

Tuning the oxygen electrocatalysis via strain on LaNiO_3 surface[†]

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1.1 Adsorption Geometry on the $\text{LaNiO}_3(001)$

The initial configurations of H, H_2O , O, OH, O_2 , and O_2H on top of surface Ni and H on top of surface Ni/O on the unstrained LaNiO_3 (LNO) surface are shown in Fig. S1. Similar initial adsorption geometries were adopted for the compressive- and tensile-strained LNO surfaces as well. The (2×2) unit cell of LNO(001) is demarked by a dotted line in all structural figures in this Supporting Information.

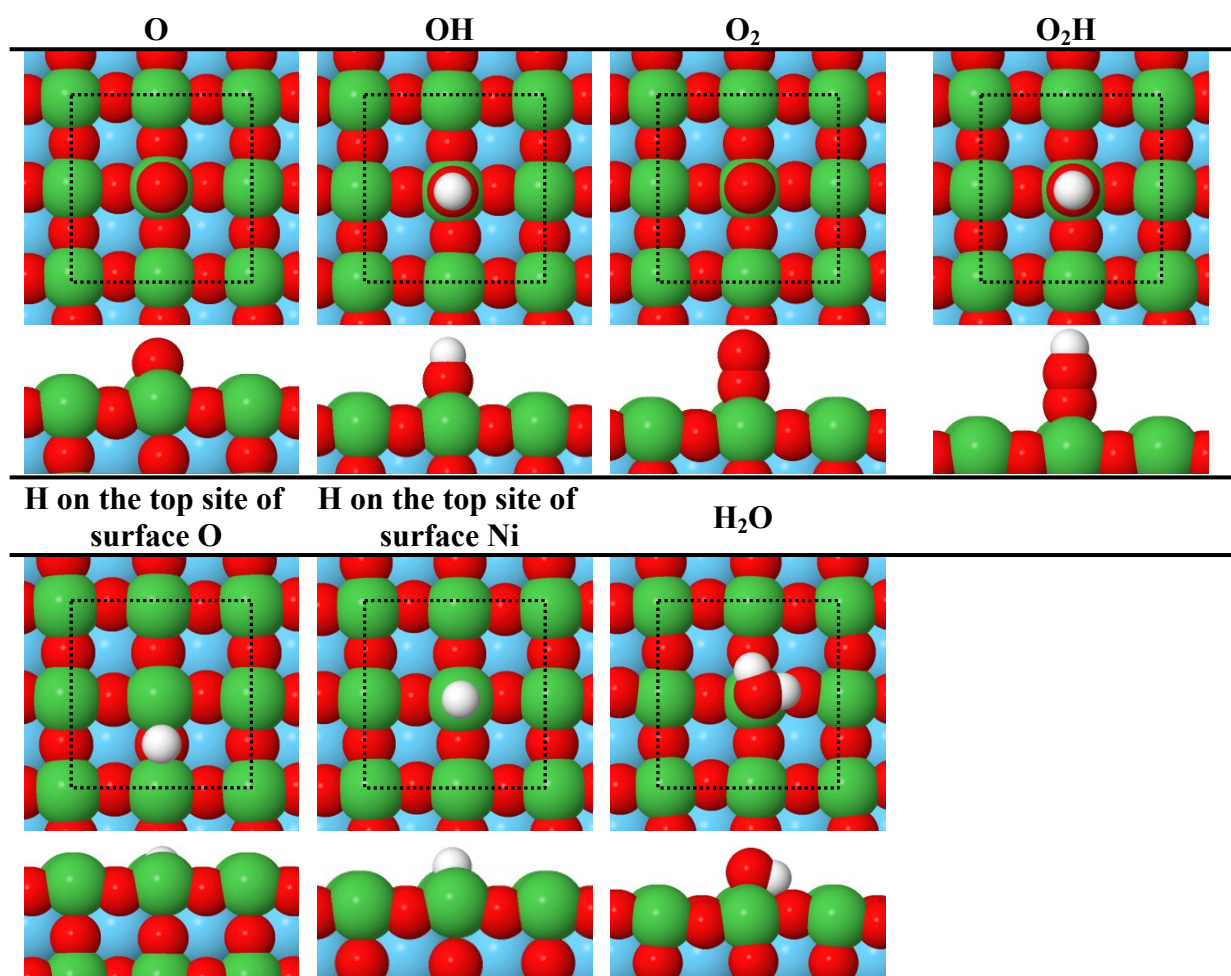


Figure S1. The initial configurations of H, H_2O , O, OH, O_2 , and O_2H on unstrained LNO(001). Green, cyan, red and white atoms represent Ni, La, O and H, respectively.

The relaxed configurations of H_2O , O, OH, and O_2 on top of surface Ni and H on top of surface Ni/O on the unstrained LaNiO_3 (LNO) surface are shown in Fig. S2. Again, similar adsorption geometries of these surface-bound molecules can be found on both the compressive and tensile strains. We observed a preference of H atom towards the adsorption on surface oxygen ions.

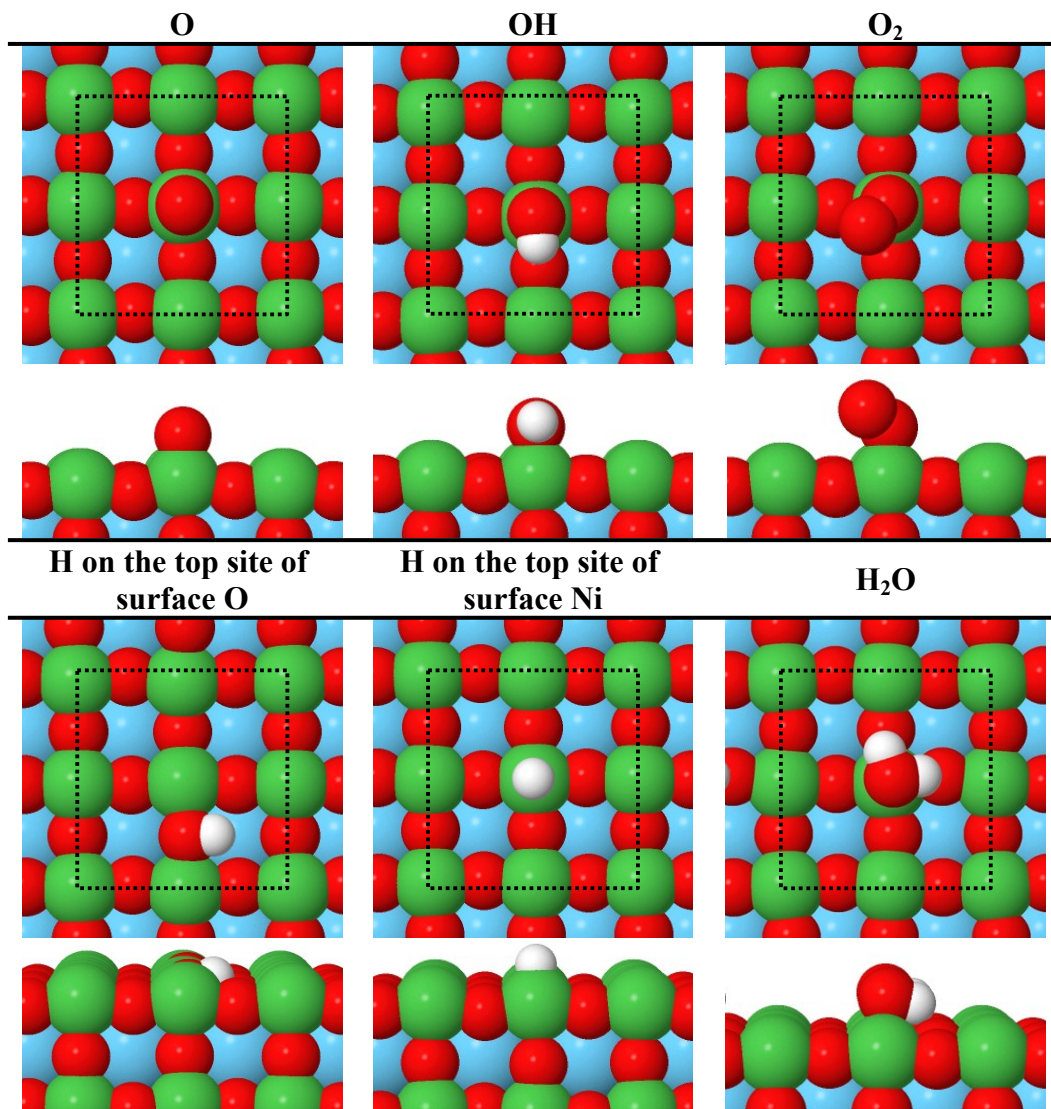


Figure S2. The relaxed configurations of H, H₂O, O, OH, and O₂ on unstrained LNO(001). Green, cyan, red and white atoms represent Ni, La, O and H, respectively.

Two different types of O₂H configurations can be seen, depending on the type of strain applied on the LNO(001) surface (Fig. S3). Inducing tensile strain leads to the dissociation of O₂H into H and O₂.

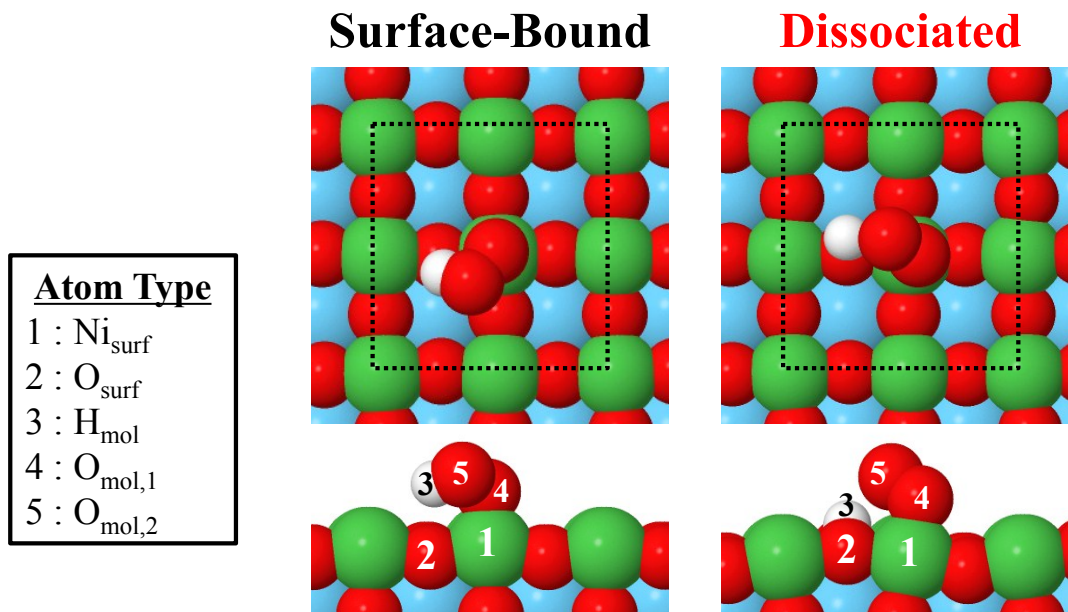


Figure S3. The relaxed configurations of surface-bound (from -3% to unstrained) and dissociated (from +1% to +3%) -O₂H on the LNO(001) surface.

Table S1 contains the geometry of both surface-bound and dissociated -O₂H on the LNO(001) surface as a function of strain. The largest structural change in the O₂H configurations is associated with the bond distance between surface Ni and H atoms.

Table S1. Change in the DFT-optimized geometry of surface-bound and dissociated O₂H on the LNO(001) surface as a function of strain (Please refer to Fig. S3 for the definition of atoms).

Strain (%)	Bond Distance (Å)				
	O _{surf} -Ni _{surf}	O _{surf} -H _{mol}	Ni _{surf} -O _{mol,1}	O _{mol,1} -O _{mol,2}	O _{mol,2} -H _{mol}
-3	1.9	2.73	1.82	1.39	0.99
-2	1.91	2.69	1.82	1.39	0.99
-1	1.94	2.56	1.82	1.38	0.99
0	1.96	2.43	1.82	1.38	0.99
1	2.08	0.98	1.87	1.27	Dissociated
2	2.12	0.98	1.86	1.28	Dissociated
3	2.18	0.98	1.85	1.28	Dissociated

Bond Angle (°)

Strain (%)	O _{surf} -Ni _{surf} -O _{mol,1}	H _{mol} -O _{mol,2} -O _{mol,1}
-3	99.7	103.2
-2	99.1	103.2
-1	98.2	103
0	97	102.9
1	93.6	Dissociated
2	93.8	Dissociated
3	94	Dissociated

1.2 Calculation of the Gibbs free energy

We can compute the Gibbs free energy of adsorption (ΔG_{ads}) on the LNO surface as shown below:

$$\Delta G_{ads} = E_{ads-surf} - E_{bare-surf} - \frac{1}{N_{ads}} \left[E_{gas} + \tilde{u}_{gas}(T, p^o) + k_B T \ln \left(\frac{p_{gas}}{p^o} \right) \right] + E_{trans} + E_{rot} + E_{vib} + TS_{con} \quad (1)$$

where $E_{ads-surf}$ and $E_{bare-surf}$ represent the DFT energy of adsorbate-covered and bare LNO(001) surfaces, respectively, at $T = 0$ K. E_{trans} , E_{rot} , E_{vib} and TS_{conf} are the translational, rotational, vibrational and configurational entropy contributions, respectively. E_{gas} is the DFT energy of an isolated adsorbate in its gas phase and N_{ads} is the number of adsorbate on the LNO surface being produced from its gas phase. $\tilde{u}_{gas}(T, p^o)$ represents the temperature-dependent chemical potential of gas-phased adsorbate at reference pressure $p^o = 1$ atm and can be calculated from thermodynamic tables.¹

Using the ideal gas and Stirling approximations, we can calculate the thermodynamic contributions such as translational, rotational and vibrational motion as follows:²

$$E = N_A k_B T^2 \left(\frac{\partial \ln q}{\partial T} \right)_V \quad (2)$$

$$q_{trans} = \left(\frac{2\pi m_{gas} k_B T}{h^2} \right)^{\frac{3}{2}} \frac{k_B T}{p_{gas}} \quad (3)$$

$$q_{rot,linear} = \frac{8\pi^2 I k_B T}{\sigma h^2} \quad (4)$$

$$q_{rot,nonlinear} = \left(\frac{\pi^{0.5}}{\sigma}\right)(I_{xx}I_{yy}I_{zz})^{0.5}\left(\frac{8\pi^2k_B T}{h^2}\right)^{1.5} \quad (5)$$

$$q_{vib} = \left(\prod_j 1 - \exp\left(-\frac{h\nu_j}{k_B T}\right)\right)^{-1} \quad (6)$$

where q_{trans} and q_{rot} define the partition function for translation and rotation of gas-phase adsorbates, respectively. m_{gas} is the molar mass of adsorbate and A is the area covered by the adsorbate on the LNO surface. q_{vib} is the vibrational partition function of the adsorbate based on a set of $3N$ harmonic oscillators with ν_j representing the DFT frequency for the normal mode j of the adsorbate. N_A and k_B represent the Avogadro and Boltzmann constant, respectively.

Now, we can derive the average energy contribution of translational, rotational, and vibrational motions for linear and non-linear molecular adsorption in terms of partition functions by applying Eqn. (3)-(6) into Eqn. (2):

$$E_{trans} = \frac{3}{2}RT \quad (7)$$

$$E_{rot,linear} = RT \quad (8)$$

$$E_{rot,nonlinear} = \frac{3}{2}RT \quad (9)$$

$$E_{vib} = N_A \sum_j \frac{h\nu_j}{2} + \frac{h\nu_j \exp\left(-\frac{h\nu_j}{k_B T}\right)}{1 - \exp\left(-\frac{h\nu_j}{k_B T}\right)} \quad (10)$$

Finally, the configuration entropy can be measured utilizing the expression below:

$$TS_{conf} = k_B T \ln \frac{N!}{n!(N-n)!} \quad (11)$$

where N represents the total number of surface sites and n is the number of occupied surface

sites. The computed ΔG_{ads} of H, H₂O, O, OH, O₂, and O₂H on the unstrained LNO(001) surface are summarized in Table S2 at $T = 300$ K and $p_{gas} = 1$ atm.

Table S2. Gibbs free energy of adsorption (ΔG_{ads}) for H, H₂O, O, OH, O₂, and O₂H on the unstrained LNO(001) surface at $T = 300$ K and $p_{gas} = 1$ atm.

(eV/molecule)	<i>O₂ Adsorption</i>		<i>O Adsorption</i>	
	Gas State	Surface-bound State	Gas State	Surface-bound State
E_{DFT}	-9.857	-678.021	-9.857	-671.613
E_{vib}	0.149	0.230	0.149	0.097
E_{trans}	0.039	0.000	0.039	0.000
E_{rot}	0.026	0.000	0.026	0.000
$E_{bare - surf}$		-668.237		-668.237
TS_{conf}		0.036		0.036
$\tilde{u}_{gas}$		-0.548		-0.548
$k_B T \ln \left(\frac{p_{gas}}{p^o} \right)$		0.000		0.000
ΔG_{ads}		0.673		1.852

(eV/molecule)	<i>OH Adsorption</i>		<i>H Adsorption</i>	
	Gas State	Surface-bound State	Gas State	Surface-bound State
E_{DFT}	-7.581	-677.847	-6.770	-673.766
E_{vib}	0.276	0.407	0.104	0.098
E_{trans}	0.039	0.000	0.039	0.000
E_{rot}	0.026	0.000	0.026	0.000
$E_{bare - surf}$		-668.237		-668.237
TS_{conf}		0.036		0.036
$\tilde{u}_{gas}$		-0.476		-0.319
$k_B T \ln \left(\frac{p_{gas}}{p^o} \right)$		0.000		0.000
ΔG_{ads}		-1.452		-1.935

(eV/molecule)	<i>O₂H Adsorption</i>		<i>H₂O Adsorption</i>	
	Gas State	Surface-bound State	Gas State	Surface-bound State
E_{DFT}	-13.246	-682.480	-14.217	-683.189
E_{vib}	0.447	0.538	0.646	0.732
E_{trans}	0.039	0.000	0.039	0.000
E_{rot}	0.039	0.000	0.039	0.000
$E_{bare - surf}$		-668.237		-668.237
TS_{conf}		0.036		0.036

$\tilde{u}_{gas}$	-0.609	-0.484
$k_B T \ln \left(\frac{p_{gas}}{p^o} \right)$	0.000	0.000
ΔG_{ads}	-0.339	-0.207

We can see that the translational, rotational, vibrational, and configurational entropy contributions to the LNO system are relatively small (less than ~ 0.1 eV/molecule), and, thus, we neglect them when determining the overall trends in Gibbs free energy for our study.

In order to observe the trends in adsorption energetics of surface-bound species, ΔE_{ads} of O, OH, O₂, and O₂H on the top of surface Ni are summarized as a function of strain in Table S3.

Table S3. ΔE_{ads} of H₂O, O, OH, O₂, and O₂H on the top of surface Ni as a function of strain.

ΔE_{ads} (eV/molecule)					
Strain (%)	H ₂ O	O	OH	O ₂	O ₂ H
-3	-0.528	1.472	-2.074	0.027	-1.048
-2	-0.582	1.491	-2.078	0.023	-1.050
-1	-0.709	1.521	-2.068	0.035	-1.043
0	-0.735	1.552	-2.030	0.073	-0.997
1	-0.766	1.514	-2.031	0.076	Dissociated
2	-0.847	1.203	-2.103	0.023	Dissociated
3	-1.012	0.940	-2.187	-0.018	Dissociated

The strong preference of H atom towards the surface O over Ni as a function of strain can be seen in Table S4.

Table S4. ΔE_{ads} of H on the top of surface Ni and O as a function of strain.

ΔE_{ads} of H (eV/molecule)		
Strain (%)	On the top of surface Ni	On the top of surface O
-3	0.197	-2.090
-2	0.192	-2.105
-1	0.212	-2.147

0	0.270	-2.144
1	0.296	-2.145
2	0.285	-2.161
3	0.317	-2.168

1.3 Derivation of theoretical overpotential

We have adopted the derivation of the theoretical overpotential (η_{theor}) for studying the activity of oxygen electrocatalysis already described in the literature.³⁻⁸ If we set the reference potential to that of the Standard Hydrogen Electrode (SHE), we can relate the hydrogen in the gas phase ($H_{2,gas}$) to the solvated proton (H^+) and electron (e^-) in the system:



Then, the chemical potential (μ) of protons, electrons, and hydrogen can be described as below:

$$\mu_{H^+} + \mu_{e^-} = 0.5\mu_{H_{2,gas}} \quad (13)$$

$$\mu_{H^+} = u_{H^+}^o + k_B T \ln a_{H^+} \quad (14)$$

$$\mu_{e^-} = u_{e^-}^o - e\Delta V \quad (15)$$

$$\mu_{H_{2,gas}} = u_{H_2}^o + k_B T \ln p_{H_2} \quad (16)$$

Here, p_{H_2} shows the partial pressure of gas-phased hydrogen, a_{H^+} describes the activity of protons, and $e\Delta V$ defines the shift in electron energy when a bias is applied. $u_{H^+}^o$, $u_{e^-}^o$, and $u_{H_2}^o$ indicate the chemical potentials of protons, electrons and hydrogen under standard conditions ($T = 298.15$ K, $p_{H_2} = 1$ bar, and $a_{H^+} = 1$). Under these conditions, we can derive the additional relationship:

$$u_{H^+}^o + u_{e^-}^o = 0.5u_{H_2}^o \quad (17)$$

Another important assumption we need to make relates H_2O in the liquid phase to the gas phase. At $T = 298.15$ K, the chemical potential of liquid-phase H_2O is equal to that of gas-

phase H₂O at a pressure of ~0.035 bars.⁸ Thus, the chemical potential of liquid-phase H₂O can be approximated as:

$$\mu_{H_2O_{liquid}} = \mu_{H_2O_{gas}} \quad (18)$$

Under standard conditions, recalling Eqn. (1), the chemical potential of gas-phase molecules will be:

$$u_{gas}^o = E_{gas} + \tilde{u}_{gas}^o \quad (19)$$

where, again, E_{gas} is the DFT energy of an isolated adsorbate in its gas phase and $\tilde{u}_{gas}^o$ represents the temperature-dependent chemical potential of gas-phase adsorbates under standard conditions from thermodynamic tables.¹

Next, we derive the appropriate expressions for reaction pathway #1 (please refer to Table 1 in the main text), starting from the step (1), $\Delta G_{1,1}$:



$$\Delta G_{1,1} = E_{H_2O^*} - E_* - \mu_{H_2O_{liquid}} \quad (21)$$

where $E_{H_2O^*}$ and E_* are simply the DFT energy of the H₂O-adsorbed state and bare LNO surface, respectively. If we apply Eqn. (18) and (19) to Eqn. (21):

$$\Delta G_{1,1} = E_{H_2O^*} - E_* - (E_{H_2O} + \tilde{u}_{H_2O}^o) \quad (22)$$

Next, for the subsequent step (2) of reaction pathway #1, $\Delta G_{1,2}$:



$$\Delta G_{1,2} = E_{OH^*} + E_{H^*} - E_{H_2O^*} - E_* \quad (24)$$

where, again, E_{OH^*} and E_{H^*} represents the DFT energy of -OH and H-adsorbed states,

respectively. Now, for step (3) of reaction pathway #1, $\Delta G_{1,3}$:



$$\Delta G_{1,3} = E_{OH^*} + E_* + \mu_{H^+} + \mu_{e^-} - E_{OH^*} - E_{H^*} \quad (26)$$

We can apply Eqns. (14)-(16) to Eqn. (26) to get the following expression for $\Delta G_{1,3}$:

$$\Delta G_{1,3} = E_{OH^*} + E_* + k_B T \ln a_{H^+} + k_B T \ln p_{H_2} + u_{H^+}^o + u_{e^-}^o - e\Delta V - E_{OH^*} - E_{H^*} \quad (27)$$

Then, under standard conditions ($T = 298.15$ K, $p_{H_2} = 1$ bar, and $a_{H^+} = 1$), Eqn. (27) can be defined using Eqn. (17) and (19) as follows:

$$\Delta G_{1,3} = E_{OH^*} + E_* + 0.5(E_{H_2} + \tilde{u}_{H_2}^o) - e\Delta V - E_{OH^*} - E_{H^*} \quad (28)$$

