T T T
0.4932210298896660 0.8136378115891993 0.2544959985253356 T T T
0.6657453758828025 0.4503054866339192 0.2555260763504487 T T T
0.6745122029554885 0.1358293815546669 0.3023509531619637 T T T
0.5766378559157668 0.0570337906405675 0.3049378906254330 T T T

1% strain with *OOH:

1.00000000000000

7.8283686000000001 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.8283686000000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.0000000000000000
Ni Ru O H
4 4 26 1
Selective dynamics
Direct
0.2500000000000000 0.7500000000000000 0.0782836859999989 F F F
0.7500000000000000 0.2500000000000000 0.0782836859999989 F F F
0.2480343054657649 0.2180635785034377 0.2272692832936443 T T T
0.7020803329936035 0.7593136940523173 0.2274481676870714 T T T
0.2500000000000000 0.2500000000000000 0.0782836859999989 F F F
0.7500000000000000 0.7500000000000000 0.0782836859999989 F F F
0.2644660599426681 0.7135739916031438 0.2330346817322296 T T T
0.7515753463611288 0.2586321400090963 0.2274927564292655 T T T
0.2500000000000000 0.2500000000000000 0.0000000000000000 F F F
0.0000000000000000 0.2500000000000000 0.0782836859999989 F F F
0.2500000000000000 0.0000000000000000 0.0782836859999989 F F F
0.2500000000000000 0.7500000000000000 0.0000000000000000 F F F
0.0000000000000000 0.7500000000000000 0.0782836859999989 F F F
0.2500000000000000 0.5000000000000000 0.0782836859999989 F F F
0.7500000000000000 0.2500000000000000 0.0000000000000000 F F F
0.5000000000000000 0.2500000000000000 0.0782836859999989 F F F
0.7500000000000000 0.0000000000000000 0.0782836859999989 F F F
0.7500000000000000 0.7500000000000000 0.0000000000000000 F F F
0.5000000000000000 0.7500000000000000 0.0782836859999989 F F F
0.7500000000000000 0.5000000000000000 0.0782836859999989 F F F
0.2470038672509024 0.2488450948301978 0.1515776378654043 T T T
0.9821172610127462 0.2479267726522071 0.2403656459373938 T T T
0.2617944194038933 -0.0004393330558827 0.2524948444305077 T T T
0.2394267540437207 0.7770982676479725 0.1683486591882917 T T T
0.0889696076992439 0.7461814746056972 0.2718169788378201 T T T
0.2651695455044278 0.4930243256147519 0.2288766617390032 T T T
0.7492187239804352 0.2553420270201545 0.1592673894897918 T T T
0.5146405134460359 0.2401081277393290 0.2424463063969829 T T T
0.7333728255858859 0.0140257336891749 0.2413462575589404 T T T
0.7536230855423917 0.7505464178920845 0.1565070619397164 T T T
0.4697026587567464 0.7474029285186993 0.2593588531869482 T T T
0.7395272879683851 0.4902730362318460 0.2412481413211271 T T T
0.7362372833164698 0.2258283708549396 0.3218969169329384 T T T
0.8699347460057260 0.2928953509538313 0.3492115215710893 T T T
0.8488675239853560 0.2554275539240504 0.3864246719238120 T T T

2% strain clean:

1.00000000000000
7.9058771999999999 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.9058771999999999 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.0000000000000000
Ni Ru O
4 4 24
Selective dynamics
Direct
0.2500000000000000 0.7500000000000000 0.0790587720000033 F F F
0.7500000000000000 0.2500000000000000 0.0790587720000033 F F F
0.2500000000000000 0.2500000000000000 0.2310047350213059 T T T
0.7500000000000000 0.7500000000000000 0.2310047350213059 T T T
0.2500000000000000 0.2500000000000000 0.0790587720000033 F F F
0.7500000000000000 0.7500000000000000 0.0790587720000033 F F F
0.2500000000000000 0.7500000000000000 0.2287490038265501 T T T
0.7500000000000000 0.2500000000000000 0.2287490038265501 T T T
0.2500000000000000 0.2500000000000000 0.0000000000000000 F F F
0.0000000000000000 0.2500000000000000 0.0790587720000033 F F F
0.2500000000000000 0.0000000000000000 0.0790587720000033 F F F
0.2500000000000000 0.7500000000000000 0.0000000000000000 F F F
0.0000000000000000 0.7500000000000000 0.0790587720000033 F F F
0.2500000000000000 0.5000000000000000 0.0790587720000033 F F F
0.7500000000000000 0.2500000000000000 0.0000000000000000 F F F
0.5000000000000000 0.2500000000000000 0.0790587720000033 F F F
0.7500000000000000 0.0000000000000000 0.0790587720000033 F F F
0.7500000000000000 0.7500000000000000 0.0000000000000000 F F F
0.5000000000000000 0.7500000000000000 0.0790587720000033 F F F
0.7500000000000000 0.5000000000000000 0.0790587720000033 F F F
0.2500000000000000 0.1548038780301353 T T T
0.9764745641267651 0.2500000000000000 0.2436174956846812 T T T
0.2500000000000000 0.9764745641267651 0.2436174956846812 T T T
0.2500000000000000 0.7500000000000000 0.1603605107143168 T T T
0.0235254358732349 0.7500000000000000 0.2436174956846812 T T T
0.2500000000000000 0.5235254358732349 0.2436174956846812 T T T
0.7500000000000000 0.2500000000000000 0.1603605107143168 T T T
0.5235254358732349 0.2500000000000000 0.2436174956846812 T T T
0.7500000000000000 0.0235254358732348 0.2436174956846812 T T T
0.7500000000000000 0.7500000000000000 0.1548038780301353 T T T
0.4764745641267651 0.7500000000000000 0.2436174956846812 T T T
0.7500000000000000 0.4764745641267651 0.2436174956846812 T T T