A similar approach can be further taken from the step (3) to (10) in reaction pathway #1, which result in the following definitions of ΔG :

$$\Delta G_{1,4} = E_{OH^*} + E_{H_2O^*} - E_{OH^*} - E_* - (E_{H_2O} + \tilde{u}_{H_2O}^o) \quad (29)$$

$$\Delta G_{1,5} = 2E_{OH^*} + E_{H^*} - E_{OH^*} - E_* - E_{H_2O^*} \quad (30)$$

$$\Delta G_{1,6} = 2E_{OH^*} + E_* + 0.5(E_{H_2} + \tilde{u}_{H_2}^o) - e\Delta V - 2E_{OH^*} - E_{H^*} \quad (31)$$

$$\Delta G_{1,7} = E_{O_2H^*} + E_{H^*} - 2E_{OH^*} \quad (32)$$

$$\Delta G_{1,8} = E_{O_2H^*} + E_* + 0.5(E_{H_2} + \tilde{u}_{H_2}^o) - e\Delta V - E_{O_2H^*} - E_{H^*} \quad (33)$$

$$\Delta G_{1,9} = E_{O_2^*} + E_{H^*} - E_{O_2H^*} - E_* \quad (34)$$

$$\Delta G_{1,10} = 2E_* + (E_{O_2} + \tilde{u}_{O_2}^o) + 0.5(E_{H_2} + \tilde{u}_{H_2}^o) - e\Delta V - E_{O_2^*} - E_{H^*} \quad (35)$$

η_{OER} can then be determined from the highest value of ΔG (from the potential-determining step) amongst the possible reaction pathways.

$$G_{OER} = \max[\Delta G_{1,1}, \Delta G_{1,2}, \Delta G_{1,3}, \Delta G_{1,4}, \Delta G_{1,5}, \Delta G_{1,6}, \Delta G_{1,7}, \Delta G_{1,8}, \Delta G_{1,9}, \Delta G_{1,10}] \quad (36)$$

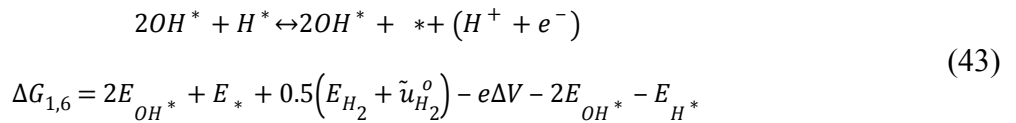
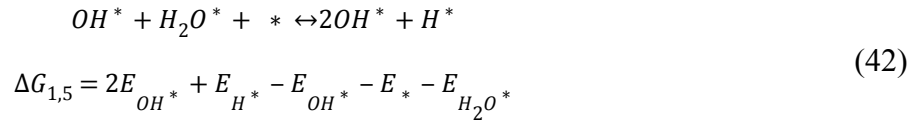
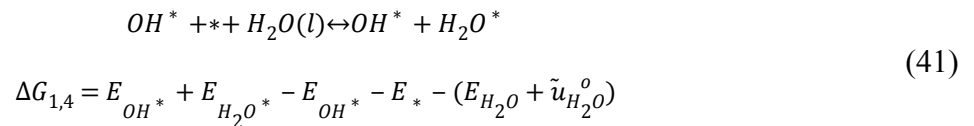
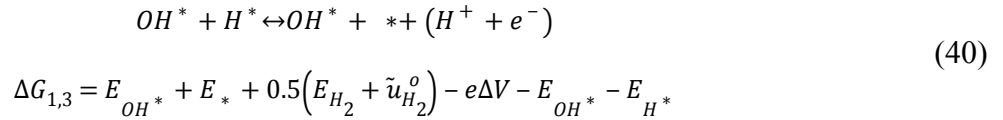
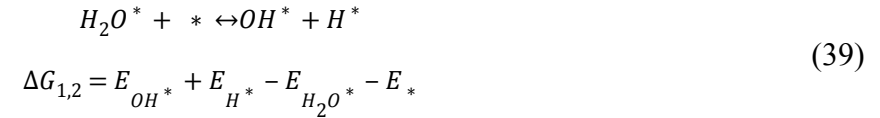
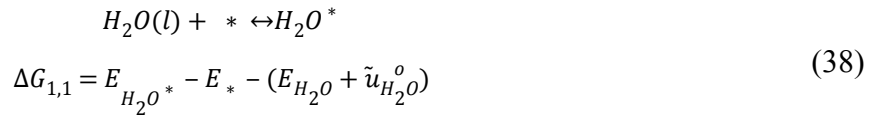
$$\eta_{OER} = \frac{G_{OER}}{e} - 1.23 \text{ V} \quad (37)$$

Again, we can repeat similar procedures for reaction pathway #2 (refer to Table 1) for the LNO system. Thus, the overall η_{OER} can be determined from the reaction pathway which yields the lowest value of η_{OER} .

1.4 Reaction pathways for the reversible OER and ORR on LNO(001)

The full list of definitions of ΔG for OER pathway #1 and #2, based on the SHE model, are summarized below:

Reaction Pathway #1:



$$\Delta G_{1,7} = E_{O_2H^*} + E_{H^*} - 2E_{OH^*}$$

$$O_2H^* + H^* \leftrightarrow O_2H^* + * + (H^+ + e^-)$$

$$\Delta G_{1,8} = E_{O_2H^*} + E_* + 0.5(E_{H_2} + \tilde{u}_{H_2}^o) - e\Delta V - E_{O_2H^*} - E_{H^*} \quad (45)$$

$$O_2H^* + * \leftrightarrow O_2^* + H^*$$

$$\Delta G_{1,9} = E_{O_2^*} + E_{H^*} - E_{O_2H^*} - E_* \quad (46)$$

$$O_2^* + H^* \leftrightarrow 2* + O_2 + (H^+ + e^-)$$

$$\Delta G_{1,10} = 2E_* + (E_{O_2} + \tilde{u}_{O_2}^o) + 0.5(E_{H_2} + \tilde{u}_{H_2}^o) - e\Delta V - E_{O_2^*} - E_{H^*} \quad (47)$$

Reaction Pathway #2:

$$H_2O(l) + * \leftrightarrow H_2O^*$$

$$\Delta G_{2,1} = E_{H_2O^*} - E_* - (E_{H_2O} + \tilde{u}_{H_2O}^o) \quad (48)$$

$$H_2O^* + * \leftrightarrow OH^* + H^*$$

$$\Delta G_{2,2} = E_{OH^*} + E_{H^*} - E_{H_2O^*} - E_* \quad (49)$$

$$OH^* + H^* \leftrightarrow OH^* + * + (H^+ + e^-)$$

$$\Delta G_{2,3} = E_{OH^*} + E_* + 0.5(E_{H_2} + \tilde{u}_{H_2}^o) - e\Delta V - E_{OH^*} - E_{H^*} \quad (50)$$

$$OH^* + * + H_2O(l) \leftrightarrow OH^* + H_2O^*$$

$$\Delta G_{2,4} = E_{OH^*} + E_{H_2O^*} - E_{OH^*} - E_* - (E_{H_2O} + \tilde{u}_{H_2O}^o) \quad (51)$$

$$OH^* + H_2O^* + * \leftrightarrow 2OH^* + H^*$$

$$\Delta G_{2,5} = 2E_{OH^*} + E_{H^*} - E_{OH^*} - E_* - E_{H_2O^*} \quad (52)$$

$$2OH^* + H^* \leftrightarrow 2OH^* + * + (H^+ + e^-)$$

$$\Delta G_{2,6} = 2E_{OH^*} + E_* + 0.5(E_{H_2} + \tilde{u}_{H_2}^o) - e\Delta V - 2E_{OH^*} - E_{H^*} \quad (53)$$

$$2OH^* + * \leftrightarrow O_2^* + 2H^* \quad (54)$$

$$\begin{aligned}
\Delta G_{2,7} &= E_{O_2^*} + 2E_{H^*} - E_* - 2E_{OH^*} \\
O_2^* + 2H^* &\leftrightarrow O_2^* + H^* + * + (H^+ + e^-) \\
\Delta G_{2,8} &= E_{O_2^*} + E_{H^*} + E_* + 0.5(E_{H_2} + \tilde{u}_{H_2}^o) - e\Delta V - E_{O_2^*} - 2E_{H^*} \\
O_2^* + H^* &\leftrightarrow 2* + O_2 + (H^+ + e^-) \\
\Delta G_{2,9} &= 2E_* + (E_{O_2} + \tilde{u}_{O_2}^o) + 0.5(E_{H_2} + \tilde{u}_{H_2}^o) - e\Delta V - E_{O_2^*} - E_{H^*}
\end{aligned} \tag{55}$$

$$\tag{56}$$

The full list of definition of ΔG for ORR pathway #1 and #2 are exactly opposite to that for OER (at $\Delta V = 0$ V). N.B. We found that the incorporation of the adsorption/desorption steps of H and H₂O into the SHE model is critical for accurately describing the OER activity on strained LNO(001). Therefore, we attempted to revise the conventional four-electron-transfer mechanism^{3, 7-9} in order to study the ORR activity. However, such modification of the four-electron-transfer pathway resulted in steps that did not involve any electron transfer (i.e. no longer potential-dependent and thermodynamically uphill at 0 V) and thus made it impossible to apply the SHE model for identifying the potential-determining steps and, ultimately, calculating the theoretical ORR overpotentials for LNO(001). This was not the case for the OER pathway. To circumvent this limitation, we decided to search for a descriptor that could be used to predict the ORR overpotential. Our results showed that the largest ΔG of the ORR pathways at 0 V seemed to adequately predict the overpotential and was, thus, useful for high-throughput exploration of such reactions.

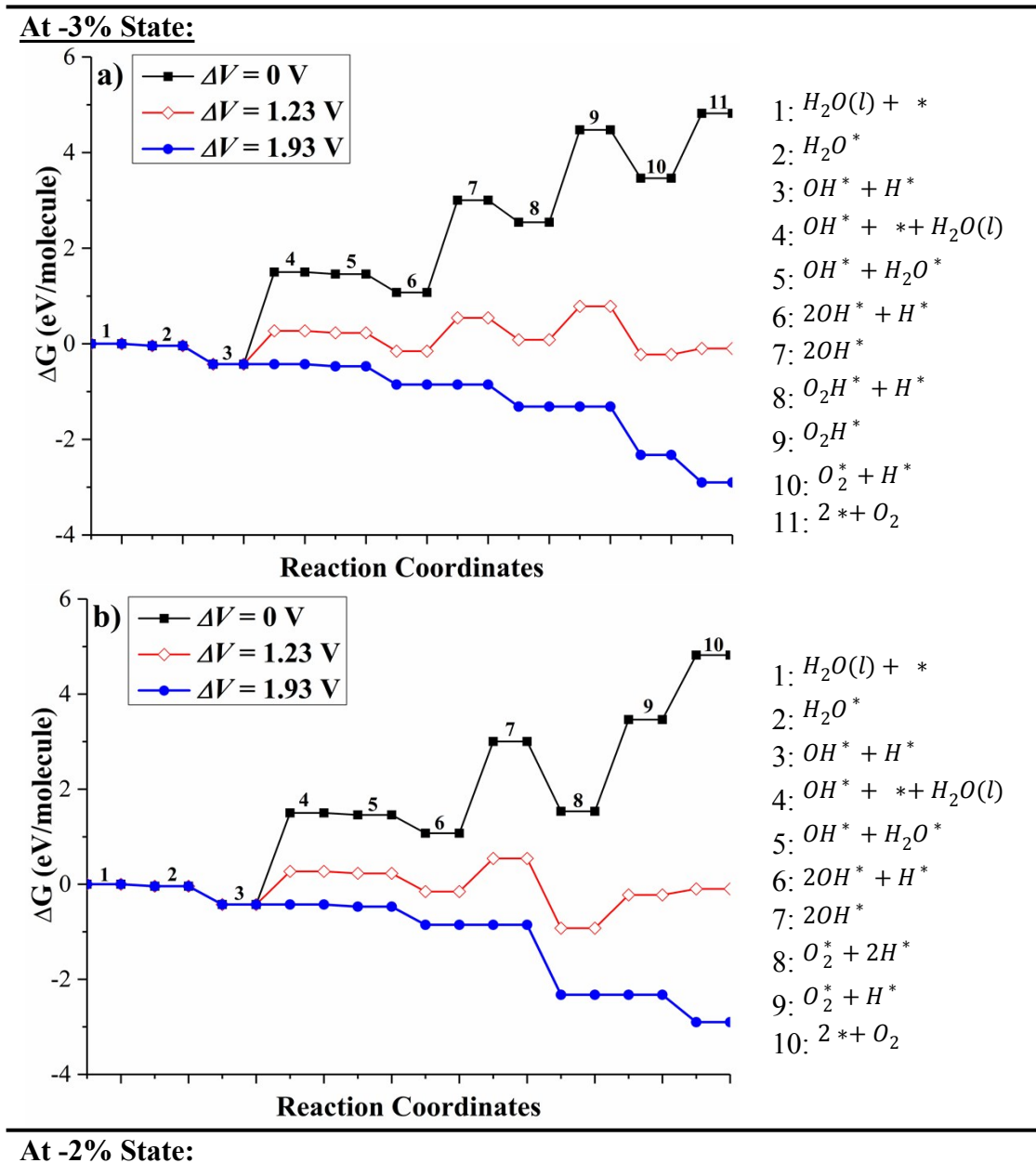
We also summarized the computed values of largest ΔG in the reaction pathways for the OER and ORR mechanisms at $\Delta V = 0$ V (ΔG^{OER} and ΔG^{ORR} , respectively) and resulting η_{OER} in Table S5.

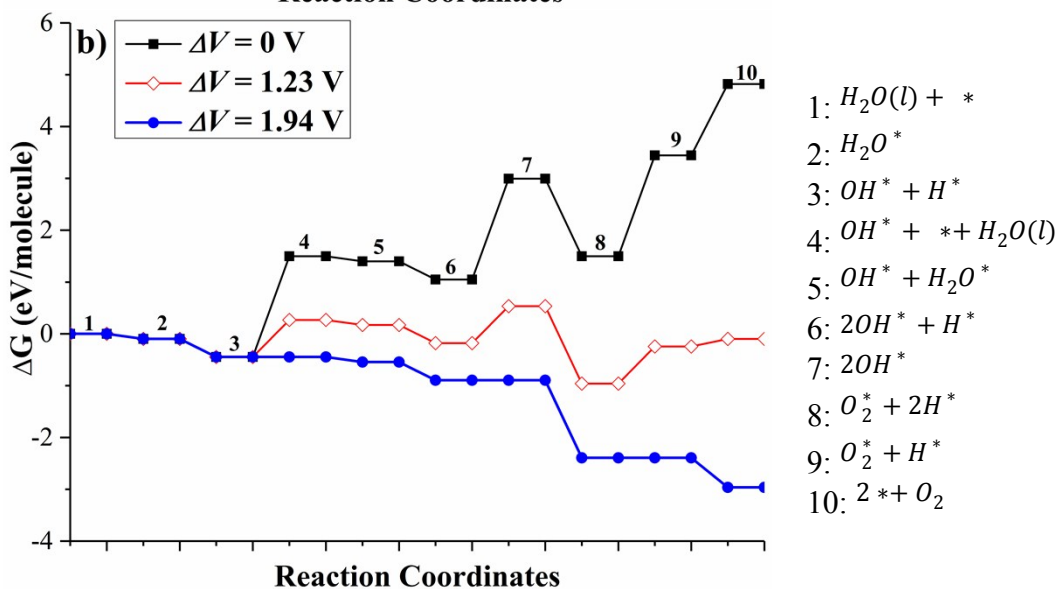
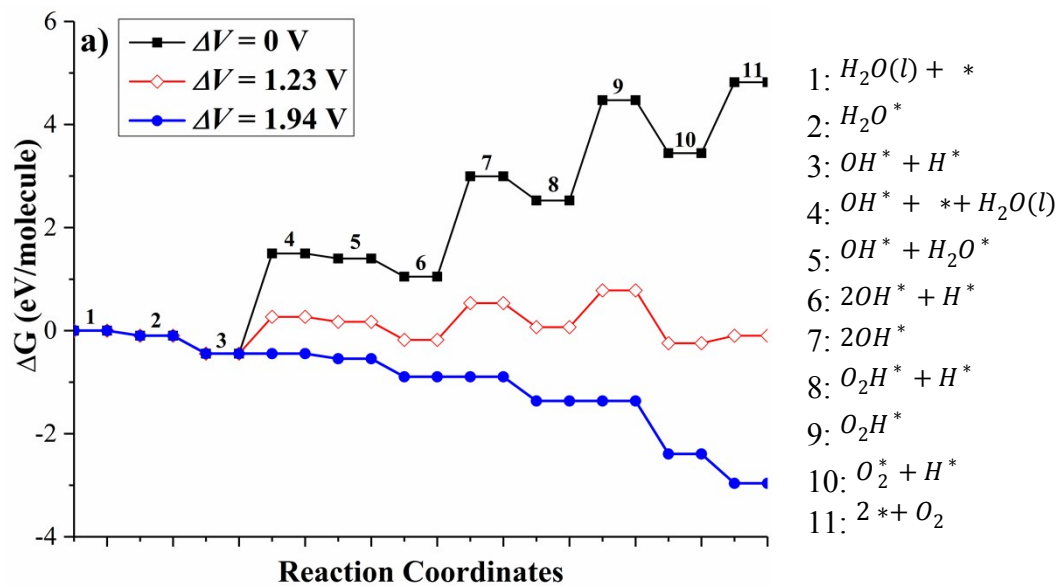
Table S5. ΔG^{OER} , ΔG^{ORR} , and η_{OER} as a function of strain.

Strain (%)	ΔG^{OER} (eV/molecule)	ΔG^{ORR} (eV/molecule)	η_{OER} (V)
-3	1.9302	1.0106	0.7002
-2	1.9460	1.0286	0.7160
-1	1.9880	1.0657	0.7580
0	1.9847	1.0699	0.7547
1	1.9858	1.6172	0.7558

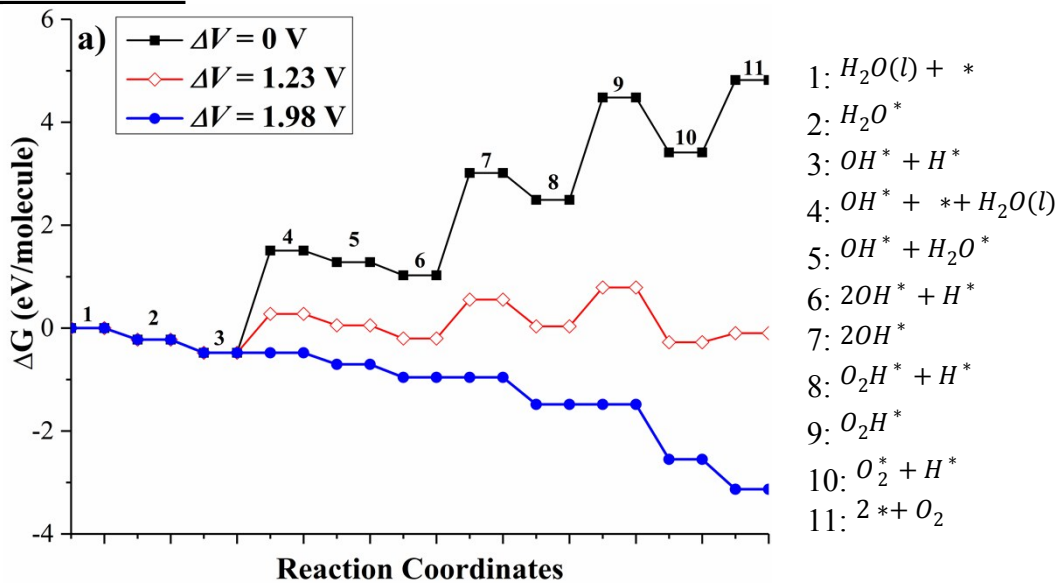
2	2.0017	1.5587	0.7717
3	2.0087	1.4450	0.7787

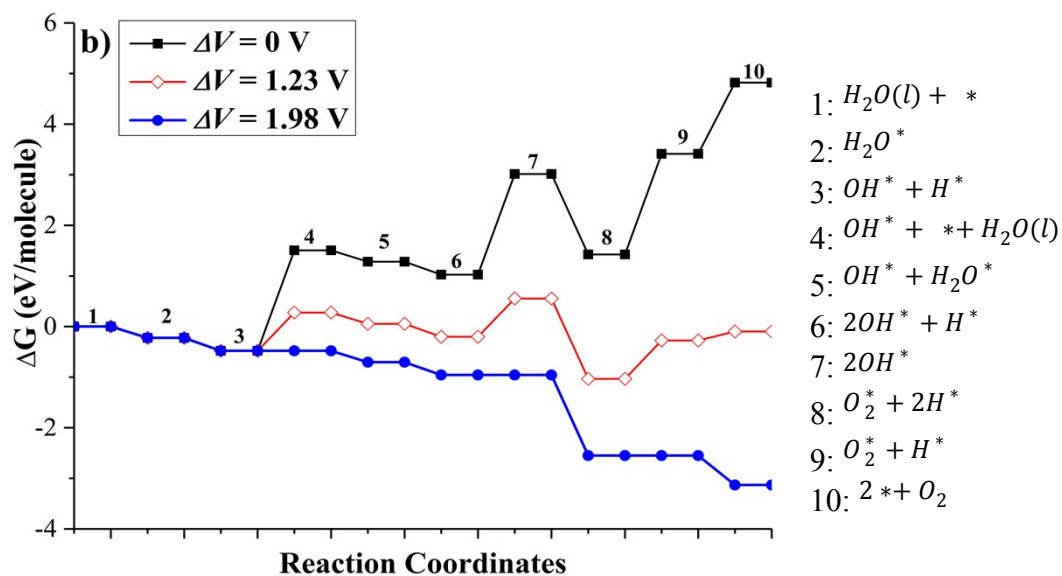
Also, Gibbs free energy diagram of OER pathway #1 and #2 were presented as a function of strain in Fig. S4 below:



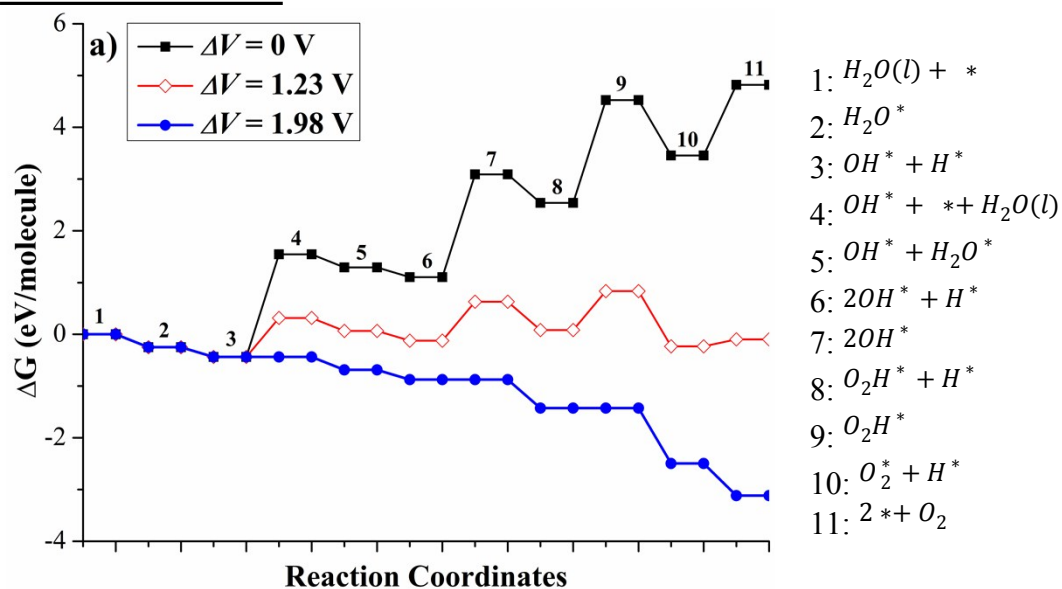


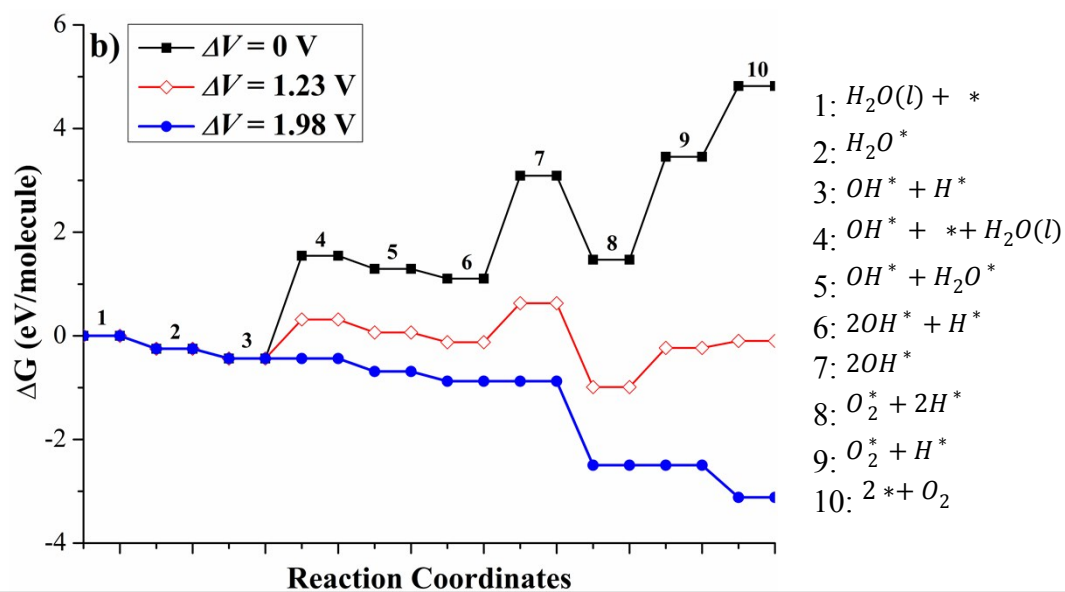
At -1% State:



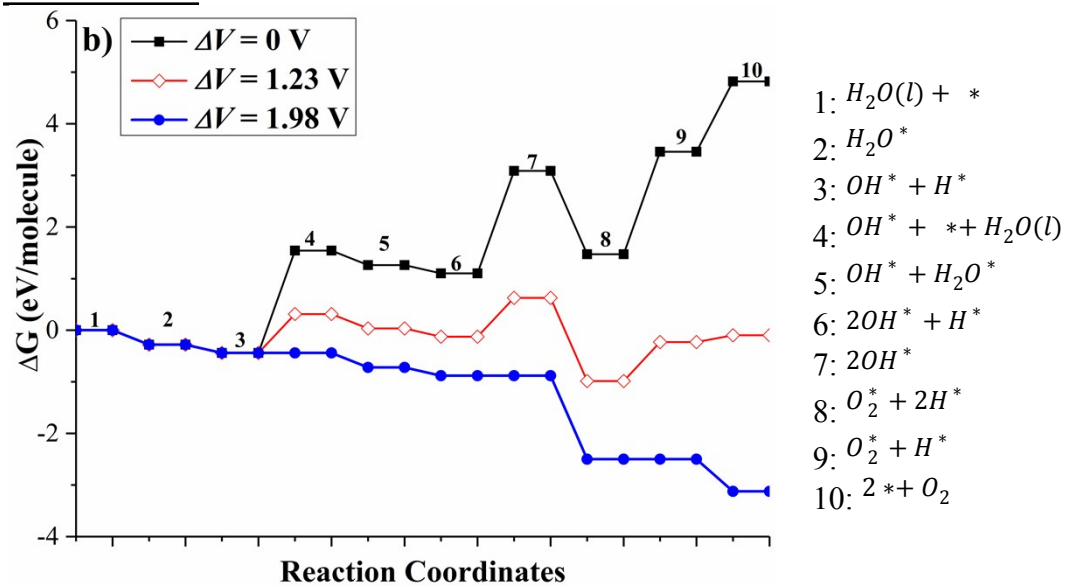


At Unstrained State:

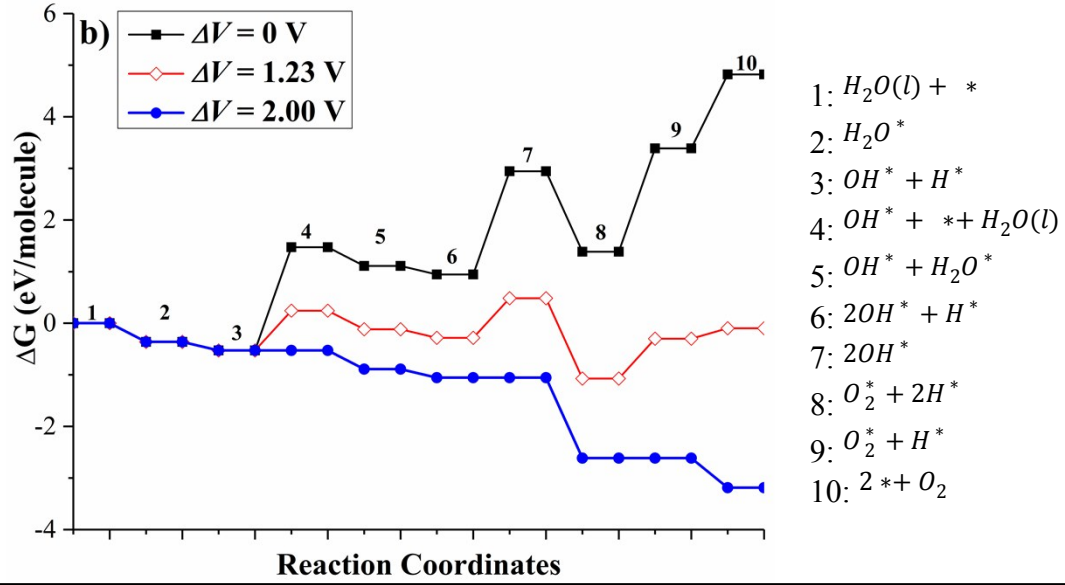




At +1% State:



At +2% State:



At +3% State:

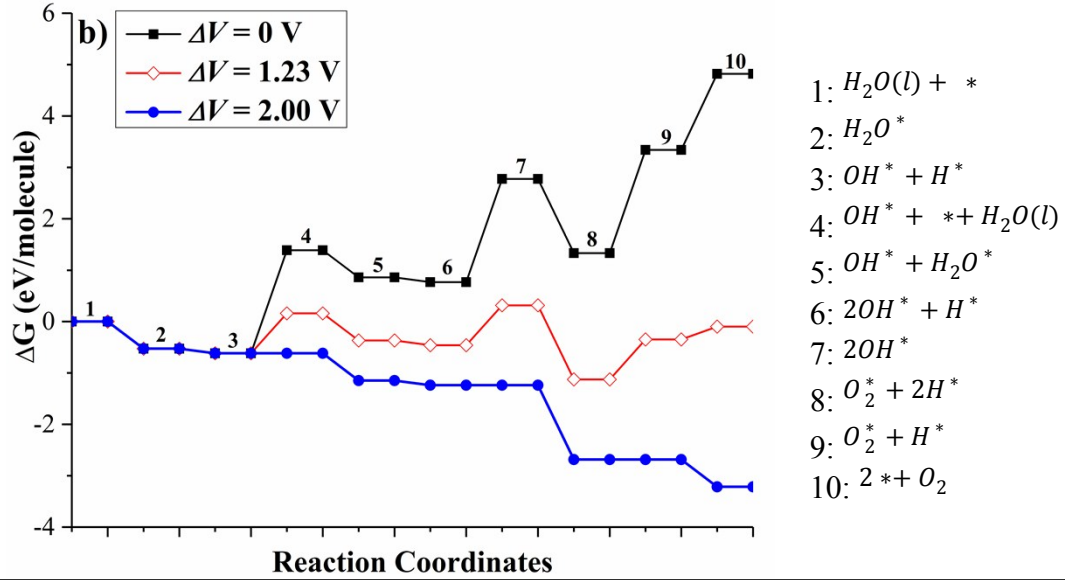
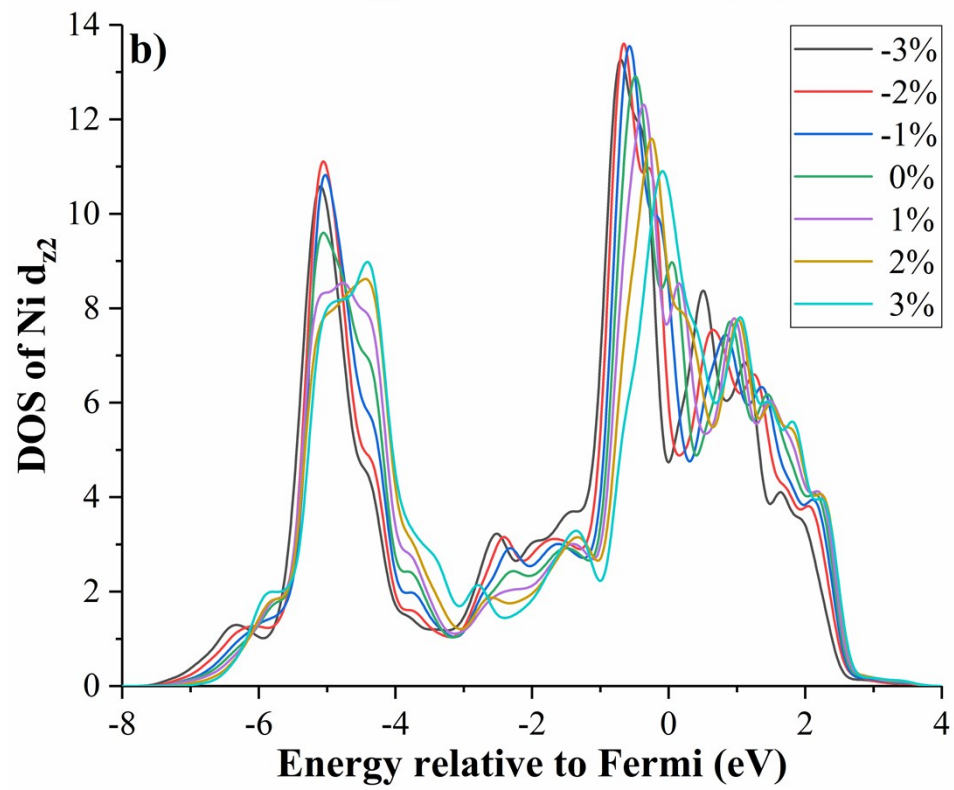
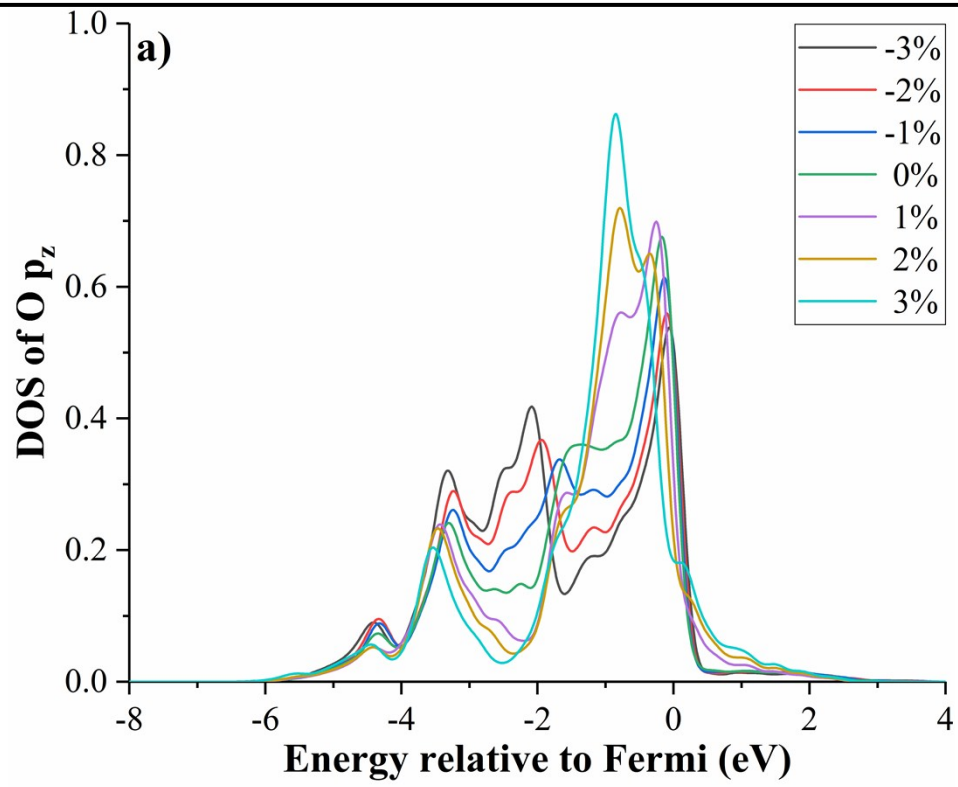


Figure S4. Gibbs free energy diagram of OER pathway a) #1 and b) #2 on the LNO(001) as a function of strain at $\Delta V = 0 \text{ V}$ (black solid squares), 1.23 V (red open diamonds) and the magnitude where all the steps become downhill (blue solid circles).

1.5 Electronic structure of strained LNO(001) surfaces

Fig. S5 presents the density of states (DOS) for the surface $O p_z$ on the bare LNO(001) surfaces and the adjacent surface $Ni d_{z^2}$ and $d_{x^2-y^2}$ after adsorption of H on the surface O.



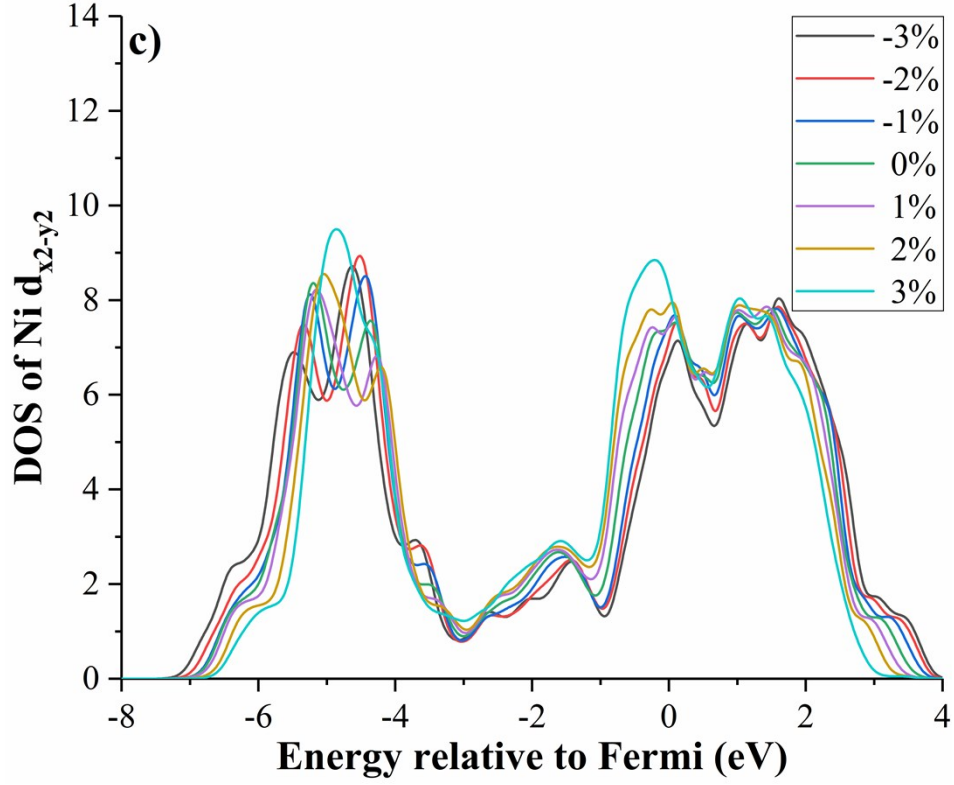


Figure S5. DOS of a) the surface O p_z on the bare LNO(001) surfaces, along with b) the surface Ni d_{z^2} and c) the surface Ni $d_{x^2-y^2}$ after H adsorption on the surface O

Table S6 summarizes the band centers of surface O p_z on the bare LNO(001) (O p_z center) and the band centers of surface Ni e_g after H adsorption on the surface O (Ni e_g center), along with their corresponding η_{OER} .

Table S6. O p_z center, Ni e_g center, and corresponding η_{OER} as a function of strain.

Strain (%)	O p_z Center	Ni e_g Center	η_{OER} (V)
-3	-1.203	0.337	0.7002
-2	-1.149	0.328	0.7160
-1	-0.982	0.311	0.7580
0	-0.951	0.313	0.7547
1	-0.823	0.313	0.7558
2	-0.780	0.300	0.7717
3	-0.767	0.286	0.7787

2.1 Summary of the periodic simulation cells used in our DFT calculations

The detailed information of our periodic simulation cells containing the fully-relaxed

unit cells and atomic coordinates is provided below in the VASP POSCAR format for the important intermediate states we explored on the LNO(001) surface.

-3% Strain State:

O ₂ adsorbed on the surface:										OH adsorbed on the surface:									
La Ni O										La Ni O H									
1.000000000000000										1.000000000000000									
7.4168595000000002		0.000000000000000			0.000000000000000					7.4168595000000002		0.000000000000000			0.000000000000000				
-0.1172806200000000		7.3694668400000003			0.000000000000000					-0.1172806200000000		7.3694668400000003			0.000000000000000				
0.0443473400000000		0.0366662800000000			40.0172788900000000					0.0443473400000000		0.0366662800000000			40.0172788900000000				
20	20	62								20	20	61	1						
Selective dynamics										Selective dynamics									
Direct										Direct									
0.0150382105500275	0.0031030551290024	0.1003744200777849	T	T	T					0.0120890985302816	0.0065610766256695	0.1003680692585050	T	T	T				
0.5121534480932439	0.0061279513127908	0.1003340844978322	T	T	T					0.5088108458486098	0.0107215461650931	0.1003541362136175	T	T	T				
0.0108206936031403	0.5065100652171662	0.1003031271102081	T	T	T					0.0076320350347950	0.5111986793252588	0.1003229895439925	T	T	T				
0.5155184452202864	0.5047897986226876	0.1003391526057088	T	T	T					0.5129112409612355	0.5082370344357962	0.1003114260545210	T	T	T				
0.0036677916433379	0.0024111554822346	0.1980695737120488	T	T	T					0.0005667245031346	0.0028150527526815	0.1980358137766158	T	T	T				
0.5002197913643830	0.0024889562079315	0.1980387889643860	T	T	T					0.4969023754415350	0.0037984389807630	0.1980327762190392	T	T	T				
0.0011645757052509	0.5024531932964705	0.1980222511814092	T	T	T					0.9977674773605101	0.5038493197600127	0.1980378748630329	T	T	T				
0.5036238675848255	0.5014028278035797	0.1980218931163253	T	T	T					0.5004516939651886	0.5016410365917161	0.1980301692647148	T	T	T				
0.0076849979988435	0.0030948962570096	0.2978760648327374	T	T	T					0.0052295263032476	0.0071907232264027	0.2978657208036991	T	T	T				
0.5089630120431469	0.0028915236777266	0.2979256974230550	T	T	T					0.5066723425905254	0.0064874482671592	0.2980104393954408	T	T	T				
0.0086004227021833	0.5035318490339826	0.2979787318204121	T	T	T					0.0063930673590858	0.5072145848903779	0.2979810439811966	T	T	T				
0.5083649480027814	0.5035543060186920	0.2978100613406169	T	T	T					0.5059670245065448	0.5075943692380367	0.2978973279977311	T	T	T				
0.0098287962859558	0.0027426365948809	0.3986558537688840	T	T	T					0.0087277083313538	0.0077912144701239	0.3986164884531676	T	T	T				
0.5100556423719403	0.0032208173347883	0.3985066469689510	T	T	T					0.5088109393168051	0.0084334631893457	0.3985601421467083	T	T	T				
0.0089341310225329	0.5033225221696115	0.3985805834092548	T	T	T					0.0076888764024662	0.5084523799957517	0.3985541869107183	T	T	T				
0.5098704577945241	0.5037094802307690	0.3986045249324024	T	T	T					0.5086851084448214	0.5088523392149170	0.3987158532593610	T	T	T				
0.0107050689770884	0.0034277999414436	0.5039972162684936	T	T	T					0.0107748027997470	0.0088162621363662	0.503963883837320	T	T	T				
0.5092537095010559	0.0039299104073720	0.5043800481252606	T	T	T					0.5099422152447192	0.0087665625923517	0.5042894467756112	T	T	T				
0.0108496339374465	0.5022303529316835	0.5041911486651732	T	T	T					0.0108829116142910	0.5080804979218086	0.5041693343599511	T	T	T				
0.5089713159548851	0.5024765834198949	0.5041664054739823	T	T	T					0.5092614817128260	0.5082604081230565	0.5039684455175569	T	T	T				
0.2570163766325289	0.2541374777832886	0.1454859960894677	T	T	T					0.2537445366714132	0.2564994776458080	0.1454595993268066	T	T	T				
0.7573910341291321	0.2530369077795617	0.1457105924098376	T	T	T					0.7544041114413048	0.2552821866196575	0.1457240119134785	T	T	T				
0.2574204129870369	0.7530973253250217	0.1457301816757466	T	T	T					0.752544999992979159	0.7553099475850976	0.1457299520605144	T	T	T				
0.7570366843998569	0.7541552531527433	0.1458845178783697	T	T	T					0.7537446678841515	0.7564963538783981	0.1458977577976566	T	T	T				
0.2562863122673036	0.2533864897200214	0.2469611492041509	T	T	T					0.2536155502511666	0.2561301093788958	0.2470026456217883	T	T	T				
0.7566549754876131	0.2525365409985802	0.2467543542648062	T	T	T					0.7540986173242092	0.2552658139300899	0.2467804121548909	T	T	T				
0.2565811965428274	0.7523998704827726	0.2467445815481644	T	T	T					0.2541217555071438	0.75524445151728979	0.2467737326367263	T	T	T				
0.7563514405757520	0.7534584314874445	0.2466431774484321	T	T	T					0.7534909839496530	0.7562477713094162	0.2466659503058335	T	T	T				
0.2589910818948342	0.2529382372950653	0.3474759191649259	T	T	T					0.2573776448038818	0.2574151428523366	0.3475209753407387	T	T	T				
0.7588061227672750	0.2536155660098561	0.3475415152204832	T	T	T					0.7568882336541763	0.2580845840133154	0.3475918880462734	T	T	T				
0.2588008652560070	0.7535217038594095	0.3475461928874555	T	T	T					0.2568924865503366	0.7580806314143549	0.3475890987337887	T	T	T				
0.7589936255058100	0.7529463473271090	0.3475429866738597	T	T	T					0.7573407097229032	0.7573417729376707	0.3475843995532831	T	T	T				
0.2600545678359755	0.2534511873809420	0.4486565488898530	T	T	T					0.2592588259804390	0.2589010039047057	0.4487097517895188	T	T	T				
0.7599151569556104	0.2530827273678380	0.4491578942925925	T	T	T					0.7595982756456247	0.2583345805854496	0.4491547697163727	T	T	T				
0.2602046927547212	0.7530993627703032	0.4491582115665104	T	T	T					0.2595738680492924	0.7585667655137103	0.4491579564868347	T	T	T				
0.7579793221082074	0.7534514105012259	0.4494486158926957	T	T	T					0.7594056821503479	0.7587359749778105	0.4494012103654358	T	T	T				
0.2583772888478871	0.2535077793696908	0.5556699840386998	T	T	T					0.2598319597310994	0.2582298741708441	0.5553245759516090	T	T	T				
0.7595795060838668	0.2531134825462984	0.5529281622773472	T	T	T					0.7597317382290103	0.2582977598686040	0.5529805068978937	T	T	T				
0.2591844267165335	0.7527461193661964	0.5527564656745902	T	T	T					0.2595231014720038	0.7566959957348545	0.5527936828589660	T	T	T				
0.7592050350889518	0.7528262356049293	0.5515661720734520	T	T	T					0.7594609811784279	0.7573937474705412	0.5515408902682207	T	T	T				
0.2599603700772193	0.2465385606299958	0.0906008326195529	T	T	T					0.2589921299526523	0.2477941523105913	0.0906873472664350	T	T	T				
0.7528653988663144	0.2603356086124005	0.09000064835916379	T	T	T					0.7469872596078755	0.2628388552662456	0.0900114151096413	T	T	T				
0.2530066897532007	0.76052418159564120	0.08994943176973014	T	T	T					0.247345545494154806	0.7633601920633503	0.0899742334745457	T	T	T				
0.7598227148504098	0.74646006049505516	0.0896942435257397	T	T	T					0.75940450167895801	0.7476772708465329	0.0896732877653173	T	T	T				
0.2534975040173513	0.2595764204977667	0.19428220334495494	T	T	T					0.2481588028852852	0.2627863091616950	0.1941805378062025	T	T	T				
0.758442493231958	0.246436351932272	0.19467046728523012	T	T	T					0.7576177693123248	0.247985240644148	0.1946582147400252	T	T	T				
0.2583077911681073	0.74632337220667171	0.1947106198278674	T	T	T					0.2575376088667017	0.7477156678442655	0.1946917027156206	T	T	T				
0.7538037063613520	0.7594638565969244	0.1949514613568191	T	T	T					0.7484198350134916	0.7622256947588426	0.194925619356147	T	T	T				
0.2594064460042024	0.249443705598820	0.2986832709186300	T	T	T					0.25892844009625867	0.71922720054471395	0.29872364503034438	T	T	T				
0.7567236803266928	0.2572353779260740	0.2988242816287933	T	T	T					0.7527601795406528	0.2622080790761296	0.298899532892684	T	T	T				
0.2566855488229453	0.7569604080766473	0.2988124288674354	T	T	T					0.2529846461248534	0.76245460560561321	0.2988821375346804	T	T	T				
0.7596908133020711	0.7489654831150604	0.2988182345834061	T	T	T					0.7588641441643562	0.752003382461657	0.2988473817203617	T	T	T				
0.2582001186414513	0.2558758517015227	0.3977919183357272	T	T	T					0.2557664807422866	0.6200801329649420	0.3979362070035555	T	T	T				
0.7602704002227980	0.2502832414536214	0.3967660954038896	T	T	T					0.7604200980350996	0.2542023134209970	0.3968138919223554	T	T	T				
0.2602906734121400	0.7504862855468962	0.3967280223080065	T	T	T					0.2600868503069922	0.7540438653886842	0.3967749618646397	T	T	T				
0.7582838952283172	0.7560243370043631	0.39673625318204948	T	T	T					0.7560575708663432	0.7616628114968048	0.396458052671502	T	T	T				
0.2604784467457388	0.2514084096912385	0.4944648146699707	T	T	T					0.2607027333646482	0.2558077800446520	0.4946451253550024	T	T	T				
0.7587226652117990	0.2544416504046207	0.4951741020943742	T	T	T					0.7586664578166601	0.2600159224621748	0.495186126632321	T	T	T				
0.2592916353926834	0.754066369089201	0.4952158312083323	T	T	T					0.2587730008090000	0.7605082572250907	0.4952378280377046	T	T	T				
0.7597635070748792	0.7517010903920201	0.4957058421031024	T	T	T					0.7603460869177796	0.7564854316223397	0.4956836532225412	T	T	T				
0.2140592969846126	0.0030234860591747	0.1461430074137859	T	T	T					0.2112003024209602	0.0052667760013565	0.1462480362511396	T	T	T				
0.7984307380444806	0.0039068839036124	0.1425838175370908	T	T	T					0.7948716489490121	0.0061305485393767	0.1424646057428020	T	T	T				
0.2986376495659253	0.5041901715988012	0.1425669157522188	T	T	T					0.2950824963019302	0.5								