2% strain with *O:

1.00000000000000
7.9058771999999999 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.9058771999999999 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.0000000000000000
Ni Ru O
4 4 25
Selective dynamics
Direct
0.2500000000000000 0.7500000000000000 0.0790587720000033 F F F
0.7500000000000000 0.2500000000000000 0.0790587720000033 F F F
0.3383543171008964 0.1860099559459372 0.2178738252130656 T T T
0.7515392771810354 0.8113086185914337 0.2233964130322469 T T T
0.2500000000000000 0.2500000000000000 0.0790587720000033 F F F
0.7500000000000000 0.7500000000000000 0.0790587720000033 F F F
0.2283382403388083 0.7752083955366573 0.2347816757066021 T T T
0.8121836308719879 0.2993630664615811 0.2498096835827617 T T T
0.2500000000000000 0.2500000000000000 0.0000000000000000 F F F
0.0000000000000000 0.2500000000000000 0.0790587720000033 F F F
0.2500000000000000 0.0000000000000000 0.0790587720000033 F F F
0.2500000000000000 0.7500000000000000 0.0000000000000000 F F F
0.0000000000000000 0.7500000000000000 0.0790587720000033 F F F
0.2500000000000000 0.5000000000000000 0.0790587720000033 F F F
0.7500000000000000 0.2500000000000000 0.0000000000000000 F F F
0.5000000000000000 0.2500000000000000 0.0790587720000033 F F F
0.7500000000000000 0.0000000000000000 0.0790587720000033 F F F
0.7500000000000000 0.7500000000000000 0.0000000000000000 F F F
0.5000000000000000 0.7500000000000000 0.0790587720000033 F F F
0.7500000000000000 0.5000000000000000 0.0790587720000033 F F F
0.2388584919406103 0.2350836221087733 0.1567812715107546 T T T
0.0262310660609814 0.2770656289099531 0.2464358960806551 T T T
0.2901595688964171 -0.0161899293918498 0.2554708035803415 T T T
0.2656281307902298 0.7372067891831828 0.1680735579091260 T T T
0.0066302470340959 0.7965453543065428 0.2388363211178866 T T T
0.2634390803091571 0.6146876528236502 0.2783242443128263 T T T
0.7598701019115172 0.2456261264468709 0.1753259359087792 T T T
0.5532266902003923 0.2524929561118884 0.2327294119931911 T T T
0.7637640213109760 0.0503974397277920 0.2362323787577149 T T T
0.7752335400744604 0.7399307079810387 0.1541089567053879 T T T
0.5338024777277915 0.7805337273830303 0.2440235993553919 T T T
0.7779688715434742 0.5120558851762214 0.2425344119677312 T T T
0.7637720589667273 0.2606582184112692 0.3148161854943973 T T T

2% strain with *OH:

1.00000000000000
7.9058771999999999 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.9058771999999999 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.0000000000000000
Ni Ru O H
4 4 25 1
Selective dynamics
Direct
0.2500000000000000 0.7500000000000000 0.0790587720000033 F F F
0.7500000000000000 0.2500000000000000 0.0790587720000033 F F F
0.1520334849570785 0.3182670817450750 0.2193761578078172 T T T
0.7978805627267052 0.6983111420044923 0.2244367463682885 T T T
0.2500000000000000 0.2500000000000000 0.0790587720000033 F F F
0.7500000000000000 0.7500000000000000 0.0790587720000033 F F F
0.2492013629075115 0.7495668295557253 0.2333979794353505 T T T
0.7294844135788060 0.1861047205353400 0.2307791269406888 T T T
0.2500000000000000 0.2500000000000000 0.0000000000000000 F F F
0.0000000000000000 0.2500000000000000 0.0790587720000033 F F F
0.2500000000000000 0.0000000000000000 0.0790587720000033 F F F
0.2500000000000000 0.7500000000000000 0.0000000000000000 F F F
0.0000000000000000 0.7500000000000000 0.0790587720000033 F F F
0.2500000000000000 0.5000000000000000 0.0790587720000033 F F F
0.7500000000000000 0.2500000000000000 0.0000000000000000 F F F
0.5000000000000000 0.2500000000000000 0.0790587720000033 F F F
0.7500000000000000 0.0000000000000000 0.0790587720000033 F F F
0.7500000000000000 0.7500000000000000 0.0000000000000000 F F F
0.5000000000000000 0.7500000000000000 0.0790587720000033 F F F
0.7500000000000000 0.5000000000000000 0.0790587720000033 F F F
0.2252619409178658 0.2964604868380591 0.1557065871311158 T T T
-0.0422156929842430 0.2220986796454429 0.2412722282833245 T T T
0.2200369023526637 0.9546460149475492 0.2525399083948380 T T T
0.2521357147404734 0.7497848395616384 0.1654066664461388 T T T
0.0118708057175569 0.7259315703646103 0.2549898814786362 T T T
0.1919823428723152 0.5258580536582792 0.2539542729077031 T T T
0.7417360194613929 0.1980649585746085 0.1617719833515860 T T T
0.5153212848754534 0.2218634796723019 0.2398063598095750 T T T
0.7371171794789891 -0.0290150041900040 0.2455545812521185 T T T
0.7528025521028558 0.7579184287919043 0.1531662350342423 T T T
0.4511090077733818 0.7129091869602801 0.2546555075555496 T T T
0.7260011633963127 0.4798403232889648 0.2239342877705209 T T T
0.7381867578552577 0.3192571809582734 0.3002605127448819 T T T
0.6195345773414249 0.3494114806639030 0.3073914335205777 T T T

2% strain with *OOH:

1.00000000000000
7.9058771999999999 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.9058771999999999 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.0000000000000000
Ni Ru O H
4 4 26 1
Selective dynamics
Direct
0.2500000000000000 0.7500000000000000 0.0790587720000033 F F F
0.7500000000000000 0.2500000000000000 0.0790587720000033 F F F
0.3567022074621277 0.1811737861821296 0.2177681121729409 T T T
0.8073515885069831 0.8679914664823656 0.2099194380891891 T T T
0.2500000000000000 0.2500000000000000 0.0790587720000033 F F F
0.7500000000000000 0.7500000000000000 0.0790587720000033 F F F
0.3074556129746231 0.7559776038664621 0.2355671540213191 T T T
0.7723262597791192 0.2820658636796538 0.2321315314926401 T T T
0.2500000000000000 0.2500000000000000 0.0000000000000000 F F F
0.0000000000000000 0.2500000000000000 0.0790587720000033 F F F
0.2500000000000000 0.0000000000000000 0.0790587720000033 F F F
0.2500000000000000 0.7500000000000000 0.0000000000000000 F F F
0.0000000000000000 0.7500000000000000 0.0790587720000033 F F F
0.2500000000000000 0.5000000000000000 0.0790587720000033 F F F
0.7500000000000000 0.2500000000000000 0.0000000000000000 F F F
0.5000000000000000 0.2500000000000000 0.0790587720000033 F F F
0.7500000000000000 0.0000000000000000 0.0790587720000033 F F F
0.7500000000000000 0.7500000000000000 0.0000000000000000 F F F
0.5000000000000000 0.7500000000000000 0.0790587720000033 F F F
0.7500000000000000 0.5000000000000000 0.0790587720000033 F F F
0.2489708557693816 0.2035344073301267 0.1564046853025922 T T T
0.9685247867795294 0.2038171729940419 0.2467541339866426 T T T
0.3056604783297795 0.9684957421557728 0.2535543500070332 T T T
0.2432276986239520 0.7245244830463156 0.1714051983196149 T T T
0.9849630547919668 0.8569575148946111 0.2409058736856679 T T T
0.2046519882640997 0.6293791536758552 0.2789732016619381 T T T
0.7739088429830968 0.3031506089946160 0.1640655503579541 T T T
0.5344321771223035 0.2870066691096256 0.2455836175849934 T T T
0.6958439188734676 0.0383462447892247 0.2360541499315419 T T T
0.7397463789666215 0.7494217249856874 0.1579907850960553 T T T
0.5123296599735903 0.6983372933725827 0.2387197106388563 T T T
0.7871839767626545 0.4821107984723870 0.2575186134761555 T T T
0.7383677416739303 0.2218546387937063 0.3314320436925282 T T T
0.8766077632119400 0.2691340453539759 0.3591701874041633 T T T
0.8515756362063858 0.2349418266608998 0.3964882383915204 T T T

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