0.3143418290385881	0.5042946856844663	0.4475307682017244	T	T	T	0.3140871593608764	0.5097132507467323	0.4479597472852892	T	T	T
0.7100285240218800	0.5030113501919118	0.4462104493975283	T	T	T	0.7098283041312530	0.5082153521255975	0.4461012071867569	T	T	T
0.2653841820935409	0.0032060803533431	0.5453988635901971	T	T	T	0.2661649851509503	0.0093360673617695	0.5458485087030744	T	T	T
0.7528385027507337	0.0036774041808108	0.5468610288311601	T	T	T	0.7532569482715711	0.0088444123261704	0.5470495729953582	T	T	T
0.2547113988326785	0.50119920569818402	0.5451404805553852	T	T	T	0.25472299763342552	0.5075981795877634	0.5450889759845947	T	T	T
0.7694485472389716	0.5021122979589844	0.5471863860446378	T	T	T	0.7701168178202847	0.5072528217042183	0.5472924840974119	T	T	T
0.0072290917059774	0.2952048336630143	0.1438092962167703	T	T	T	0.0040529540750323	0.2967697883817715	0.1432470576114619	T	T	T
0.5068857747365755	0.2117167089236297	0.1450151952510913	T	T	T	0.5037456910442952	0.2139187722454493	0.1456084803282732	T	T	T
0.0066216042004945	0.7119793987020074	0.1449508223398631	T	T	T	0.0034587292079796	0.7143076380130884	0.1455253806738522	T	T	T
0.5075637131276850	0.7950745199726156	0.1438729804732937	T	T	T	0.5045400514581787	0.7966210911244931	0.1433219225651202	T	T	T
0.0070681278700577	0.3004056788480073	0.2465792602296526	T	T	T	0.0044980609659478	0.3033943971990661	0.2471264929752754	T	T	T
0.5059860642011883	0.2062305803258780	0.2457795500261311	T	T	T	0.5033440311045686	0.2093595905416601	0.2452332339044959	T	T	T
0.0061373136923376	0.7061227560462979	0.2458553906516395	T	T	T	0.0034849765423203	0.7093173927448617	0.2453663245833246	T	T	T
0.5068933840876085	0.8002714748468155	0.2466827982870667	T	T	T	0.5043196091405480	0.8034638570688769	0.2472380752316779	T	T	T
0.0086906874196431	0.2034060990091528	0.3468069481310526	T	T	T	0.0068809068148284	0.2083247516777103	0.3465096771480874	T	T	T
0.5091584643754270	0.3038670457903525	0.3472250310355252	T	T	T	0.5073831804242170	0.3083684441154977	0.3476719474003751	T	T	T
0.0094907402147676	0.8033513134561222	0.3471347010006863	T	T	T	0.0076691335147663	0.8081798343895567	0.3474075223848521	T	T	T
0.5083433741895954	0.70365521021605668	0.3466571682841085	T	T	T	0.5065424117731374	0.7085526172550517	0.3464471784358310	T	T	T
0.0102450336547304	0.3053041527348361	0.4472271070968887	T	T	T	0.0097453000210617	0.3117782027490341	0.4474630900605628	T	T	T
0.5100021001229965	0.2019427312355453	0.4467285415808364	T	T	T	0.5093829911115297	0.2079119064473834	0.4465530029396186	T	T	T
0.0094331419136991	0.7031736930258810	0.4466365168281591	T	T	T	0.0088410583790931	0.7088633640034525	0.4464700306276905	T	T	T
0.5107522458692224	0.8049683169016044	0.4470301754330095	T	T	T	0.5103221494939562	0.8103827055315782	0.4471810419383304	T	T	T
0.0102428725582751	0.2462866312655264	0.5451048922475302	T	T	T	0.0103528621597120	0.2523824521682166	0.5449659241053592	T	T	T
0.5094038257531587	0.2588310968054487	0.5455703711812032	T	T	T	0.5099718005530091	0.2640313118979064	0.5450321372569407	T	T	T
0.0103697230759754	0.7601122260324694	0.5462648089045816	T	T	T	0.0106996821741640	0.7669075194430192	0.5460962996684822	T	T	T
0.5087839105149105	0.7456321857593033	0.5462859960762603	T	T	T	0.5089197749215483	0.7512627895789920	0.5459393444938321	T	T	T
0.2628969639756146	0.2461473340235556	0.6016944565467344	T	T	T	0.2596206698886345	0.2466193796048660	0.5997803837504101	T	T	T
0.152546584922272	0.3410080927307891	0.6176656588218915	T	T	T	0.2613793225291214	0.1159135952558699	0.6043254628002428	T	T	T

O adsorbed on the surface:						H adsorbed on the surface (O):					
La Ni O						La Ni O H					
1.0000000000000000						1.0000000000000000					
7.4168595000000002						7.4168595000000002					
-0.1172806200000000						-0.1172806200000000					
0.0443473400000000						0.0443473400000000					
20	20	61				20	20	60	1		
Selective dynamics						Selective dynamics					
Direct						Direct					
0.0122872602728954	0.0069055524667379	0.1005469342158485	T	T	T	0.0125819279155476	0.0076149284227920	0.1002566092167975	T	T	T
0.5088417096374189	0.0112448647113072	0.1005782677747605	T	T	T	0.5078433325745134	0.0115215136001555	0.1002553032629384	T	T	T
0.0076338496529702	0.5117466566531530	0.1005551753903361	T	T	T	0.0073242923012325	0.5113380154362365	0.1002712762621661	T	T	T
0.5131315597165390	0.50858358788760399	0.1004616247017752	T	T	T	0.5126040005541121	0.5075956608058942	0.1002423079255417	T	T	T
0.0007728952038068	0.0024044932439429	0.1981551356871929	T	T	T	0.9991376243638268	0.0021240554145123	0.1980113178687698	T	T	T
0.4972629121366746	0.0036627042119732	0.1982299958116073	T	T	T	0.4956298485863451	0.0037157310120036	0.1980058494102637	T	T	T
0.9982322851825318	0.5036465006728096	0.1982238560288032	T	T	T	0.9957562374141189	0.5038158300097805	0.1981091070611913	T	T	T
0.5007345991810420	0.5013959944065596	0.1981420649574972	T	T	T	0.4990747242184957	0.5020775409029042	0.1980630367484366	T	T	T
0.0053255494824799	0.0068662346061678	0.2978767479041214	T	T	T	0.0034787891485082	0.0070410360324261	0.2977472282746755	T	T	T
0.5066996935038465	0.0063123408638437	0.2980997224983523	T	T	T	0.5040412475779883	0.0066533222818896	0.297956838771015	T	T	T
0.0064157727360998	0.5069698314358867	0.2980276059173120	T	T	T	0.0037294209713784	0.5067329922468097	0.2980339147427411	T	T	T
0.5059979860872234	0.5072830785350075	0.2978985635500243	T	T	T	0.5032264836646946	0.5071683417389680	0.2981541031543529	T	T	T
0.0087202953871060	0.0073401394856732	0.39850733093160453	T	T	T	0.0055259552340501	0.0080506127430072	0.3981851435522904	T	T	T
0.508794277230367	0.0077304603085677	0.3984853244862072	T	T	T	0.5050664196779874	0.0078828334559070	0.3981848480393775	T	T	T
0.0077327225965803	0.5080228804147308	0.3984487107388280	T	T	T	0.0044320814706320	0.5080290022046545	0.3989810239606228	T	T	T
0.5088493248456838	0.5081764823579364	0.3985785086817805	T	T	T	0.5044387652673991	0.5081191893116542	0.3993468866086200	T	T	T
0.0105957039814319	0.0088427804710070	0.5037371724271713	T	T	T	0.0037379091372471	0.0086690313561007	0.5019824255887008	T	T	T
0.5097228251947186	0.0088242478568867	0.5039380639218705	T	T	T	0.5131440123507274	0.0077066871673765	0.5025071866346340	T	T	T
0.0105217906942091	0.5078105624988376	0.5039639542340298	T	T	T	0.0094659311759509	0.5088143818309843	0.5038384062595265	T	T	T
0.5089365757741561	0.5079816064983589	0.5038123125467227	T	T	T	0.5087276537802364	0.5076292077588563	0.5050027312360745	T	T	T
0.2540006182187255	0.2566373665967800	0.1456823037630053	T	T	T	0.2528920450924118	0.2566526319389141	0.1457256473738966	T	T	T
0.7547318788877643	0.2554766311542873	0.1459285626879229	T	T	T	0.7537442545493446	0.2553355571240770	0.1457884876213029	T	T	T
0.2547834712321357	0.7554788565933346	0.1459265681625244	T	T	T	0.2536647383299949	0.7552794911708359	0.1457175375816419	T	T	T
0.7539208772247601	0.756613457949885	0.1461081526439348	T	T	T	0.7529085799345598	0.7566133202272006	0.1457570255477926	T	T	T
0.2536461446562816	0.2559268745684836	0.2470825645019080	T	T	T	0.2521028464596628	0.2561957108959019	0.2467911065706648	T	T	T
0.7542150601341561	0.2550588321637223	0.2468948793765881	T	T	T	0.7524794725554068	0.2551408161514007	0.2467582459176927	T	T	T
0.2542269578979479	0.7550567378852879	0.2468895484220209	T	T	T	0.2526785007212783	0.7550011455743177	0.2467904265958862	T	T	T
0.7534626316410342	0.7560212291429286	0.2467837715669570	T	T	T	0.7517975521273531	0.7560084417724096	0.2467585072546487	T	T	T
0.2574214679308482	0.256690329468698	0.3474887929370916	T	T	T	0.2548951816242451	0.2578659480294870	0.3477216481204677	T	T	T
0.7569887426793056	0.2575818528175265	0.3475544188572694	T	T	T	0.7545844135044167	0.2579012625697017	0.3476902083428110	T	T	T
0.2569453019025169	0.7575851177606515	0.3475659633508970	T	T	T	0.2544114610850202	0.7570819446469923	0.3477214495692818	T	T	T
0.7573992463071563	0.7569012956467572	0.3475583053871422	T	T	T	0.7549924643904157	0.7568862784484475	0.3476919429746033	T	T	T
0.2593403262765005	0.2585277569031719	0.4484400620392979	T	T	T	0.2581314218963314	0.2565916998039379	0.4495650478252942	T	T	T
0.7596497647277094	0.2579936364162227	0.4489934634977443	T	T	T	0.7578005720532590	0.2584948750739812	0.4491013606190135	T	T	T
0.2595703398592488	0.7578977605763573	0.4489939707331336	T	T	T	0.2580289116879624	0.7596488568999228	0.4495608176782835	T	T	T
0.7594790695890967	0.7582380864540531	0.4492985566574229	T	T	T	0.7574726669882150	0.7576484274969971	0.4491071463587257	T	T	T
0.2594040172839207	0.2579903544912543	0.5569505954339860	T	T	T	0.2574224258617779	0.2623626171308713	0.5532153356184686	T	T	T
0.7593499531396882	0.2582175462527904	0.5531841282301933	T	T	T	0.7618336605006385	0.2580031106663293	0.5512187080767457	T	T	T
0.2593272094779533	0.7581458419310608	0.5529962343598946	T	T	T	0.2579012849164636	0.7533555007928888	0.55232945095978697	T	T	T
0.7591285949356463	0.7580639476688690	0.5511442801539856	T	T	T	0.7621377898258920	0.7583044984050838	0.5512016572571946	T	T	T
0.2597951020267499	0.2476657568038297	0.0909020608102788	T	T	T	0.2590192067841289	0.2466345162248752	0.0899549755001107	T	T	T
0.7472429842537489	0.2632255245981413	0.0904004815333759	T	T	T	0.7466232443946879	0.2644124590760287	0.0897523083308650	T	T	T
0.2472848331035634	0.7636974754260608	0.0902138742424810	T	T	T	0.2465065695984928	0.7643666759431799	0.0899491996213180	T	T	T
0.759526908689240	0.7475254461566053	0.0890987815337249	T	T	T	0.7590738941381034	0.7466169771434940	0.08989778618574777	T	T	T
0.2481057734264818	0.26258919107198804	0.1944189760171758	T	T	T	0.2469150287560076	0.263033657828770	0.1947063819731342	T	T	T
0.7582607111216639	0.2481600698629491	0.1948757677080741	T	T	T	0.7566602427532528	0.2471908448780018	0.1947981616839302	T	T	T
0.2582113436980610	0.7478272900843356	0.1948893241436630	T	T	T	0.2565407790699041	0.7470369023989335	0.1946782514955114	T	T	T
0.7482030038747939	0.7618210588782570	0.1951975720639810	T	T	T	0.7471713145417100	0.7628428051066704	0.1947604074599556	T	T	T
0.2589734741262256	0.2517558613052005	0.1983136207738670	T	T	T	0.2581835847138892	0.2507608097575676	0.2898613856864546	T	T	T
0.7528910081711310	0.2614259888295125	0.2988665342560005	T	T	T	0.7497192150365349	0.262984294306619	0.2989876496461618	T	T	T
0.2528989898054746	0.7618787444040360	0.298734945984681	T	T	T	0.2515200027046623	0.7628247003002588	0.2989769843665263	T	T	T
0.7589790110001563	0.7519732408988960	0.298348901630263	T	T	T	0.7562226770395876	0.7506664287068652	0.2989950433191007	T	T	T
0.2557717126359001	0.2621912366605020	0.39768680720761674	T	T	T	0.2512128881706714	0.2657839323248094	0.3969952815280929	T	T	T
0.7604073210695377	0.2539885105797287	0.3967771989577524	T	T	T	0.7598634343737454	0.2518710670127868	0.3967732104158769	T	T	T
0.2601304337967365	0.7535779162984747	0.3967334836812024	T	T	T	0.2566175581250342	0.7496561288740917	0.3970169278735447	T	T	T
0.7560140321437566	0.7610782640280997	0.3963663613980776	T	T	T	0.75477840150538638	0.763859031360500	0.3967797393035749	T	T	T
0.2607508546700284	0.2556315603680046	0.4940184308076196	T	T	T	0.2617331351490064	0.2414739012221792	0.490486077348821	T	T	T
0.7583990973940355	0.2599149731002897	0.4950859638321896	T	T	T	0.7556223376643182	0.2605144258592383	0.4964275815590044	T	T	T

0.2585149981035603	0.7597801157105956	0.4951193255917152	T	T	T	0.2581099320898744	0.7743855233961185	0.4960419922690080	T	T	T
0.7602923458482540	0.7561873879841817	0.4956280391105261	T	T	T	0.7571717028346904	0.7555522764736768	0.4954366032678791	T	T	T
0.2113882532068833	0.0054294910496538	0.1464030182225393	T	T	T	0.2102632862328681	0.0054951200324802	0.1463905265334763	T	T	T
0.7951691735261885	0.0062647272353428	0.1426921567368902	T	T	T	0.7941383085447133	0.0063596429446060	0.1422153505792473	T	T	T
0.2953557668058111	0.5066975298510268	0.1425538011981350	T	T	T	0.2942098960659969	0.5063136674650173	0.1422000799528694	T	T	T
0.7116150029663555	0.5056314957378759	0.1463182883343915	T	T	T	0.71022345770279067	0.5054786135916817	0.1463614876080440	T	T	T
0.2075590772189224	0.0052202350949711	0.2446951513917834	T	T	T	0.2059785268204809	0.0051767696701784	0.2445284860422511	T	T	T
0.8024273802229683	0.0061409326231296	0.2478662697417731	T	T	T	0.8009022638524332	0.0060625136713694	0.2479279210133836	T	T	T
0.3024884572576989	0.5059424473757109	0.2478526236752708	T	T	T	0.3012990331782023	0.5061184150530540	0.2479664289782415	T	T	T
0.7071877339215964	0.5050591076548242	0.2448944428266630	T	T	T	0.7057483898482605	0.5051675152582987	0.2445564984624860	T	T	T
0.3084081850752055	0.0081176107147087	0.3481213699209242	T	T	T	0.3055561569696673	0.0081246056697763	0.3485132737237117	T	T	T
0.7076495175763667	0.0067922225755736	0.3461122141816882	T	T	T	0.7048161984605193	0.0069245889238872	0.3459244428778527	T	T	T
0.2074955341658421	0.5065734234355296	0.3461439581921370	T	T	T	0.2039256329334835	0.5069411141710863	0.3458753894232190	T	T	T
0.8086344558670182	0.5077169846001376	0.3478257497531646	T	T	T	0.8069180295806282	0.5079948856395395	0.3484178122854529	T	T	T
0.2091214594970307	0.0072353201971021	0.4459861257276938	T	T	T	0.2086751112040943	0.0075807806077124	0.4449499941358294	T	T	T
0.8128074651713847	0.0085584582129974	0.4474593226323763	T	T	T	0.8110872904598747	0.0085806220278593	0.4486446961701133	T	T	T
0.3141113675560888	0.5091929673081497	0.4477285520729943	T	T	T	0.3123081504582632	0.5086659315336645	0.4501232532080983	T	T	T
0.7101256333942605	0.5077653524179506	0.4459537123418776	T	T	T	0.7100695647379258	0.5075781764653665	0.4455930606128116	T	T	T
0.2642992752892009	0.0093190678658597	0.5449528841139764	T	T	T	0.2823085747476025	0.0078457970791244	0.5646004336964431	T	T	T
0.7541565262493878	0.0094100805144959	0.5464940124936672	T	T	T	0.7420523080899168	0.0080653768653775	0.5463738308749593	T	T	T
0.2554170765896810	0.5076039291791657	0.5448324012096480	T	T	T	0.2494144950746008	0.5078667399440735	0.542851518949831	T	T	T
0.7677137525735570	0.5071530111896573	0.5469489706744833	T	T	T	0.7721576262095178	0.5083261877867941	0.5465681271431198	T	T	T
0.0044020946093486	0.29770444257568072	0.1434393059345589	T	T	T	0.0035451357675798	0.2969973512431814	0.1432566451050097	T	T	T
0.5040308809662347	0.2141983081993812	0.1459290316348985	T	T	T	0.5028220944915022	0.2141533280785449	0.1456084789423412	T	T	T
0.0037379832613881	0.7144871856916800	0.1458690184792459	T	T	T	0.0026969256232414	0.7140579757861572	0.1456174981842989	T	T	T
0.5047787818018892	0.2081940532030219	0.1435136424699584	T	T	T	0.5036191935301843	0.7970804583218677	0.1432344349954256	T	T	T
0.0045205402591045	0.3030039592533577	0.2473129828677600	T	T	T	0.0028423692591037	0.3031668160589205	0.2473435160174652	T	T	T
0.5034193715476806	0.2093702179012373	0.2453762572149506	T	T	T	0.5019625291219307	0.2092217983219370	0.2452287770273854	T	T	T
0.0035403495431009	0.7094319072705521	0.2454706117489467	T	T	T	0.0019701729014112	0.7092771011737606	0.2454295641231145	T	T	T
0.5043241116582997	0.803093534389631	0.2474385891567940	T	T	T	0.5027794868931286	0.8034083702892211	0.2471705506818066	T	T	T
0.0068472372825996	0.2081940532030219	0.3464966368011861	T	T	T	0.0042700862574251	0.2079568787854445	0.3462310128722144	T	T	T
0.5075226758240632	0.3074626023644516	0.3475489748037059	T	T	T	0.5052600297358567	0.3084600038079169	0.3481757435533947	T	T	T
0.0077483672592296	0.8072778475992801	0.3473878026455051	T	T	T	0.005264251203176	0.8079408271920666	0.3473787571636646	T	T	T
0.5065971463249540	0.7084482575096667	0.3463899329662445	T	T	T	0.5041583362756095	0.7077640530723958	0.3469642684503211	T	T	T
0.0098246384582392	0.3110696917931324	0.4472808817727886	T	T	T	0.0087064017770700	0.3101939583107687	0.4483204636235196	T	T	T
0.5095004608090660	0.2077938628484504	0.4463405428795982	T	T	T	0.5073300624972515	0.2085008409725932	0.4460516274757571	T	T	T
0.0088927754882323	0.7083531391854373	0.4463669695562472	T	T	T	0.0074611179128534	0.7076581512040064	0.4474834421827743	T	T	T
0.5103818959404550	0.8095379652345038	0.4470933059661521	T	T	T	0.5083459266792567	0.8094789489332828	0.4468629856783770	T	T	T
0.0106942302468172	0.2535379843812494	0.5450235659817649	T	T	T	0.0112186547462402	0.238908454089051	0.5445019038617630	T	T	T
0.5087975250647139	0.2630759988331180	0.5451172805241564	T	T	T	0.5073680594054794	0.2597302439215217	0.5456344687648607	T	T	T
0.0106161439352722	0.7652519885248368	0.5460970872710033	T	T	T	0.0117935895042975	0.7784995821136128	0.5446888047394086	T	T	T
0.50840022709833719	0.7520668064221591	0.5459258092377725	T	T	T	0.5073950088733860	0.7561153778988424	0.5454200483081372	T	T	T
0.2592391092108313	0.2569953201520731	0.5986256239834464	T	T	T	0.4100971482393114	0.0115050162303163	0.5711410050523281	T	T	T

O ₂ H adsorbed on the surface:						H ₂ O adsorbed on the surface:					
La Ni O H						La Ni O H					
1.0000000000000000						1.0000000000000000					
7.4168595000000002						7.4168595000000002					
0.0000000000000000						0.0000000000000000					
-0.1172806200000000						-0.1172806200000000					
7.3694668400000003						7.3694668400000003					
0.0000000000000000						0.0000000000000000					
0.0443473400000000						0.0443473400000000					
0.0366662800000000						0.0366662800000000					
40.0172788900000000						40.0172788900000000					
20	20	62	1			20	20	61	2		
Selective dynamics						Selective dynamics					
Direct						Direct					
0.0151843067602613	0.0053113996213980	0.1007149791204185	T	T	T	0.0132730754697505	0.0051251927698994	0.1002893103598604	T	T	T
0.5115868019737988	0.0099356286304584	0.1007288199925469	T	T	T	0.5077244055955267	0.0083090626169799	0.1002661450901010	T	T	T
0.0105704151580142	0.5102997354359786	0.1007125213104487	T	T	T	0.0086444956674152	0.5073549261812452	0.1003163163306586	T	T	T
0.5158368685215251	0.5072826546581410	0.1006782029760913	T	T	T	0.5123810743057435	0.5004438228891662	0.1003156786264479	T	T	T
0.0039821702099445	0.0009512875534270	0.1984429089325985	T	T	T	0.0003133167655267	0.0040458309217549	0.1980328075322414	T	T	T
0.5003667690382585	0.0024535289063579	0.1984944155136290	T	T	T	0.4971960716488555	0.0016619918622167	0.1980156284731785	T	T	T
0.0011431536579991	0.5023016228783632	0.1984720335890913	T	T	T	0.9972414320528042	0.5017750056819497	0.1980695437575638	T	T	T
0.5038899781845245	0.4999121492770939	0.1984337338374047	T	T	T	0.5005389985757769	0.5006083550280966	0.1980998391706364	T	T	T
0.0091275956897903	0.0072828450586702	0.2983612296085241	T	T	T	0.0058232543556057	0.0036533773144711	0.2978235122146333	T	T	T
0.5105890192911602	0.0063249792800377	0.2984982458307783	T	T	T	0.5064985365346737	0.0035542408052846	0.2979414041234468	T	T	T
0.0103083424030501	0.5070824619721606	0.2984658926979193	T	T	T	0.0065899540400853	0.5032914874227815	0.2979812892656858	T	T	T
0.5098298862903334	0.5073643393225260	0.2983240824099695	T	T	T	0.5054640905690655	0.5035865669147450	0.2978891248753230	T	T	T
0.0124401899417563	0.0082904923122697	0.3991953951349316	T	T	T	0.0079912044470014	0.0032689779942514	0.3987337990333756	T	T	T
0.5126804537059613	0.0091102047127882	0.3990737633026029	T	T	T	0.5082509439652358	0.0041836021184967	0.3984951027117293	T	T	T
0.0116778741806556	0.5090673822279470	0.3990100125330969	T	T	T	0.0066445168932623	0.5035175458821817	0.3986265083521650	T	T	T
0.5124870025567603	0.5093994310848800	0.3991494323315621	T	T	T	0.5069460999053065	0.5040333880832547	0.3987198421260476	T	T	T
0.0141734662279731	0.0103995357062345	0.5045955458669766	T	T	T	0.0073533689052235	0.0020622573214338	0.5030129986891434	T	T	T
0.5133409012156918	0.0099745367439326	0.5045333391904236	T	T	T	0.5096049260544427	0.0035663818736785	0.5036248072316402	T	T	T
0.0141150549424935	0.5086530292850284	0.5048839869300537	T	T	T	0.0062044471406934	0.5051993579980751	0.5038419925165428	T	T	T
0.5122152444111023	0.5091104164449618	0.5043829919242739	T	T	T	0.5076155537010673	0.5054825966816490	0.5041612761336970	T	T	T
0.2567981647719861	0.25512204038438684	0.1458984453908414	T	T	T	0.2536641179735650	0.2539868310823351	0.1460262896107658	T	T	T
0.7575744174647809	0.2539201012135521	0.1461403129466277	T	T	T	0.7542424210052098	0.2528040548820267	0.1458044945621451	T	T	T
0.2575890818370397	0.7538896349375364	0.1461951719287381	T	T	T	0.2542907775316672	0.7527450521746579	0.1457835321802836	T	T	T
0.7566856556654642	0.7551823919512159	0.1461319610981138	T	T	T	0.7537515366673249	0.7539824887898131	0.145634554886642	T	T	T
0.2571618852281361	0.25541993210997386	0.2474477221147861	T	T	T	0.2534015441726148	0.2534927761439969	0.2468133414644647	T	T	T
0.7577086935808239	0.25453132766991132	0.2472330644512872	T	T	T	0.7539074252635393	0.2523771774451227	0.246734565816040	T	T	T
0.2577100290159748	0.7545072912754165	0.2472010393579751	T	T	T	0.2539180962801495	0.7523912884269630	0.2466776731196038	T	T	T
0.7570547415988571	0.7555640281540263	0.2471092650881275	T	T	T	0.7533867562231856	0.7534788789173238	0.2467743911539158	T	T	T
0.2612711715098541	0.2575601164030559	0.3480043391433512	T	T	T	0.2566362407769390	0.2531939938247154	0.2477284737465034	T	T	T
0.7606490677640158	0.2584356213077257	0.348076560431291	T	T	T	0.7564033394056776	0.2540895205561555	0.3475714162553061	T	T	T
0.2606786186595083	0.5754858001236022	0.3480750615793832	T	T	T	0.2562844736285314	0.7540935454746536	0.34795962975979951	T	T	T
0.7612329923360264	0.7576160029025090	0.3480680893535322	T	T	T	0.7567154249748897	0.7531818795444620	0.3475461120417814	T	T	T
0.2624317790633626	0.556958613243600	0.449785663535808	T	T	T	0.2575240396041172	0.2542907495138377	0.4494248756856951	T	T	T
0.7630309670237025	0.2593141013824294	0.4496634155947490	T	T	T	0.7571460259286877	0.2541115137118337	0.4489490036503829	T	T	T
0.2628679441896224	0.7592356686732771	0.4496015013399020	T	T	T	0.2578317018734701	0.7533813350026916	0.4489194295783441	T	T	T
0.7629128995808827	0.7594871212155923	0.4499041062197335	T	T	T	0.7570585262839305	0.7538451080600133	0.4489894511481821	T	T	T
0.2639336801422658	0.2587934557299647	0.5559089731647688	T	T	T	0.2556227863734299	0.2515946438731251	0.5495620049123435	T	T	T
0.7612388772657397	0.259793886268144	0.5532651627300922	T	T	T	0.7603239286829052	0.2524296749975948	0.5526257537642997	T	T	T
0.2633846219901699	0.759554110019823	0.5529170165402775	T	T	T	0.2570500793233046	0.7563055001232222	0.5526805307294788	T	T	T
0.7622114022281323	0.7588321972453045	0.5520357398777591	T	T	T	0.7585389908684135	0.7545956432468452	0.5521167643320579	T	T	T
0.2620747814051612	0.2461710598196305	0.0909982115726038	T	T	T	0.2581931968074823	0.2446505162098833	0.089197894632938	T	T	T
0.7495196604645500	0.2617108832806707	0.0903856370389207	T	T	T	0.7475367247770939	0.2613290476083512	0.08909131665072540	T	T	T
0.2491890647343240	0.761570840286242	0.0901890892672199	T	T	T	0.2476109773536953	0.7611330822968576	0.0900027069275239	T	T	T

0.7619358061615955	0.7461354910919056	0.0900464715187681	T	T	T	0.7587665071924447	0.7450260132164902	0.0901898491394385	T	T	T
0.2512529182104331	0.2612372861464536	0.1946751291270701	T	T	T	0.2490827505691482	0.2600625407082734	0.195777894963514	T	T	T
0.7613541613045669	0.2467389036437453	0.1951163648969612	T	T	T	0.7566757027258273	0.2455170773693651	0.1948068647674429	T	T	T
0.2614551239905580	0.7465734392508736	0.1952495467931570	T	T	T	0.2566876387830953	0.7454656804996598	0.1947613129593344	T	T	T
0.7510824470848974	0.7610169461009022	0.1953775290159641	T	T	T	0.7490965513975169	0.7599427743171815	0.1945057530696886	T	T	T
0.2634105744536228	0.2519798417122274	0.2991982787902643	T	T	T	0.2581018763347281	0.2488691045702369	0.2978768487271933	T	T	T
0.7559844883299078	0.26214411927060459	0.2993819122508654	T	T	T	0.7533628489520380	0.2575281411340508	0.2988215175855076	T	T	T
0.2558351424566965	0.7623548757316811	0.2993395156786391	T	T	T	0.2535074365381772	0.7575686272551814	0.2988447461413090	T	T	T
0.7636660860680422	0.7519871560014195	0.2993232794440814	T	T	T	0.7577844503232659	0.7492347236725230	0.2989812274123020	T	T	T
0.2592362688729892	0.2622807036866490	0.3983974121193299	T	T	T	0.2554592858725129	0.2555999784232733	0.3968897708287730	T	T	T
0.7642787770321249	0.2553683603609826	0.3972752281676009	T	T	T	0.7584647879601881	0.2515077395630348	0.3968083812129025	T	T	T
0.2644859991765998	0.7554807582077387	0.3971503416258386	T	T	T	0.2581226790025991	0.7515288147493123	0.3968841947414052	T	T	T
0.7588712041234658	0.7620767745162027	0.3969106619055438	T	T	T	0.7555574556876251	0.7558471985677443	0.3966626591410871	T	T	T
0.2638907715612575	0.2585011271444344	0.4950635803885888	T	T	T	0.25891346467446547	0.2538149089393431	0.4986305591418420	T	T	T
0.7619270528337836	0.2607301382147114	0.4957180919579116	T	T	T	0.7555378529858492	0.2549508627298608	0.4947507807010407	T	T	T
0.2615506585384608	0.760241413760457	0.4958037386243461	T	T	T	0.2574872732255093	0.7534726651528079	0.4946824790049079	T	T	T
0.7644180917531358	0.75779816316619059	0.4961357392080714	T	T	T	0.7572568391652175	0.7531653688297276	0.4951696705826527	T	T	T
0.2141679612238079	0.0038462326088862	0.1465569149255899	T	T	T	0.2111323741330230	0.0032142194788808	0.1463747239476603	T	T	T
0.7982989271445717	0.0047611889195807	0.1428881909293906	T	T	T	0.7948752329370347	0.0038558065736500	0.1423594654521483	T	T	T
0.2985490044888834	0.5051007488760893	0.1428419694744889	T	T	T	0.2946412780165047	0.5035139206008019	0.14242154960659574	T	T	T
0.7142816781701171	0.504179299603057	0.1465540462909232	T	T	T	0.7108281456324383	0.5028149370322529	0.1462883792069027	T	T	T
0.2107602342246366	0.0046675188505034	0.2449986034444578	T	T	T	0.2070983369427284	0.0022664678778610	0.2446810532009950	T	T	T
0.8065156352021390	0.0056211362665479	0.2482975821245432	T	T	T	0.8025284359545907	0.0033975816247809	0.2477569402481063	T	T	T
0.3065953614481813	0.5054279529275902	0.2482743300075754	T	T	T	0.3024807203969664	0.5037440065020414	0.24780815976020770	T	T	T
0.7105418963348100	0.5045522371576965	0.2451286747348931	T	T	T	0.7070424524602710	0.5026464865212207	0.2447452127956215	T	T	T
0.3129073821843562	0.0088690791092105	0.3484703121369179	T	T	T	0.3086235615847961	0.0043351703833604	0.3476931804824014	T	T	T
0.7111022415382138	0.0075816754344610	0.3466156246569767	T	T	T	0.7064330489218262	0.0032614337281031	0.3463858477629564	T	T	T
0.2109653623217369	0.5072635323114625	0.3467170267304027	T	T	T	0.2064325469346445	0.5029392064641486	0.3463748945006700	T	T	T
0.8128609115836483	0.5085605147915615	0.3483415508828998	T	T	T	0.8086383633483876	0.5040551063711320	0.3477156824778499	T	T	T
0.2117072391679145	0.0086054832993554	0.4470092768432536	T	T	T	0.2053911964256058	0.0037636760296570	0.4472150373276180	T	T	T
0.8156099873273233	0.0098636810626402	0.4478895749458118	T	T	T	0.8087547285252492	0.0044491646116022	0.4469530056739373	T	T	T
0.3168080974646088	0.5106224632368307	0.4480909041264027	T	T	T	0.3112277084374140	0.5039459519173511	0.4476776865614030	T	T	T
0.7127200875025181	0.5090663904201875	0.4467915485848835	T	T	T	0.7071325178142061	0.5035917124183886	0.4463165050500940	T	T	T
0.2707676009455753	0.0099872556569665	0.5451907338247750	T	T	T	0.2676339585156882	0.0008114403066995	0.5435564844479800	T	T	T
0.7558813882644415	0.0101427260552427	0.5475965037853570	T	T	T	0.7431835921304980	0.0040044760579703	0.5472368697885339	T	T	T
0.2580457242162026	0.5088544734604667	0.5455298807911930	T	T	T	0.2453900886584603	0.5073022725010562	0.5451834965151267	T	T	T
0.7736922671103983	0.5086064103567836	0.5476545862541400	T	T	T	0.7691184645417396	0.5034877730766899	0.5476949596103535	T	T	T
0.0071970924376359	0.2956904935989613	0.1436024907924462	T	T	T	0.0044871155808749	0.2941519485268687	0.1435899475930404	T	T	T
0.5068010887297447	0.2122846545459609	0.1461041923497035	T	T	T	0.5031380294295374	0.2117858960752714	0.1453856652955245	T	T	T
0.0065238752761658	0.7126617064751031	0.1460820788287123	T	T	T	0.0035808037981633	0.7112918244326580	0.1454155624575379	T	T	T
0.5074045397941020	0.7955052647677832	0.1435944124952471	T	T	T	0.5042098069738375	0.7945208630465977	0.1434456187283586	T	T	T
0.0080130528358922	0.3029333807120196	0.2478517457136959	T	T	T	0.0038365651678130	0.3005507048252185	0.2470000973109370	T	T	T
0.5069010258987987	0.20871317016642	0.2455093494323322	T	T	T	0.5036011984977578	0.2065018281802771	0.245518896392232	T	T	T
0.0070175744488252	0.7085669694488532	0.2455536588757994	T	T	T	0.0032278465499976	0.7064679864873153	0.2455679282601170	T	T	T
0.5078821355633067	0.8030553106092171	0.2479538205687390	T	T	T	0.5042099726575842	0.8004649638568325	0.2468824352522589	T	T	T
0.0107766142262591	0.2086891238794877	0.3469294767096613	T	T	T	0.0063226844270452	0.2038768882128106	0.3465616837843584	T	T	T
0.5112268533077042	0.3088143602787810	0.3482408857481758	T	T	T	0.5068189517049168	0.3041409873145736	0.3473503363231751	T	T	T
0.0115708503219025	0.8087015859847568	0.3481144453964546	T	T	T	0.0071130077621364	0.8041248404859135	0.3473523287004746	T	T	T
0.5104502898852346	0.7089450120636798	0.346723855021410	T	T	T	0.5059039692170562	0.7041063066185289	0.3466804121379964	T	T	T
0.0130033479505940	0.3125471424822719	0.4479671085678731	T	T	T	0.0083021933935460	0.3059642883939350	0.4474973443385591	T	T	T
0.5127864994808462	0.2091592044852462	0.4470256735068053	T	T	T	0.5064889880911149	0.2028521102825312	0.4468670128764266	T	T	T
0.0122952131828029	0.7100632587331575	0.4467177885091971	T	T	T	0.0068325271448679	0.7046144217326867	0.4464585969284970	T	T	T
0.5135855630284780	0.8114184155710504	0.4478569247681961	T	T	T	0.5081197400170282	0.8050278825512874	0.4468510607699451	T	T	T
0.0128467874887050	0.2523782466545228	0.5461812698045776	T	T	T	0.0044141090836635	0.2441473312479868	0.5433481307612468	T	T	T
0.5122723597993541	0.2661414030150198	0.5458853380006587	T	T	T	0.5107552094629293	0.2654885073445167	0.5454868475091109	T	T	T
0.0138091330919394	0.7687778681315578	0.5471154476161715	T	T	T	0.0078537862959231	0.7661515698071969	0.5462044551859615	T	T	T
0.5127169477935212	0.7513400146150957	0.5464246206933581	T	T	T	0.5069558077950212	0.7416384054837998	0.5468926863060676	T	T	T
0.2547331477447230	0.2700795847471298	0.6013437533239809	T	T	T	0.2856335586626676	0.2839553033868792	0.5997740273326909	T	T	T
0.1654456801060476	0.1213205591145510	0.6152406778535848	T	T	T	0.2622182931530193	0.4149231244890435	0.5986196921668596	T	T	T
0.0370026438661739	0.1485505850501525	0.6115228554989756	T	T	T	0.4178282473619948	0.2764633959600066	0.5979491108788226	T	T	T

-2% Strain State:

O ₂ adsorbed on the surface:						OH adsorbed on the surface:					
La Ni O						La Ni O H					
1.0000000000000000						1.0000000000000000					
7.4933220000000000						7.4933220000000000					
-0.1209078500000000						-0.1209078500000000					
0.0457189100000000						0.0457189100000000					
20	20	62				20	20	61	1		
Selective dynamics						Selective dynamics					
Direct						Direct					
0.0077551383794792	0.0055983919235981	0.1013798032369481	T	T	T	0.0052800281286470	0.0046624534454439	0.1013174822005201	T	T	T
0.5070853424980417	0.0067147891636718	0.1013640064426184	T	T	T	0.5039547784396938	0.0063345888327674	0.1013803450842660	T	T	T
0.0068663042368330	0.5075084505971835	0.1013472104013879	T	T	T	0.0036237276963600	0.5070980022550453	0.1013488106609460	T	T	T
0.5092425619727834	0.5065222487393954	0.1013724537065439	T	T	T	0.5067320833365293	0.5056758921452298	0.1013469976386017	T	T	T
0.0090341429014922	0.0075338410821986	0.101399030151760	T	T	T	0.0076044323335353	0.0070124152038107	0.198229365135968	T	T	T
0.5085520798003531	0.0076511098631215	0.1980250084772666	T	T	T	0.5070432021544649	0.0067030485998893	0.1980428185789589	T	T	T
0.0091014910173585	0.5071951126687297	0.1980063798317421	T	T	T	0.0076550016789158	0.5066732630808547	0.1980252880513011	T	T	T
0.5088578678085289	0.5067446685267155	0.1982590341305211	T	T	T	0.5074913153052091	0.50622453566687	0.1982463298656461	T	T	T
0.0086501880435405	0.0075124200942837	0.2974353437291305	T	T	T	0.0076025103554400	0.0070772333956737	0.2974754556596704	T	T	T
0.5092752698657662	0.0072629119753274	0.2975181523086019	T	T	T	0.5081071794579309	0.01976640468239	0.2975383417485138	T	T	T
0.0091842361502067	0.5079597360362312	0.2974865068621542	T	T	T	0.0078841311029935	0.5079826991939703	0.2975374684910147	T	T	T
0.5095987206218053	0.5079627384322714	0.2974501818954346	T	T	T	0.5084465209298130	0.5080859098005854	0.29743536762752907	T	T	T
0.0095106434142481	0.0077803204077393	0.3977850805057156	T	T	T	0.0077659978620343	0.5080339047842621	0.3978435825361806	T	T	T
0.5100482940669582	0.0084545299939296	0.3976098492978203	T	T	T	0.5084959106880210	0.0087678515685580	0.3976103155721603	T	T	T
0.006886562904937	0.5084815632517263	0.3976288832947518	T	T	T	0.0072832327212254	0.5086814730525636	0.3976666564409621	T	T	T
0.5093449388514526	0.5089158774457054	0.3978005884073980	T	T	T	0.5075708664418045	0.5091937552980017	0.3978401097125427	T	T	T
0.0097224754026405	0.0093799722471850	0.5026394790742286	T	T	T	0.0076133190750117	0.0088164226284017	0.5023494057296475	T	T	T
0.5084067549903855	0.0092137581255089	0.5026280073572471	T	T	T	0.5069988061817193	0.006948915862065	0.5024649203873720	T	T	T
0.0094679914439063	0.5080696801136423	0.5026338100617493	T	T	T	0.0073454960605018	0.5078314349188579	0.5025868172899625	T	T	T
0.5079607936850327	0.507724830646436	0.502676956758528	T	T	T	0.5066432321610885	0.5076810416054988	0.50258871635672868	T	T	T

0.2587497793884834	0.2572286099119021	0.1456462020578567	T	T	T	0.2568539831103168	0.2566607126658527	0.1456211927999799	T	T	T
0.7589126548788530	0.2570100754558831	0.1458046821578868	T	T	T	0.7571123924475383	0.2564041640755952	0.1457854885734483	T	T	T
0.2588553597397397	0.75704354854449676	0.1458325488360719	T	T	T	0.2571321019477087	0.7564346143350361	0.145811170336189	T	T	T
0.7587067108359565	0.7572038807081118	0.145963961767512	T	T	T	0.7569216498791931	0.7566702938572362	0.1459551639760586	T	T	T
0.2590382578473048	0.2574756429672689	0.2466481032761815	T	T	T	0.2576179592129916	0.2573897713105561	0.2466783442388691	T	T	T
0.7589903090421372	0.2573156661352379	0.2464408056063744	T	T	T	0.7576589734747745	0.2569842440286544	0.2464666780051654	T	T	T
0.2590326614376705	0.7573493835715497	0.2464466993131121	T	T	T	0.2576191463796391	0.7570149108499101	0.2464575172724668	T	T	T
0.7589923216073524	0.7574778855865109	0.2463585549959193	T	T	T	0.7576350484148183	0.7573722064737540	0.2463747857078150	T	T	T
0.2593700304002197	0.25800993995547899	0.3467481773672781	T	T	T	0.2578606305696224	0.2581978122205796	0.3467771302784156	T	T	T
0.7593238846029801	0.2581488455634662	0.3467787129475465	T	T	T	0.7577336332763260	0.2584564722754155	0.3468247143698447	T	T	T
0.2592709577519002	0.7581249812273823	0.3468009449321189	T	T	T	0.2576514817968472	0.7583908932174195	0.3468346776325090	T	T	T
0.7593798316381701	0.7580203696142693	0.3467697557684273	T	T	T	0.7578526930695503	0.7581889897956893	0.3468177071968604	T	T	T
0.2592307725318493	0.2586380416022100	0.4473720758133065	T	T	T	0.2572951180673222	0.2586448729753119	0.4474427654072884	T	T	T
0.7592460602550107	0.2584843581376986	0.4478154503420252	T	T	T	0.7573646141686602	0.2586096973996129	0.4478280052170695	T	T	T
0.2593542532134412	0.7583864534862030	0.4478421302710049	T	T	T	0.2575535052451985	0.7585176071173558	0.4478601066022793	T	T	T
0.7591769390473168	0.7584985646877908	0.4480467010399246	T	T	T	0.7573198184326273	0.7585826492309073	0.4480298240338899	T	T	T
0.2572456968375202	0.2573934672690412	0.5529816421152020	T	T	T	0.2572199278619690	0.2572483547617244	0.5526282131245553	T	T	T
0.7583471809675284	0.2582052384815251	0.5505435464434322	T	T	T	0.7592202507985425	0.2573762693127664	0.5506828598142608	T	T	T
0.2581142464556470	0.7584461745984853	0.5502857545966022	T	T	T	0.2572144158391613	0.7575475791534547	0.5503194505164545	T	T	T
0.7583109630575122	0.2587677626858495	0.5492767842992606	T	T	T	0.7584597198538540	0.7576012424126917	0.5492722036642623	T	T	T
0.2608472633837634	0.2556289137706544	0.091871156035706	T	T	T	0.2600477123085415	0.2534517101017639	0.0918962027763424	T	T	T
0.7582721887775120	0.2600918626100343	0.0913583014160716	T	T	T	0.7562130798424137	0.2606004831960320	0.0913750665559760	T	T	T
0.2580972001004809	0.7601787546407837	0.0913341316439586	T	T	T	0.2563524677027189	0.7606491547058031	0.0913634462510973	T	T	T
0.7610156169658076	0.7555402708113534	0.0910967246482196	T	T	T	0.7604158872602887	0.7536856997711654	0.0911412241316243	T	T	T
0.2576984522673996	0.2587984956407454	0.1942568493780626	T	T	T	0.2556964695880810	0.2592799038419542	0.1942163734299105	T	T	T
0.7596679263877559	0.2556583821131505	0.1946669400268969	T	T	T	0.7586112932783597	0.2544779254063559	0.1946203446354120	T	T	T
0.2597732586880634	0.7556414821311066	0.1947393594385484	T	T	T	0.2585672733668760	0.7544140184015992	0.1946973368225626	T	T	T
0.7576929200974594	0.7586152636413510	0.1949715266634937	T	T	T	0.7559078807079508	0.7590453283163656	0.1949427395506823	T	T	T
0.2605207953497146	0.2569173305710485	0.2979483232673513	T	T	T	0.2592337612180049	0.2574067816004714	0.2979514423532644	T	T	T
0.7580766075914671	0.2590641840949242	0.2980150471136588	T	T	T	0.7566655715361057	0.2591023976013689	0.2980862635132547	T	T	T
0.2581147611809104	0.7592084010751076	0.2980077658586571	T	T	T	0.2564844799583849	0.7590246366902874	0.2980489620177225	T	T	T
0.7605177053365824	0.7566941004617693	0.2979408752947968	T	T	T	0.7593983530835906	0.7573373901832284	0.2979960645162154	T	T	T
0.2579458545840894	0.2593875225040140	0.3968045663164823	T	T	T	0.2567381509846279	0.2586514210203387	0.3969643181483414	T	T	T
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0.2602093746439532	0.7573820093480286	0.3957201325294609	T	T	T	0.2589659345903636	0.7583142197818216	0.3957547071325598	T	T	T
0.7581317212756035	0.7592460356048264	0.3954368974236667	T	T	T	0.7566953307472711	0.7587899376223732	0.3955099576966744	T	T	T
0.2601038568146304	0.2582080831787904	0.4934285672590613	T	T	T	0.2577700500161236	0.2586386336096543	0.4936440689382277	T	T	T
0.7580684691197671	0.2588492593945915	0.4940718010477051	T	T	T	0.7567428416247229	0.2579767679644712	0.4940805139089065	T	T	T
0.2585232050073077	0.7584461465124339	0.4941677576713805	T	T	T	0.2571731525014391	0.7580710401548669	0.4941931267709867	T	T	T
0.759330141236635	0.7581353545979305	0.4944932820170056	T	T	T	0.7578282551767789	0.7587340324729693	0.4945074093528581	T	T	T
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0.7159574030608968	0.0065938444506932	0.1445994335619701	T	T	T	0.7141651727804723	0.0060307612624106	0.1444061865252345	T	T	T
0.2159406562331578	0.5069741922009695	0.1445710036265164	T	T	T	0.2140556719390831	0.5063811837370660	0.1443325199947318	T	T	T
0.8018242833685106	0.50754444105488210	0.1453891866152574	T	T	T	0.8002623391267341	0.5069805971985548	0.1456529463041676	T	T	T
0.2121988545539323	0.0070893650479638	0.2456489283843620	T	T	T	0.2109571384407851	0.0069201589543731	0.2454521165141554	T	T	T
0.8062135632188104	0.00787603404457036	0.2461929371145991	T	T	T	0.8052451385843367	0.0076504354813102	0.2463248552791472	T	T	T
0.3063265794415156	0.5076742212646783	0.2461724855002873	T	T	T	0.3052728229965084	0.5074706950676540	0.2462779243822766	T	T	T
0.7122217644852120	0.5068269392771109	0.2457100202907882	T	T	T	0.7109710019426336	0.5066334209329294	0.2456276834395982	T	T	T
0.3084197714806398	0.0087982749500400	0.3465725815614596	T	T	T	0.3067786377741512	0.0091050731151438	0.3464344193956082	T	T	T
0.7111221668252948	0.0076312483664958	0.3458718069761591	T	T	T	0.7093280503806692	0.0078933227534175	0.3460246004608988	T	T	T
0.2107299013166788	0.5072770717329737	0.3460477792067198	T	T	T	0.2089289738642088	0.5074549535024788	0.3462517604955083	T	T	T
0.8081896760399955	0.5084674074465575	0.3462800893354268	T	T	T	0.8066205232679319	0.5087432802538634	0.3462993381300362	T	T	T
0.2097076057997079	0.0087819433522323	0.4456095428271772	T	T	T	0.2069754169441494	0.0076006698608332	0.4459105036522598	T	T	T
0.8086854663682619	0.00780074369437381	0.4456609554724228	T	T	T	0.8063377746336078	0.0090670063792464	0.4455585452309735	T	T	T
0.3099371680154141	0.5094555191348951	0.4458969837968478	T	T	T	0.3072822866010396	0.5095940343393426	0.4457749021569572	T	T	T
0.7110572960294439	0.5081214142283832	0.4453033994142505	T	T	T	0.7079604572091478	0.5082731577521357	0.4456377827095885	T	T	T
0.2637236625285680	0.0089587634268596	0.5430650979488679	T	T	T	0.2613366222118708	0.0080485194070730	0.5427020069173382	T	T	T
0.7527764237012416	0.0090857960360380	0.5446701063095460	T	T	T	0.7484849282821547	0.0085703912212327	0.5449083600558061	T	T	T
0.2541901146076043	0.5081290444352194	0.5432718470676187	T	T	T	0.2526608465962597	0.5079281649477543	0.5429247198452026	T	T	T
0.7656666024901793	0.50761643128373869	0.5448533776116893	T	T	T	0.7606120983209261	0.5068071108720927	0.5445417981363262	T	T	T
0.0083422389576094	0.2149199368708579	0.1447750051715116	T	T	T	0.0064172605774837	0.2141297713756545	0.1446156348343382	T	T	T
0.5094582906078770	0.2991288211425968	0.1452231374723390	T	T	T	0.5076191073139750	0.2986471131960742	0.1452538496781597	T	T	T
0.0090546590508722	0.7991552750374223	0.1453535089684197	T	T	T	0.0073425612286569	0.7986576027513205	0.1453468393686158	T	T	T
0.5085995656263568	0.7150220217420423	0.1448224681177365	T	T	T	0.5068101828724479	0.7142445530595020	0.1447259550931908	T	T	T
0.0095503233456529	0.3035729662334141	0.2459882171286588	T	T	T	0.0081714375159360	0.3035580723125516	0.2461181296052846	T	T	T
0.5084585137982326	0.2112134039137496	0.2455389215162514	T	T	T	0.5070914561014433	0.2110181270747068	0.2454555739623168	T	T	T
0.0087384983660718	0.7113462177905768	0.2456056201015070	T	T	T	0.00730432334658235	0.7109310285480310	0.2455190767805903	T	T	T
0.5093058675900145	0.8036166249471959	0.2461044569827637	T	T	T	0.5079227627998050	0.8035379983946919	0.2461964463605098	T	T	T
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0.5095308272348705	0.30631317289969792	0.3465986647223011	T	T	T	0.5079574692038404	0.3065441295191015	0.3466519301559227	T	T	T
0.0098913680344332	0.8056653737401299	0.3464317361060555	T	T	T	0.0082691008411559	0.8061579928487209	0.346529077087363	T	T	T

0.0087829488425214	0.0075696430144585	0.1983092432994727	T	T	T	0.0066441883074103	0.0069035267355272	0.1983364360749552	T	T	T
0.5083758021256962	0.0073761645041677	0.1980556968095277	T	T	T	0.5066988285205067	0.0068597774319842	0.1980691487770195	T	T	T
0.0089273639782933	0.50726066131106346	0.1980598291760385	T	T	T	0.0067997254097422	0.5069348000335647	0.1981744462598753	T	T	T
0.5086462966933879	0.5070154207728760	0.1982931149688006	T	T	T	0.5066931906438710	0.5067922784959324	0.1984723641800200	T	T	T
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0.5091285117318822	0.0072715286817592	0.2975504243202962	T	T	T	0.5056879355035175	0.0078211392211345	0.2975522891199738	T	T	T
0.0089242472627265	0.5080285909301171	0.2975020035625369	T	T	T	0.0054547860282653	0.5076864435094888	0.2975264683105580	T	T	T
0.5092989967298807	0.5078993446216474	0.2974665606092489	T	T	T	0.5059713972524499	0.5079765869269737	0.2978117647879450	T	T	T
0.0094686946023095	0.0079563427467769	0.3977393866083416	T	T	T	0.0059794818209303	0.0088036277230112	0.3972788193044195	T	T	T
0.5099367753580233	0.0082397347251144	0.3976397390621489	T	T	T	0.5057692125409514	0.0084654284641472	0.3972941106463123	T	T	T
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0.5096093688684742	0.5087016237678829	0.3977707904928419	T	T	T	0.5049197572313233	0.5088052341325431	0.3985310901769674	T	T	T
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0.0097049218178462	0.5079133303998318	0.5024920633132968	T	T	T	0.0089561368666015	0.5094995455090592	0.5020367352342654	T	T	T
0.5084327197143427	0.5080793750338374	0.5023573683336450	T	T	T	0.5102440480743309	0.5079541492267814	0.5032553305399313	T	T	T
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0.7586934310079642	0.2572010492918642	0.1458586618255411	T	T	T	0.7570211845047907	0.2567206850518793	0.1459789288955769	T	T	T
0.2587073491717430	0.7572527924756168	0.1458671945836687	T	T	T	0.2569985835595106	0.7566471243342833	0.1459644442119970	T	T	T
0.7585355712658186	0.7574415595607564	0.1459919238719639	T	T	T	0.7568359651511685	0.7569114395482472	0.1459936783312469	T	T	T
0.2588277763781179	0.2575151345361751	0.2466703568075529	T	T	T	0.2568365623737099	0.2574477512294426	0.2465732118857283	T	T	T
0.7587953146858334	0.2574041486379883	0.2464880880522355	T	T	T	0.7564785498703922	0.2574138561151433	0.2465565730020854	T	T	T
0.2588332030222444	0.7574663189958097	0.2464946923768220	T	T	T	0.2568056210734602	0.7573196687563323	0.2465767517139079	T	T	T
0.7587554031526970	0.7575324286116519	0.2464044318215692	T	T	T	0.7565860269314207	0.7574096210712925	0.2465654577402734	T	T	T
0.2593867653603937	0.2579421520991214	0.3467442405339891	T	T	T	0.2567080118320202	0.2591919563142848	0.3469491310764008	T	T	T
0.7592064695347167	0.5080652094523225	0.3467955691256770	T	T	T	0.7566251253115162	0.2584482069321137	0.3469008465281036	T	T	T
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0.7593483122634740	0.7579261657898883	0.3467920107892998	T	T	T	0.7567677593417155	0.7583352723716457	0.3469251705979083	T	T	T
0.2593490118752330	0.2585404992552659	0.4472243283752203	T	T	T	0.2589420825060768	0.2567322098754655	0.4482632014428869	T	T	T
0.7595022024693723	0.2583657390868245	0.4477923527238055	T	T	T	0.7588543017378204	0.2591188127039992	0.4476750878625339	T	T	T
0.2594936784930225	0.7582541938753046	0.4478278121296408	T	T	T	0.2586996433214214	0.7605170562164671	0.4482435640134387	T	T	T
0.7594706332541972	0.7584566168257726	0.4480406476223300	T	T	T	0.7584749466816247	0.7580826106537457	0.4476638290065166	T	T	T
0.2587405434601504	0.2584411779322811	0.5547177223018168	T	T	T	0.2574431439304450	0.2635812335969796	0.5504708752870482	T	T	T
0.7587146041221450	0.2584188610640293	0.5508597312429657	T	T	T	0.7616617037293267	0.2589048302733243	0.5490123601328154	T	T	T
0.2587608246717057	0.7583642888485974	0.5506560651346361	T	T	T	0.2580049046892583	0.7530868155531434	0.5504851959290095	T	T	T
0.7587551931466892	0.7583890309294165	0.5492604879406798	T	T	T	0.7619274921131678	0.7585243442292039	0.5498880910217556	T	T	T
0.2608402075274557	0.2560869276018507	0.0919525004232844	T	T	T	0.2599230143364525	0.2535764612052853	0.0914568314630512	T	T	T
0.7572650839123775	0.2605856571706143	0.0914396787161076	T	T	T	0.7567896057024338	0.2601167660522544	0.0914403461928345	T	T	T
0.2572947819455779	0.7604213152670999	0.0914277366541555	T	T	T	0.2570023558437680	0.7602851175664659	0.0914630771239838	T	T	T
0.7608074406968477	0.7561055401684087	0.0912583197773605	T	T	T	0.7596106011849554	0.7538328627350653	0.0914118555497802	T	T	T
0.25730702512021321	0.2589071588399506	0.1942522835152486	T	T	T	0.2553109940775699	0.2595413805431355	0.1948562153911905	T	T	T
0.7597662726871862	0.255772635383305	0.1947192722209327	T	T	T	0.7582686871237502	0.2550330613913526	0.1949030575143856	T	T	T
0.2597804681825502	0.7559250438560402	0.1947766295282084	T	T	T	0.2578014461587385	0.7546806472392118	0.1948774478193324	T	T	T
0.7573692256257766	0.7588740813813289	0.1949812027652479	T	T	T	0.7561359210814503	0.7590783839009514	0.1949375080469829	T	T	T
0.2604677709214592	0.2566741328848152	0.298056623292258	T	T	T	0.2596758282517875	0.2545734109949787	0.2981300605561139	T	T	T
0.7579301099094052	0.2591242863762666	0.2980274411185908	T	T	T	0.7536935149095225	0.2610209744331191	0.2981032511269262	T	T	T
0.2578861616385259	0.7595097433799151	0.2979990397992439	T	T	T	0.2559828300951844	0.7616136055817014	0.2981181907628262	T	T	T
0.7605181108654862	0.7568520998581484	0.2979593118250186	T	T	T	0.7577222422986460	0.7555271726350007	0.2981478691823455	T	T	T
0.2582015837142744	0.2598821110323890	0.3967275120067586	T	T	T	0.2531416650344390	0.2663702779187307	0.3960047377509286	T	T	T
0.7603327560528425	0.7573461403457430	0.3957818126304170	T	T	T	0.7611388236619909	0.2529783169254783	0.3958245603271983	T	T	T
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0.7582406285178002	0.7592261334846601	0.3954741749926814	T	T	T	0.7565219525058036	0.7632129271866248	0.3958269533509981	T	T	T
0.2596496840693548	0.2575736485401215	0.4929494315593796	T	T	T	0.2619077034354867	0.2402826957447991	0.4950118867661175	T	T	T
0.7587784484312917	0.2587905825672467	0.4941684676503749	T	T	T	0.7566350728332569	0.2611035968901803	0.4941886694032852	T	T	T
0.2587377249378300	0.7588523470266757	0.4942914199740349	T	T	T	0.2587331327899386	0.7768867058102613	0.4949864269212341	T	T	T
0.7595735991020111	0.7581322455941697	0.4945625133816441	T	T	T	0.7576752283689434	0.7562908531857975	0.4941712128927291	T	T	T
0.3018784772849759	0.0074517536954203	0.1453897346556613	T	T	T	0.3001310873033668	0.0071326492426338	0.1457367231482782	T	T	T
0.7158365165106420	0.0068441327441028	0.1446491090506373	T	T	T	0.7139574200102879	0.0063736880266610	0.1445873385952355	T	T	T
0.2157203054334576	0.5071843056117015	0.1446365090739137	T	T	T	0.2139883820333129	0.5064203465050809	0.1445175343062173	T	T	T
0.8016651330383757	0.5077159119156601	0.1454358636685575	T	T	T	0.8002865202763557	0.5071264504888997	0.1457122275935231	T	T	T
0.2119520459740447	0.0071495986991010	0.2457019851669884	T	T	T	0.2097939015115985	0.0069693777954923	0.2456055137502060	T	T	T
0.8058881601555792	0.0079332607178349	0.2462580009470238	T	T	T	0.8039362048720138	0.0078170646114951	0.2464816589534051	T	T	T
0.3060135650422894	0.5077475691135198	0.2462075032303754	T	T	T	0.3041459518435510	0.5077421752999797	0.2465762609404025	T	T	T
0.7120160652853248	0.5069469782011563	0.2457294287411339	T	T	T	0.7095791971461822	0.5070197633088492	0.2457633005933887	T	T	T
0.3083568349057642	0.0086135049772130	0.3466412440673262	T	T	T	0.3044490081062040	0.0088173407017616	0.3473496720253855	T	T	T
0.7111626190469297	0.0075011057412903	0.3458928490833686	T	T	T	0.7081533915294999	0.0079320667233529	0.3456361278434109	T	T	T
0.2109962529492035	0.5072937142071144	0.3459429107503683	T	T	T	0.2076820772183920	0.5079249514007531	0.3452812898549434	T	T	T
0.8079372882844702	0.5083851454719448	0.3463456227585262	T	T	T	0.8057304059119161	0.5089168346026879	0.3469874976126837	T	T	T
0.2103263754908290	0.0073822538724946	0.4453932965886893	T	T	T	0.2125948997686648	0.0080800014628946	0.4434270717634285	T	T	T
0.8089885250992067	0.0087374418647476	0.4456831827606889	T	T	T	0.8093542412293679	0.0090848901160256	0.4472922289835310	T	T	T
0.3102578567665154	0.5094014703618862	0.4459388334226002	T	T	T	0.3102191845837751	0.5089839715041999	0.4489919443129253	T	T	T
0.7111683514163570	0.5080021723290871	0.4453526272594683									

O ₂ H adsorbed on the surface:										H ₂ O adsorbed on the surface:									
La Ni O H										La Ni O H									
1.000000000000000										1.000000000000000									
7.493322000000000		0.000000000000000			0.000000000000000			0.000000000000000			7.493322000000000		0.000000000000000			0.000000000000000			
-0.120907850000000		7.445440999999998			0.000000000000000			0.000000000000000			-0.120907850000000		7.445440999999998			0.000000000000000			
0.045718910000000		0.037800290000000			39.856726879999965						0.045718910000000		0.037800290000000			39.856726879999965			
20	20	62	1							20	20	61	2						
Selective dynamics										Selective dynamics									
Direct										Direct									
0.0090729757397101	0.0041190426632110	0.1018139533710557	T	T	T					0.0053748221213975	0.0053317912137716	0.1015289123220242	T	T	T				
0.5082929180656073	0.0046849308964175	0.1017520209143165	T	T	T					0.5031814542588485	0.0062498970137542	0.1015221080191048	T	T	T				
0.0079725404545617	0.5055281191627534	0.1017449256907483	T	T	T					0.0037133801658663	0.5072639429943533	0.1015018071215231	T	T	T				
0.5107040745176891	0.5050098920699542	0.1017956085491211	T	T	T					0.5067006269108770	0.5052118254736180	0.1015284743397184	T	T	T				
0.0115688827023477	0.0038368913313991	0.1987257995360942	T	T	T					0.0076638505062924	0.0067891385487955	0.1983412276749923	T	T	T				
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0.0116196395270593	0.5031828180118457	0.1984535225888788	T	T	T					0.0075100703538830	0.5066060553973656	0.1981037971665538	T	T	T				
0.5113981576877527	0.5031458577328737	0.1986892387940641	T	T	T					0.5075550605881377	0.5063431462891543	0.1983611317405385	T	T	T				
0.0111785010053401	0.0030601170530190	0.2979359423076620	T	T	T					0.0082492171102686	0.0075819763399720	0.2974394345377458	T	T	T				
0.5117423445852268	0.0027204243207063	0.2979322241444742	T	T	T					0.5082941751716848	0.0075577633428234	0.2975243698720089	T	T	T				
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0.5120494146661909	0.5034105541904567	0.2978759198174654	T	T	T					0.5083328432689614	0.5079260467102051	0.2975052886345969	T	T	T				
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0.0112974595515824	0.5034315901227391	0.3981633642716051	T	T	T					0.0075958439808466	0.5090235458825811	0.3976462932793297	T	T	T				
0.5119770286116573	0.5041221826668451	0.3982394385688063	T	T	T					0.5083745323898511	0.5099353240539937	0.3980468382084021	T	T	T				
0.0130018634233252	0.0029147924560647	0.5027743407516410	T	T	T					0.0098347772457809	0.0074397600569628	0.5016243686738713	T	T	T				
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0.0134871816913282	0.5021568441190963	0.5032006482563207	T	T	T					0.0078690282405715	0.5106416619894152	0.5011417166672328	T	T	T				
0.5114348341966198	0.5022986050582529	0.5031378116155862	T	T	T					0.5115103374678657	0.5108166760724816	0.5019085858733886	T	T	T				
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0.7609533477634072	0.2539811121714660	0.1462512308989833	T	T	T					0.7572051473925575	0.2564118263284957	0.1459193591845996	T	T	T				
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0.7622240774557378	0.2521314170372035	0.5508283528811424	T	T	T					0.7630256648444773	0.2597693266792304	0.5501423310273907	T	T	T				
0.2623833203477097	0.7542868054957514	0.5507152279808792	T	T	T					0.2572123234188834	0.7559083181666781	0.5497684196928321	T	T	T				
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0.2617158734325524	0.2516027635948825	0.0923289838871553	T	T	T					0.2600912706927024	0.2529551583170413	0.0917140936933343	T	T	T				
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0.2627927475386332	0.2521934436744242	0.2984009879982605	T	T	T					0.2608827377376281	0.2554732800272492	0.2970420643213224	T	T	T				
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0.2607041078782262	0.2549969175991060	0.298501660026007	T	T	T					0.2570094526699259	0.7603930369627202	0.2980395353863877	T	T	T				
0.7629897762481946	0.7517741583517323	0.29849																	

0.0111701793255835	0.7067518290354178	0.2461640290038767	T	T	T	0.0075454033686855	0.7111356662015910	0.2455284133249022	T	T	T
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0.0117558715194892	0.2056846377078590	0.3465370294938842	T	T	T	0.0088197425555286	0.2110395380677159	0.3457450501602731	T	T	T
0.5119186805716056	0.3015052346759887	0.3469660163400196	T	T	T	0.5087635598042082	0.3069772317803111	0.3468142701714727	T	T	T
0.0122861961309341	0.8012285198663980	0.3468765085917451	T	T	T	0.0093922414838965	0.8060132862136217	0.3466620839534482	T	T	T
0.5113100615937766	0.7061235367319322	0.3463362726010033	T	T	T	0.5083013372815507	0.7109595854011286	0.3458619655290368	T	T	T
0.0124694369979687	0.3022660183580457	0.4463416846578560	T	T	T	0.0104984782181780	0.3095098560883689	0.4464756076799681	T	T	T
0.5123075097901432	0.2046754210187668	0.4459815116054111	T	T	T	0.5088933044422993	0.2114071418361367	0.4454135301615186	T	T	T
0.0118262583239542	0.7063635607657583	0.4457222289051950	T	T	T	0.0091894530430293	0.7139055179244503	0.4449592112774210	T	T	T
0.5129400542346293	0.8016918208245269	0.4460926661833325	T	T	T	0.5101565424915218	0.8082256684914495	0.4456953358750695	T	T	T
0.0123634868883230	0.2460875272506707	0.5431767098790713	T	T	T	0.0072174083886820	0.2498078575504404	0.5410752229885143	T	T	T
0.5123935071159299	0.2573190746027168	0.5436478157723651	T	T	T	0.5136171358673806	0.2740630082130141	0.5437940190322050	T	T	T
0.0128695539767544	0.7588502492014509	0.5450690131790062	T	T	T	0.0099988588892636	0.7732453002931268	0.5441278756910478	T	T	T
0.5115612648068860	0.7453082164755380	0.5447294815512118	T	T	T	0.5096087591177273	0.7479179243278586	0.5443369709381072	T	T	T
0.2738997145731521	0.2597154162831835	0.5989392833227573	T	T	T	0.2913949447106036	0.2382361551721017	0.5970954061495908	T	T	T
0.1301273840598934	0.3469586132698033	0.6130808630284046	T	T	T	0.2885054995646305	0.1059447503634472	0.5950097944670025	T	T	T
0.1588455917054292	0.4751417766604482	0.6090310813022860	T	T	T	0.4193419051513866	0.2696366244282265	0.5948085105819048	T	T	T

-1% Strain State:

O ₂ adsorbed on the surface:						OH adsorbed on the surface:					
La Ni O						La Ni O H					
1.0000000000000000						1.0000000000000000					
7.5697844400000003						7.5697844400000003					
-0.1196987700000000						-0.1196987700000000					
0.0452617200000000						0.0452617200000000					
20 20 62						20 20 61 1					
Selective dynamics						Selective dynamics					
Direct						Direct					
0.9981947313415755	0.9876093443624213	0.1023377968736431	T	T	T	0.9966114724787517	0.9914741418333982	0.1024797741905125	T	T	T
0.4864057390452112	0.9970796959237028	0.1023521976146103	T	T	T	0.4850122363245076	0.0011071698330774	0.1024541617824206	T	T	T
0.9860117320451389	0.4974199387448092	0.1023186988766697	T	T	T	0.9846170127047218	0.5012353165061785	0.1024125410868469	T	T	T
0.4985879693556050	0.4881330123691681	0.1023722560947245	T	T	T	0.4971641609786194	0.4924349395418797	0.1025176801930923	T	T	T
0.0014855223773791	0.0004909005686778	0.1983148964986759	T	T	T	-0.0000366955982797	0.0039202193835975	0.1984305009348213	T	T	T
0.5014344239111004	1.0000147759022706	0.1983059159435509	T	T	T	0.4998796458673012	0.0031235643901954	0.1983374423940089	T	T	T
0.0017279280901995	0.4999314887975004	0.1982961534175743	T	T	T	1.0001245920653534	0.5031257876247238	0.1983242906657286	T	T	T
0.5012991501559688	0.5000681530656548	0.1983474027441672	T	T	T	0.4996708087052368	0.5034147293320059	0.1984703720619171	T	T	T
0.0060728354126422	0.0035790476746433	0.2968000775051691	T	T	T	0.0050415241444099	0.0055828971057489	0.2968441597173785	T	T	T
0.5056961030714594	0.0039325920322924	0.2969191176239713	T	T	T	0.5048560902458827	0.0058503607016518	0.2968932158034510	T	T	T
0.0057587871235022	0.5045488591266686	0.2968706348444712	T	T	T	0.0049152695541872	0.5067145935998378	0.2968108053859031	T	T	T
0.5068416687729229	0.5035714977580076	0.2968730947730290	T	T	T	0.5058773309956267	0.5054755889200715	0.2969602992369685	T	T	T
0.0124506601783122	0.0087186234120228	0.3963664712879924	T	T	T	0.0120554741562451	0.0100540773419119	0.3962984168792817	T	T	T
0.5134060108455187	0.0088920876637138	0.3964517577136328	T	T	T	0.5129936657246860	0.0103978668452299	0.396468926534380	T	T	T
0.0115746926526869	0.5093485667530814	0.3964888826380063	T	T	T	0.0111100545030957	0.5105074883497980	0.3964205324913118	T	T	T
0.5121674596276257	0.5095942419458812	0.3965966431103826	T	T	T	0.5116112479570271	0.5111106727879039	0.3967071362199845	T	T	T
0.0170357303526986	0.0136034298998190	0.5004603583381413	T	T	T	0.0169046396169550	0.0144311154428777	0.5004102998814524	T	T	T
0.5162377516196165	0.0130096974537750	0.5006480419875458	T	T	T	0.5163765837991111	0.0138602442276726	0.5005254086076588	T	T	T
0.0164328603870628	0.5128594235395042	0.5006274836377111	T	T	T	0.0166812657461265	0.5144599539807718	0.5003223577662704	T	T	T
0.5152458582980731	0.5120247829760376	0.5006856026195246	T	T	T	0.5160923295621187	0.5140230433075755	0.5003627516796559	T	T	T
0.2497577168548067	0.2501160472067188	0.1458160441279214	T	T	T	0.2481710928510527	0.2538546529171115	0.1458847960885964	T	T	T
0.7510144691457903	0.2482804723338811	0.1459548386614598	T	T	T	0.7492921690217329	0.2519688212518588	0.1460065701641129	T	T	T
0.2510461106204419	0.7482880295302982	0.14596935866602170	T	T	T	0.2493486395396526	0.7519836793474761	0.1460319703209906	T	T	T
0.7497392210486585	0.7501057359922124	0.1460042343362001	T	T	T	0.7482535052093809	0.7537415269102452	0.1461043940881989	T	T	T
0.2546589855085534	0.2529505220450441	0.2462259099678429	T	T	T	0.2533194521584526	0.2554752380730337	0.2462933058341217	T	T	T
0.7549463808886537	0.25223399375662701	0.2460704752371432	T	T	T	0.7535677918703160	0.2549774529058770	0.2461143387318399	T	T	T
0.2549673177401595	0.7524126128381323	0.24607071786767558	T	T	T	0.2536286397660207	0.7550304074699257	0.2461247484430859	T	T	T
0.7544264186616128	0.7531521804688435	0.2460039971655629	T	T	T	0.7530766921771789	0.757045511080298	0.2460530446331192	T	T	T
0.2601151386134425	0.2566924727069639	0.3457286956083558	T	T	T	0.2595786196423415	0.2581810967287886	0.3457525863891895	T	T	T
0.7598918426632397	0.2571863195638299	0.3456946794452174	T	T	T	0.7592377386160278	0.2588248411506231	0.3456938274090006	T	T	T
0.2596857871343310	0.7569245672495207	0.3456968806919094	T	T	T	0.2590724817522502	0.7584387828616720	0.3457062380609699	T	T	T
0.7597759904632851	0.7569102356713305	0.3456276979550374	T	T	T	0.7590831155470019	0.7583894870267111	0.3456253314155628	T	T	T
0.2645918775368951	0.2621820409012107	0.4455638708812623	T	T	T	0.2641210444237192	0.2634194103982715	0.4456095621111157	T	T	T
0.7653696320239664	0.2613011653410274	0.4460323927575116	T	T	T	0.7651741145239725	0.2623593819889229	0.446005842080426	T	T	T
0.2652988613461171	0.76105367330971935	0.4460393202202238	T	T	T	0.2648393527216181	0.7626059743228847	0.4459802038959152	T	T	T
0.7648019294668638	0.7617622470303247	0.4462242185078849	T	T	T	0.7648439707716863	0.7630932951496563	0.4461259887032158	T	T	T
0.2638392788952217	0.2618752469105333	0.5497659594883341	T	T	T	0.2654774877724428	0.2639384214591696	0.5492700429258636	T	T	T
0.7644712781830827	0.2624846364239327	0.547504988865874	T	T	T	0.7652550252848249	0.2639823550007768	0.5472956461913920	T	T	T
0.2643224571541832	0.7624752439337886	0.5473475915886523	T	T	T	0.2648591287480427	0.7616004226630007	0.5474151239917930	T	T	T
0.7643181015459751	0.7617555461605808	0.5465113792465349	T	T	T	0.7650212166466313	0.7622458968177670	0.5464207496697289	T	T	T
0.2669704438607232	0.2356543151337412	0.0927372474493260	T	T	T	0.2651049524993662	0.2395290253133997	0.0928862975929537	T	T	T
0.7402640940779124	0.2700789214328032	0.0922905953414877	T	T	T	0.7384343776475291	0.2733565971061570	0.0924699546336108	T	T	T
0.2404504628001638	0.7701408054000162	0.0922830379240985	T	T	T	0.2389320792881539	0.7732675866848115	0.0924570734355427	T	T	T
0.7670094897460475	0.7359450535434765	0.0924084847587078	T	T	T	0.7653835795215919	0.7391963759193255	0.0924165529998215	T	T	T
0.2404746728629042	0.2646904113122858	0.1944373546299951	T	T	T	0.2393293622772100	0.2678749050803837	0.1944942939536355	T	T	T
0.7623812820491729	0.2355876450604056	0.1949701201692707	T	T	T	0.7604718799867695	0.2387247771092270	0.1949985051060904	T	T	T
0.2624482392113675	0.7355372449595149	0.1950077380631065	T	T	T	0.2605116478817095	0.7387088903796750	0.1950173485232281	T	T	T
0.7404730955264315	0.7647934314785220	0.1950832257761665	T	T	T	0.7397745451774849	0.7679346545759981	0.1952334367398377	T	T	T
0.2684536848553776	0.2413146960547444	0.2963903071312623	T	T	T	0.2668564934621613	0.242625371555629	0.2969080099807518	T	T	T
0.7461762044297338	0.2691910704833959	0.2967151376369855	T	T	T	0.7461316237769067	0.2712692551221487	0.2966800561495352	T	T	T
0.2463616428969997	0.7697352173904568	0.2966901090963255	T	T	T	0.2464604732633978	0.77198864051940	0.2967262570508669	T	T	T
0.7685657004519264	0.7410502722286076	0.2965370573399928	T	T	T	0.7665409461153559	0.7424702297211894	0.2965343864959933	T	T	T
0.2489974947420667	0.2749667306762468	0.3953346012413623	T	T	T	0.2497906531671475	0.276748049394815	0.3954943438711726	T	T	T
0.7740461359733025	0.2441490628760838	0.3941825676851576	T	T	T	0.7726576166205652	0.2460072899037056	0.3941364815239527	T	T	T
0.2723615149167605	0.7428751235105024	0.3941541249019125	T	T	T	0.2709449512179543	0.7437964814030920	0.3941786550789503	T	T	T
0.7505908180267824	0.772286996293841	0.3939087991339963	T	T	T	0.7511195929481592	0.773570392102472	0.3938795387809974	T	T	T
0.2733011664625492	0.2515446954858365	0.4918141744715041	T	T	T	0.2718832940410282	0.2512432766651822	0.4920119468228903	T	T	T
0.7586274053781584	0.2684437827739381	0.492626359728841	T	T	T	0.7596727179751189	0.269486740696230	0.4926223661291454	T	T	T
0.2593393784840286	0.7681614703247494	0.4926625280785617	T	T	T	0.2595407843825341	0.7708477507249769	0.4925923668756585	T	T	T
0.7694839187618590	0.7548585982282027	0.4929922500477836	T	T	T	0.7696500395511791	0.7564275049690106	0.4929001483854019	T	T	T
0.2871777611659998	0.9948418503631813	0.1482698017824195	T	T	T	0.28512246643479599	0.0031189541511955	0.1482728721			

0.7871085937264477	0.4995826188199651	0.1482843420925688	T	T	T	0.7851162815582496	0.5033067619827526	0.1483128753163261	T	T	T
0.2152571627331889	0.0026742377157090	0.242778022665016	T	T	T	0.2140163563800010	0.0052549576530533	0.2428479188152642	T	T	T
0.7977431554711638	0.0031967635004516	0.2479550405349892	T	T	T	0.77959310567704732	0.0058624119391211	0.2481307952445044	T	T	T
0.2979702198825010	0.5029160808965595	0.2479976213539323	T	T	T	0.2962451788584862	0.5056273841790839	0.2481768611950276	T	T	T
0.7154196283559492	0.5023626627081587	0.2427725602407047	T	T	T	0.7141538229842477	0.5049627199498553	0.2428402416915510	T	T	T
0.3040789149469146	0.0076805818049190	0.348136685264795	T	T	T	0.3035914777609907	0.0091756938869646	0.3482437526862302	T	T	T
0.7196034410378579	0.0065999215022812	0.3419390733087582	T	T	T	0.7189079878053816	0.0081299822422477	0.3418807140484719	T	T	T
0.219222348671966	0.5064024744849266	0.3420097755957650	T	T	T	0.2184711256344279	0.5078111611816296	0.3419342159961732	T	T	T
0.8040067111861976	0.5074781371444493	0.3477006010037417	T	T	T	0.8037133528893767	0.5090020822027836	0.3476477358851628	T	T	T
0.2286078991974573	0.0107283722260591	0.4406372979480247	T	T	T	0.2285327379052862	0.0118772854586231	0.4404518493374675	T	T	T
0.8138496505974638	0.0120662282152942	0.4459386163453224	T	T	T	0.8137471760758762	0.0132676912539724	0.4458601221926695	T	T	T
0.3150667651409982	0.5125836202663617	0.4465784066236860	T	T	T	0.3143875866379078	0.5138254493850989	0.4468376639743740	T	T	T
0.7282233609627283	0.5114581626451359	0.4409796835245446	T	T	T	0.7275054057700888	0.5126317261601956	0.4411340595720479	T	T	T
0.2722079529420554	0.0129641032136010	0.5411902511167374	T	T	T	0.2723058758949098	0.0145422205082738	0.5417077639706031	T	T	T
0.7630647028651520	0.0128021231276016	0.5412903511556750	T	T	T	0.7628190473706159	0.0139983239378260	0.5413237095275361	T	T	T
0.2621377295684340	0.5127321659386198	0.5401759976786981	T	T	T	0.2623520218966146	0.5141382645438231	0.5397015786639697	T	T	T
0.7762328460392287	0.5120393894901364	0.5429538496795046	T	T	T	0.7763163414146101	0.5133259745512069	0.5425476957302290	T	T	T
0.9999711629595908	0.2135225836284114	0.1427765508112125	T	T	T	0.9983589115209849	0.2179293727173667	0.1428981945099976	T	T	T
0.5011164939743298	0.2850829350067844	0.1475575574365478	T	T	T	0.4993948086106275	0.2886018249340821	0.1475988927728831	T	T	T
0.0009773084987087	0.7850299632041969	0.1476053210302984	T	T	T	0.9992088519672178	0.7886217696583021	0.1476559419127484	T	T	T
0.5002907823509540	0.7134915926641580	0.1429413471660728	T	T	T	0.4987841993397694	0.7179905436498488	0.1430833510030186	T	T	T
0.0053372813045115	0.2948077638871480	0.2474244366726838	T	T	T	0.0039340544337159	0.2968821408611854	0.2473388437479734	T	T	T
0.5043394949190552	0.2130692271932366	0.2434708750207057	T	T	T	0.5028412668583341	0.2158629056262704	0.2436039091449442	T	T	T
0.0046409816933338	0.7134726513984047	0.2433981041222519	T	T	T	0.0032468674063587	0.7161527821493043	0.2436174353199367	T	T	T
0.5050395328487650	0.794803409941409	0.2474584819984401	T	T	T	0.5036051654605574	0.7969631164651956	0.2472460109439447	T	T	T
0.0097823759841950	0.2164211313011408	0.3426995216649977	T	T	T	0.0091988334142051	0.2175537247549872	0.3429942521890475	T	T	T
0.5101255136111348	0.3001749821430107	0.3474110712908520	T	T	T	0.5095546108051112	0.3018734676840413	0.3473388437479734	T	T	T
0.0101611138444622	0.7995956458361264	0.3471199963246601	T	T	T	0.0096072408091841	0.8014821600309923	0.3468739450514718	T	T	T
0.5094004251624573	0.7169061673809184	0.3425829397448210	T	T	T	0.5087605708844196	0.7180307990096856	0.3428606410391732	T	T	T
0.0154811443253876	0.3100556898036804	0.4462277968922522	T	T	T	0.0150773789773062	0.3110740421948340	0.4460491903123487	T	T	T
0.5157046916515042	0.2242178162258100	0.4412617516131030	T	T	T	0.5153588953983361	0.2250495068777668	0.4415101832302391	T	T	T
0.0148311213775354	0.7235361894521278	0.4417313443141630	T	T	T	0.0145448292298860	0.7241995245835670	0.4417896359387407	T	T	T
0.5158762537125985	0.8087032826730081	0.4455403488342610	T	T	T	0.5157258114029123	0.8090984774435964	0.4452963036964155	T	T	T
0.0158782165275132	0.258805188740533	0.5402239330586653	T	T	T	0.0157071881150136	0.2601583128510113	0.5398187999374309	T	T	T
0.5160846281782326	0.2682951706106569	0.5413651542779342	T	T	T	0.5167183036124031	0.2687242037497481	0.5405079874318185	T	T	T
0.0160982688326674	0.7710675026802121	0.5423305453425097	T	T	T	0.0165207965597724	0.7729363150454506	0.5422907358408708	T	T	T
0.5151639444333606	0.75778836310135942	0.5412349953310827	T	T	T	0.5152698603457190	0.7596375792845619	0.541113617506921	T	T	T
0.268358927610998	0.2747048456768842	0.5962237332014865	T	T	T	0.2659927557509373	0.2581290876852507	0.5941236283351723	T	T	T
0.1694653214879324	0.1700078295238501	0.6125734645779912	T	T	T	0.2816935285779325	0.1315310967036459	0.5990281422249976	T	T	T
O adsorbed on the surface:						H adsorbed on the surface (O):					
La Ni O						La Ni O H					
1.0000000000000000						1.0000000000000000					
7.5697844400000003						7.5697844400000003					
-0.1196987700000000						-0.1196987700000000					
0.0452617200000000						0.0452617200000000					
20 20 61						20 20 60 1					
Selective dynamics						Selective dynamics					
Direct						Direct					
0.9976734212818185	0.9880417972739982	0.10224451221182152	T	T	T	0.9965368346224562	0.9889674853648690	0.1023309932932700	T	T	T
0.4863382984400891	0.9977181035862416	0.1023033077423910	T	T	T	0.4844034197178997	0.9984045634838825	0.102308379289190	T	T	T
0.9858174044467226	0.4979264099154587	0.1022090598826816	T	T	T	0.9845020762814589	0.4982949716591853	0.1023109060166340	T	T	T
0.49796237323482086	0.4885918453905490	0.1023071772884797	T	T	T	0.4966236877983625	0.4891345231674280	0.1023785082277442	T	T	T
0.0014844215250800	0.0011127695156441	0.1982853171086796	T	T	T	-0.0002992526846882	0.0012560779453034	0.1983473844380793	T	T	T
0.5015356876348100	0.0004994472840555	0.1982772452938820	T	T	T	0.4999648049229632	0.0007867736938506	0.1982284083516393	T	T	T
0.0016973427183228	0.5005076869070676	0.1982277456900175	T	T	T	-0.0003670217300973	0.5009592235326336	0.1983909351109829	T	T	T
0.5012921541052129	0.5006144119410189	0.1983619108417496	T	T	T	0.4994628582201792	0.5012105876502532	0.1984466061765314	T	T	T
0.0060137469858041	0.0039826557527714	0.2967576027083833	T	T	T	0.0048128074020934	0.0043488481330315	0.2966975766129596	T	T	T
0.5056821492752310	0.0042467386892732	0.2969106989509593	T	T	T	0.5035097420308127	0.0049483395240572	0.2967177573844895	T	T	T
0.0058574590437683	0.5049705196209622	0.2968104993882352	T	T	T	0.0028362864681130	0.5052531862933675	0.2969088148291019	T	T	T
0.5068776840517056	0.5038194334254107	0.2968765985356226	T	T	T	0.5039381563924454	0.5046915125274500	0.2972496584117091	T	T	T
0.0126210244634492	0.0088956654125106	0.3963442774785335	T	T	T	0.0102841670140704	0.0094875073489638	0.395995647411735	T	T	T
0.5136371892075602	0.0084871424874128	0.3964723695459879	T	T	T	0.5109542045805086	0.0092248344140960	0.3959622139459311	T	T	T
0.0117835801932755	0.5093307483047214	0.3964864428439914	T	T	T	0.0095977244176293	0.5095536543461406	0.3969044240738045	T	T	T
0.5124459864288697	0.5093297798510207	0.3966957108909380	T	T	T	0.5080405410980937	0.5101610535937434	0.3971994456896857	T	T	T
0.0167062315941350	0.0128305443505776	0.5004334874810582	T	T	T	0.0104024933136712	0.0123349254335216	0.4990211563075410	T	T	T
0.5157781457744199	0.0124274916081570	0.5006377864397578	T	T	T	0.5224451393674114	0.0105012578657132	0.498540356832273	T	T	T
0.0164169056582114	0.5119787239476110	0.5005170613783332	T	T	T	0.0142382898169789	0.5130385646557516	0.5000343728975466	T	T	T
0.5151650176279667	0.5113181712900403	0.5005888352659509	T	T	T	0.5170579737695026	0.5101429639766794	0.5014269982161205	T	T	T
0.2495493756550877	0.2506339655160525	0.1457904110967133	T	T	T	0.2480409350728951	0.2511481029644058	0.1459940105524215	T	T	T
0.7508945806315874	0.2489202120574287	0.1458919853869224	T	T	T	0.7493496080998554	0.2492199771635410	0.1460017164			

0.7403191853991316	0.7648592484773091	0.1950906650855475	T	T	T	0.7399404566225217	0.7652850737123464	0.1950475266552742	T	T	T
0.2685060355012319	0.2414142593163440	0.2969928825407975	T	T	T	0.2669174688184596	0.2405423244028714	0.2968376466502147	T	T	T
0.7462334034032578	0.2691934746141192	0.2966321666167598	T	T	T	0.7439722853636431	0.2709684011501645	0.2967938037040153	T	T	T
0.2462912607282145	0.7701477489134386	0.2966174929874910	T	T	T	0.2471790039232304	0.7707201673241721	0.2967872169699945	T	T	T
0.7685288009503748	0.7414495697457356	0.2964926221263065	T	T	T	0.7639844950349676	0.7405274782103448	0.2967373023181554	T	T	T
0.2491194345684455	0.2751222046999499	0.395199508383917	T	T	T	0.2483667486028618	0.2769202470808015	0.3945334537719371	T	T	T
0.7736948115964077	0.2449709032057502	0.3941788947984303	T	T	T	0.7716364087269039	0.2417336642247875	0.3942525083763845	T	T	T
0.2720997888310266	0.7427774351976746	0.3941867358904074	T	T	T	0.2662417595392734	0.7405281831764785	0.3945204964721670	T	T	T
0.7513252329083984	0.7714215179866036	0.3938985347126870	T	T	T	0.7533580267273500	0.7751066805177959	0.3942299689834181	T	T	T
0.2724351520321551	0.2502494310141040	0.4912875445707928	T	T	T	0.2716974254404588	0.2373661735934687	0.4935498466950888	T	T	T
0.7596624553914775	0.2669280544005130	0.4930340869839239	T	T	T	0.7583942617150329	0.2684593245694681	0.4926073454256059	T	T	T
0.2598946396416764	0.7673952424731491	0.4930916879008290	T	T	T	0.2620598420506817	0.7840270676913681	0.4935262025351664	T	T	T
0.7690660978860745	0.7548154512187252	0.4931287181685812	T	T	T	0.7647851241190055	0.7534570829476971	0.4926394950030915	T	T	T
0.2875206788317466	-0.0000576456568402	0.1482566868026137	T	T	T	0.2856564138186183	0.0005211595095105	0.1482977468791435	T	T	T
0.7144281664468095	0.9995603007878212	0.1419728812149052	T	T	T	0.7127873728940215	1.0000113141623446	0.1419439317373212	T	T	T
0.2143898907129889	0.4997942309569107	0.1417716846088546	T	T	T	0.2127380974646640	0.5000809685109411	0.1419257544614338	T	T	T
0.7874648902200430	0.5002350630140168	0.1481504124941948	T	T	T	0.7858832833257303	0.5005029474098908	0.1483012659224577	T	T	T
0.2151430914943561	0.0031251177320292	0.2427856529289270	T	T	T	0.2131291496897545	0.0030582230122798	0.2428809546253589	T	T	T
0.7975855194456615	0.0036676819489949	0.2478944721309513	T	T	T	0.7956183108149666	0.0037840044101280	0.2480892430036676	T	T	T
0.2978725820963874	0.5033624185551407	0.2479952792829148	T	T	T	0.2963101511993305	0.5037018901589740	0.2481961933664833	T	T	T
0.7152199323255568	0.5028889901434429	0.2428512989151971	T	T	T	0.7131991846399540	0.5029983695958402	0.2428477802797041	T	T	T
0.3043270224538594	0.0077460425236504	0.3481645232063730	T	T	T	0.3015367973403662	0.0079290619975744	0.3483273607144103	T	T	T
0.7193832928083158	0.0066984377080647	0.3420029741538083	T	T	T	0.7168176750482255	0.0070776095125871	0.3418236968889986	T	T	T
0.2192179570106293	0.5066122690469593	0.3419778430042612	T	T	T	0.2167263018046109	0.5070416304682932	0.3417456570483027	T	T	T
0.8045563201075459	0.5076195490355364	0.3475810332564019	T	T	T	0.8030302732269665	0.5079237056580561	0.3482085978706096	T	T	T
0.2299604962087927	0.0100001830421987	0.4405483085185632	T	T	T	0.2277986891554977	0.0104288797567948	0.4399091857839595	T	T	T
0.8138410415762471	0.0115290399950672	0.4458149605549784	T	T	T	0.8116157022230311	0.0114625409994425	0.4470955764136526	T	T	T
0.3148556831227974	0.5121700133918298	0.4466204988380006	T	T	T	0.3123498811936820	0.5111434955688811	0.4485777622230060	T	T	T
0.7274810414585180	0.5109092697057698	0.4413613571317094	T	T	T	0.7286796605853384	0.5104621916624398	0.4405765429453212	T	T	T
0.2697931278416983	0.0128100894013590	0.541167677293646	T	T	T	0.2828807446302720	0.0107382009200593	0.5587773914298423	T	T	T
0.7635829409240750	0.0122079498028083	0.5412417219371572	T	T	T	0.7584394267603670	0.0110660426677402	0.5404704237509437	T	T	T
0.2623614413625131	0.51059588902310548	0.5402063722501901	T	T	T	0.2603189614640675	0.5109925337525241	0.5381360340423709	T	T	T
0.7751264220161307	0.5110631383516644	0.5427228542222793	T	T	T	0.7739986595108213	0.5112626706382792	0.5420528573242980	T	T	T
-0.0000456427289216	0.2136624679640633	0.1427133928706016	T	T	T	0.9986230494019995	0.2138960177558789	0.142983130389322	T	T	T
0.5009048606447979	0.2860063760981127	0.1475264857080556	T	T	T	0.4992600154686349	0.2865635933861376	0.1475713019431170	T	T	T
0.0007344675428765	0.7859892071733919	0.1475764175007917	T	T	T	0.9993108726233855	0.7865547641200638	0.1475215038985342	T	T	T
0.5002481781541582	0.7136703142996365	0.1428510911070738	T	T	T	0.4986690832746341	0.7139997505209196	0.1430610896427001	T	T	T
0.0053102257129079	0.2951322649116159	0.2473866848716688	T	T	T	0.0032574032293345	0.2952635857593204	0.2474642394945051	T	T	T
0.5043066399135610	0.2137557718640148	0.2434079339372844	T	T	T	0.5025296438361134	0.2135315719263208	0.2435055098519120	T	T	T
0.0045744930306511	0.71404155865428192	0.2433244423280345	T	T	T	0.0025903681429126	0.7136809678292197	0.2438159629737181	T	T	T
0.5049193294376375	0.7952083081675339	0.2474449672234500	T	T	T	0.5031013037820329	0.7955766604766561	0.2471275644414448	T	T	T
0.0097256954200263	0.2163807741521519	0.3427343002150827	T	T	T	0.0076742568978366	0.2162648483433116	0.3428395958628396	T	T	T
0.5103407583886733	0.3004951434443889	0.3473894834210643	T	T	T	0.5083805644438605	0.3014027931237003	0.3477018573766454	T	T	T
0.0103045421295223	0.80036546466947094	0.3470515643004711	T	T	T	0.0084278030273636	0.8009554741739182	0.3466044524126139	T	T	T
0.5095349414911147	0.7168612299449479	0.3426407028080855	T	T	T	0.5076053660618089	0.7160913177425035	0.3437998701717790	T	T	T
0.0153339547499572	0.30902209885210494	0.4460250939485271	T	T	T	0.0150102904333627	0.3068912827508449	0.4463114687714870	T	T	T
0.5158439648902298	0.2237230664261653	0.4413053582852248	T	T	T	0.5137503724373940	0.2217718638223380	0.4418052158847610	T	T	T
0.0149456536646658	0.7223807149106548	0.4420068841180249	T	T	T	0.0140862054299632	0.7210384842433061	0.4433531597563765	T	T	T
0.5159693602833229	0.8082679614631538	0.4455092664619362	T	T	T	0.5144070060284939	0.8063222368970309	0.4446013560014206	T	T	T
0.0165000571339382	0.2587220380337025	0.5404314864595444	T	T	T	0.0168652494795497	0.2506203215504060	0.5397448221394627	T	T	T
0.5151534014890120	0.2663061666299428	0.5411699466354135	T	T	T	0.5141707528378491	0.2582315181774678	0.5419829652734514	T	T	T
0.0159575392073741	0.7686161048481970	0.5420914383432301	T	T	T	0.0169116206138978	0.7752376797511691	0.5405925849240389	T	T	T
0.5146052497035690	0.75775733902135588	0.5410704230546434	T	T	T	0.5135654390979185	0.7633444632041443	0.5411436892158805	T	T	T
0.2622136996083999	0.2643723457146736	0.5938840983450394	T	T	T	0.4053395266950372	0.0152712131626579	0.5661055964967628	T	T	T

O ₂ H adsorbed on the surface:						H ₂ O adsorbed on the surface:					
La Ni O H						La Ni O H					
1.0000000000000000						1.0000000000000000					
7.5697844440000003						7.5697844440000003					
-0.1196987700000000						-0.1196987700000000					
0.0452617200000000						0.0452617200000000					
0.0000000000000000						0.0000000000000000					
0.0000000000000000						0.0000000000000000					
0.0374222900000000						0.0374222900000000					
39.6698201000000026						39.6698201000000026					
20	20	62	1			20	20	61	2		
Selective dynamics						Selective dynamics					
Direct						Direct					
0.0019794825632908	0.9898429478869855	0.1026822522543028	T	T	T	0.9968679252976089	0.9900112854568930	0.1025999079999521	T	T	T
0.4913295714897100	0.9996348249384165	0.1027202989414998	T	T	T	0.4858829329402740	0.9982904495560647	0.1026521461532161	T	T	T
0.9911333210650215	0.5004487177127210	0.102660204481567	T	T	T	0.9855689055846578	0.4996086060990910	0.1025729163542352	T	T	T
0.5028169152146114	0.4900509870374767	0.1027043798403405	T	T	T	0.4988333674573215	0.4904828646080940	0.1027222601891892	T	T	T
0.0046677113259846	0.0027571341539614	0.1987251268506759	T	T	T	0.9999068340331495	0.0022103253516636	0.1984105312058093	T	T	T
0.5047346948700653	0.0021992193949613	0.1986761532072303	T	T	T	0.5001637036744584	0.0011799174173162	0.1983981401105752	T	T	T
0.0051892627040657	0.5019239997383294	0.1985727151761610	T	T	T	0.0004426950522307	0.5014293950337648	0.1984018887980702	T	T	T
0.5045729725444241	0.5023594621829036	0.1987387002095119	T	T	T	0.4999143908410636	0.0014078741988677	0.1985188364379994	T	T	T
0.0088765440853987	0.0052901588461410	0.2973269792120463	T	T	T	0.0048229497392249	0.0052112426883052	0.2967886559107795	T	T	T
0.5084620385345417	0.0052588413842599	0.2973897298059222	T	T	T	0.5036961610985251	0.0055428315207437	0.2968558937527437	T	T	T
0.0087372116405226	0.506283842670002	0.2972416819508953	T	T	T	0.0037479071853434	0.5060337506501887	0.2968062693388770	T	T	T
0.5099308486103891	0.5051288424765373	0.2972417590151329	T	T	T	0.5049438024189955	0.5054762286826673	0.2969248803963195	T	T	T
0.0151237171357321	0.0099196936576969	0.3968171895525680	T	T	T	0.0106220944449651	0.0103250288395602	0.3961015905461014	T	T	T
0.5159054658075833	0.0006263524902928	0.3703737226317189	T	T	T	0.5111110142083446	0.0115084110657287	0.3965622730772898	T	T	T
0.0146104949758939	0.51023865387250559	0.3968508831555837	T	T	T	0.0089351291124997	0.5113871757319782	0.3965656407837959	T	T	T
0.51519720344742542	0.5107403948793684	0.3970798210525094	T	T	T	0.5093975754323912	0.5118826115729193	0.3968950236874932	T	T	T
0.0197912812792515	0.0157914724282953	0.5135050616616687	T	T	T	0.0117560732993276	0.0131274461163116	0.4984847006110914	T	T	T
0.5196550839737618	0.014507300634854	0.5009104590831321	T	T	T	0.5194284949326916	0.0131211100244781	0.5015811655959007	T	T	T
0.0196226549671575	0.5136408549951981	0.5013665030093282	T	T	T	0.0137067390069476	0.5164166069255575	0.4987911406784971	T	T	T
0.5186876142735030	0.5107643485034553	0.50066259252381153	T	T	T	0.5199669730460812	0.5134965793050014	0.49967096219235484	T	T	T
0.2535151727416334	0.2525262060432468	0.1461727822153567	T	T	T	0.2488843896443342	0.2515049210046496	0.1459114668781161	T	T	T
0.7548102463079318	0.2507758018151736	0.1462956398521431	T	T	T	0.74977606060418074	0.2497487826645345	0.1460735569011127	T	T	T
0.2548705014076267	0.7508852565673457	0.1463083186182877	T	T	T	0.2498732834066810	0.7498658908383309	0.1460827359941266	T	T	T
0.7534945023443891	0.7524702038350518	0.1463768936655204	T	T	T	0.7487654828970693	0.7516627619350742	0.1461543771920401	T	T	T
0.2577940274295454	0.2548373009608050	0.2466252148268405	T	T	T	0.2533456113515010	0.2540764084068209	0.24626877090171506	T	T	T
0.7581958025430736	0.2544042596152547	0.24646589572913337	T	T	T	0.7534240545683889	0.2537986104138666	0.2461329867658580	T	T	T
0.2581898789554646	0.7545287190203265	0.24644584857204556	T	T	T	0.2533923946364204	0.7536990021048853	0.24612063568827509	T	T	T
0.7576066422027071	0.7550105895474595	0.2463843343203505	T	T	T	0.7529384802639030	0.7545180920966793	0.24610659759212874	T	T	T
0.2629809436063776	0.2580781747252919	0.3461604618864696	T	T	T	0.2581601468917968	0.25898932288254477	0.3459299231178714	T	T	T
0.7626362400986534	0.2585608961019679	0.3461398065010798	T	T	T	0.7578448132654287	0.2589000257605852	0.3457122235971393	T	T	T
0.2626106968798278	0.758165030399133	0.3461263737114861	T	T	T	0.2580030795275718	0.7581755650090383	0.3457974714086338	T	T	T
0.7626497651392279	0.7582523717257011	0.3460656262685893	T	T	T	0.7579092489691605	0.7583939400315273	0.3456584937896134	T	T	T

0.2669307024393394	0.2633833225854435	0.4460832647924867	T	T	T	0.2631714474904883	0.2636337957296223	0.4459127841524920	T	T	T
0.7685639776265637	0.2625049362008959	0.4465343846033115	T	T	T	0.7633104752669102	0.2622651741973238	0.4456144817470666	T	T	T
0.2677525856257097	0.7622602730627916	0.4465108769533405	T	T	T	0.2647029738038443	0.7646613454417377	0.4462215660021014	T	T	T
0.7683861012044649	0.7630189061827074	0.4467060058190164	T	T	T	0.7628779083262179	0.7637966500329300	0.4456842519958437	T	T	T
0.2705531491982175	0.2643038893592476	0.5502260810044345	T	T	T	0.2626451045178103	0.2635256462522155	0.5441065025810224	T	T	T
0.7656036282341906	0.2649020399397039	0.5479889924148762	T	T	T	0.7690874355860920	0.2645272177237232	0.54649419732902019	T	T	T
0.2686706189005729	0.7641717346554638	0.5475669158687657	T	T	T	0.2624049050507138	0.7633348418695485	0.5448473164999389	T	T	T
0.7669484777601563	0.7631268887094290	0.5469427456494640	T	T	T	0.7665115426213003	0.7617748733015554	0.5463826806711447	T	T	T
0.2710693081560322	0.2392391828074824	0.0931193735366591	T	T	T	0.2648795540661175	0.2371145696882828	0.0933595166952076	T	T	T
0.7425547564538438	0.2704505219170010	0.0926951454028914	T	T	T	0.7403590773413252	0.2704744577423980	0.0924318068656368	T	T	T
0.2424763210657183	0.7706931373694280	0.0926831957918379	T	T	T	0.2402724857351109	0.7713953064294680	0.0924485248049107	T	T	T
0.7717144075703337	0.7392702132604477	0.0926051916957790	T	T	T	0.7651604290873590	0.7375020635265990	0.0923846641847884	T	T	T
0.2434131553354372	0.2659564448210645	0.1947965540559746	T	T	T	0.2395639860601411	0.2666155619664377	0.1948669744314732	T	T	T
0.7665095888472643	0.2392682889218432	0.1953033969936617	T	T	T	0.7606124630493183	0.2372117912021879	0.1950685530410432	T	T	T
0.2669611245709139	0.7392994215486719	0.1953789164841729	T	T	T	0.2606236593012809	0.7365163817221018	0.1952701617787891	T	T	T
0.7432164077503995	0.7660224919138507	0.1955099284374031	T	T	T	0.7401720070090889	0.7660037207342548	0.1951717558580980	T	T	T
0.2708988370713935	0.2431123548989923	0.2972695162818012	T	T	T	0.2652811826447594	0.2425904852861306	0.2956946693706877	T	T	T
0.7493577572545700	0.2703461554175645	0.2971369929688308	T	T	T	0.7453473545163073	0.2707595591654751	0.2967510940679564	T	T	T
0.2489663475463507	0.7710762552288865	0.2970819663768759	T	T	T	0.2454678168777911	0.7709953379320993	0.2964302132849014	T	T	T
0.7717222801448125	0.7426938888921084	0.2969404803920194	T	T	T	0.7655686201179009	0.7424190369669772	0.2966920491265139	T	T	T
0.2522759045185494	0.2762031737458293	0.3958874042189436	T	T	T	0.2508835531593480	0.2762475357931211	0.3956291633689836	T	T	T
0.7764213620348551	0.2459639035565663	0.3946985093173161	T	T	T	0.7709499691685385	0.2456382517827403	0.3942692674405227	T	T	T
0.2758611933561205	0.7437143415485677	0.3945441350027278	T	T	T	0.2688812804343175	0.7443385754846084	0.3941951484551249	T	T	T
0.7531504847429064	0.7731188949200518	0.3943526703494314	T	T	T	0.7501369073985921	0.7741692957185158	0.3940881494022607	T	T	T
0.2746620654985390	0.2524007311887396	0.4924287407173015	T	T	T	0.2732373547875844	0.2394499145366786	0.4957403582676113	T	T	T
0.7624588786343049	0.2695193632356722	0.4931393684488588	T	T	T	0.7579425231914365	0.2692503909696380	0.492081966065102	T	T	T
0.2614970290571864	0.7698950883589153	0.4931930278401476	T	T	T	0.2599772695912261	0.7812362671406767	0.4937475198030146	T	T	T
0.7738105454086317	0.7565775842512681	0.4935023261295648	T	T	T	0.7680571855407478	0.7568310090473920	0.4923901985498117	T	T	T
0.2914045053854653	0.0019340724381643	0.1483217898873595	T	T	T	0.2853920640518094	0.0008156169473135	0.1484320770012062	T	T	T
0.7185297649516694	0.0013558513920558	0.1425920364403792	T	T	T	0.7146960003105236	0.0005099948312890	0.142123530757029	T	T	T
0.2185227872525191	0.5017873613882569	0.1424936098478273	T	T	T	0.2147897013663269	0.5008982662118296	0.1419821306523937	T	T	T
0.7910568670821735	0.50021284789597577	0.1482944757594997	T	T	T	0.7849757868039740	0.5011648674142513	0.1482330509758772	T	T	T
0.2179730284421336	0.05426728915912832	0.2432670091958916	T	T	T	0.21430786467390118	0.0036760968353582	0.2427501841815359	T	T	T
0.8011041001737446	0.0052527486681004	0.2482570661256718	T	T	T	0.7959475906221047	0.0046172487635686	0.2480773459030786	T	T	T
0.3013514823271999	0.5050266348488880	0.2482769397336234	T	T	T	0.2958952217194367	0.5043777250408853	0.2480428765002803	T	T	T
0.7180211521347399	0.5042362654664300	0.2432953001354900	T	T	T	0.7139334358861309	0.5038063290762944	0.2429844906274597	T	T	T
0.3067462149312299	0.00898598605913731	0.3485496630009039	T	T	T	0.3025698160795983	0.0095853082748472	0.3480006183203877	T	T	T
0.7222138011114340	0.0079317341562759	0.3424553533729448	T	T	T	0.7167148490653286	0.0083422143097815	0.342059859250361	T	T	T
0.2217645316161029	0.50769204948637655	0.3424840903808726	T	T	T	0.2159212120460789	0.5076439104118255	0.3421338044667223	T	T	T
0.8069516664361540	0.5088426743680502	0.3480460991259832	T	T	T	0.8026606199910016	0.5089803522686460	0.3478609205594672	T	T	T
0.2322730242774319	0.0116212952511015	0.4408327787961778	T	T	T	0.2249179343279315	0.0133549328668400	0.4406691496637256	T	T	T
0.8172724907152545	0.0138260196430205	0.4464328617540411	T	T	T	0.8122089556584741	0.0134687282261099	0.4458959869292786	T	T	T
0.3177112514933222	0.5137919404180264	0.4471101548246746	T	T	T	0.3117510039451574	0.5142216097621687	0.4480769921332990	T	T	T
0.7301745567256503	0.5126450229814207	0.4417048305621602	T	T	T	0.7277452065495259	0.5129458501984385	0.4408545218104580	T	T	T
0.2767976411104360	0.0145681695164038	0.5413117230941999	T	T	T	0.2988243119940442	0.0095410684187925	0.5486957758283866	T	T	T
0.7655840480753288	0.0148091753641612	0.5422226171280926	T	T	T	0.75963300354435874	0.0140033907530486	0.5418550928592188	T	T	T
0.2658128584891261	0.5145033013623397	0.5402179741799013	T	T	T	0.2587540620355391	0.5140213237598635	0.5368611203220952	T	T	T
0.7801855506326054	0.5136589273768676	0.5434661577830628	T	T	T	0.7872500165821785	0.5136459687056883	0.5429197122020643	T	T	T
0.0038621034407529	0.2160950853167943	0.1430636730902695	T	T	T	0.9990179646493578	0.2154895990651839	0.1431862331757248	T	T	T
0.5049582145968782	0.2876861998570347	0.1479978877075195	T	T	T	0.5001620052891594	0.2856874491498415	0.1475681171024284	T	T	T
0.0047089243233611	0.7876660672191584	0.1480580901518269	T	T	T	0.9998878237076472	0.7858917381925942	0.1475457777736701	T	T	T
0.5041634781958598	0.7160232450240901	0.1430928219815236	T	T	T	0.4992264478396458	0.7157735703740661	0.1432440178714283	T	T	T
0.0085407028314878	0.2969673822458295	0.2477936435204761	T	T	T	0.0035503726690675	0.2954690639039163	0.2472737977952777	T	T	T
0.5075333851715214	0.2149569791430021	0.2438229081174320	T	T	T	0.5031243831055957	0.2147677596805840	0.24352812705002725	T	T	T
0.0078390413110445	0.7153257313613202	0.2436249685326728	T	T	T	0.0028713331808644	0.7146688653566354	0.2436853774606325	T	T	T
0.5082659533584025	0.7967992208965474	0.2479406146029191	T	T	T	0.5036143737051476	0.7957158284798760	0.2473640183082078	T	T	T
0.0125639775612608	0.2176041172537820	0.3432716946940646	T	T	T	0.0085149842805317	0.2172560591507891	0.3430480650824728	T	T	T
0.5129686761849588	0.30174700484878513	0.3477973124717026	T	T	T	0.507803889893663	0.3032190281108856	0.3472942706163062	T	T	T
0.0131458745452078	0.8014937863127196	0.3475915612775463	T	T	T	0.0084994910899119	0.8017932074648368	0.3469306038000112	T	T	T
0.5123038749940668	0.7182804254042130	0.3429238974481975	T	T	T	0.5074630970272855	0.7173445874418708	0.3430516887510243	T	T	T
0.0182289915272668	0.3117334645253895	0.4467112801231140	T	T	T	0.01469486266077623	0.3099521885198063	0.4461355455173954	T	T	T
0.5185797259345737	0.2252419143517844	0.4420009154745470	T	T	T	0.5132225961685455	0.2254061528232632	0.4418759669555268	T	T	T
0.0177866248212191	0.72451089469779965	0.4419456664211930	T	T	T	0.0136412216350020	0.7249807437375922	0.4422658038965988	T	T	T
0.5189690790515350	0.8093286721135020	0.44616308084071620	T	T	T	0.5140762091371927	0.8102767893800696	0.4453039064616995	T	T	T
0.0180272792683999	0.2592109703332698	0.5418038721566226	T	T	T	0.0150147810496477	0.2537862603034909	0.5376731195176233	T	T	T
0.5185331670199631	0.2708108507038910	0.5415096829842987	T	T	T	0.5213441265920692	0.2813062014615126	0.5419167399608710	T	T	T
0.0193932515939508	0.7788282260482132	0.5430948768786146	T	T	T	0.0174269629143781	0.7807709604719343	0.5406384813314643	T	T	T
0.5187910707011879	0.7588120136979126	0.5412276119261598	T	T	T	0.5177408304304990	0.7508259485312613	0.5405725481496299	T	T	T
0.2629846292601564	0.2829272933953744	0.5959765493033538	T	T	T	0.2861791448216874	0.2464244718541047	0.5941166514132707	T	T	T
0.1608525743719611	0.1486558885866181	0.6103907234115693	T	T	T	0.2953442508401143	0.1153462569566631	0.5896274699451458	T	T	T
0.0390738291454877	0.1831285755587868	0.6045679769077615	T	T	T	0.4100809766355008	0.2882309182171614	0.594298004249756	T	T	T

0% Strain State:

0.5056496740874555	0.0031543143696094	0.2957839101514209	T	T	T	0.5042643575251338	0.0050125386774709	0.2958335706128639	T	T	T
0.0059464112365117	0.5034056315964091	0.2958306940293653	T	T	T	0.0051132028753920	0.5048874108142206	0.2958155523684871	T	T	T
0.5066973314628109	0.5025090415845072	0.2959188328002547	T	T	T	0.5057732348496614	0.5042060766739986	0.2959078459046543	T	T	T
0.0143638012414399	0.0099076413335715	0.3937370243277092	T	T	T	0.0135023047833812	0.0121907692353677	0.3937854273937955	T	T	T
0.5156483498537366	0.0101911440372850	0.3938305086513359	T	T	T	0.5148419677576518	0.0123724870520435	0.3939611487577664	T	T	T
0.0133210663775954	0.51081944662139489	0.3939826128563764	T	T	T	0.0127896749597127	0.5129471800767806	0.3939566824674686	T	T	T
0.5138801632825245	0.5111495537124412	0.3940380410984244	T	T	T	0.5133014737242468	0.5129849441353582	0.3941323328954967	T	T	T
0.0199275369431011	0.0162876974463275	0.4962750324907406	T	T	T	0.0193093488506422	0.0180257493175219	0.4963655151405844	T	T	T
0.5188639654654009	0.0154246477137201	0.4964044988666036	T	T	T	0.5186404939650947	0.0172834768515341	0.4964912455024530	T	T	T
0.0181567679982283	0.5164682517264207	0.4965208942629815	T	T	T	0.0177143610502949	0.5192742713085875	0.4962686385942286	T	T	T
0.5177656829222935	0.5143804164194733	0.4965402731811585	T	T	T	0.5182139473131017	0.5173831264779963	0.4962771576539463	T	T	T
0.2477988346018414	0.2484857741964138	0.1472354664492766	T	T	T	0.2454355749478116	0.2494588682906937	0.1471969371241862	T	T	T
0.7495452083589869	0.2458855911992018	0.1472714417274813	T	T	T	0.7471670013735688	0.2470676266512517	0.1472337526068959	T	T	T
0.2496099187054148	0.7459341832568307	0.1472657827360123	T	T	T	0.2473305505225986	0.7469871290895853	0.1472561681114229	T	T	T
0.7479094443307467	0.7483553559457646	0.1472559212525641	T	T	T	0.7455969814365893	0.7495190487126691	0.1472351035386386	T	T	T
0.2537648165305456	0.25114460861092944	0.2458452273730780	T	T	T	0.2524454440356179	0.2528937170408985	0.2458612656936667	T	T	T
0.7538296608054894	0.2510805754199262	0.2457577527177767	T	T	T	0.7524875697992047	0.2525518547474115	0.2457462146422873	T	T	T
0.2539559966343844	0.7511139697715264	0.2457490212884223	T	T	T	0.2525890737832417	0.7525855817274421	0.2457744897497247	T	T	T
0.7536641683722531	0.7514858633132991	0.2456834891673906	T	T	T	0.7523873689120248	0.7528911900857783	0.2456897017643984	T	T	T
0.2617156131490050	0.2569076732834872	0.3437302300116568	T	T	T	0.2608717439752719	0.2587292112847443	0.3437941678616388	T	T	T
0.7614324300079500	0.2574555260115873	0.3436183073912066	T	T	T	0.7605388027526182	0.2592176408101607	0.3436530655540031	T	T	T
0.2611127035920127	0.7571234037340521	0.3435998738857608	T	T	T	0.2602705025195833	0.7588993898154209	0.3436488163552031	T	T	T
0.7610356277448309	0.7573309719375004	0.3434937701867590	T	T	T	0.7601608285056333	0.7591550571018364	0.3435112108710058	T	T	T
0.2669879363764944	0.2644616825744916	0.4420090524517956	T	T	T	0.2663167939801527	0.2666744136388037	0.442116136973040	T	T	T
0.7680241424946952	0.2635050009644017	0.4424784612833914	T	T	T	0.7676166040228476	0.2655603795915631	0.4425483317481781	T	T	T
0.2679164389125850	0.7632630715598774	0.4424548709471972	T	T	T	0.2672261947830100	0.7657635888782515	0.4424780827581653	T	T	T
0.7673010673708245	0.7639587716840847	0.4425901874018057	T	T	T	0.7669404032144608	0.7663262570347158	0.4425803761960037	T	T	T
0.2653381851664224	0.2645441628302450	0.5441630885293111	T	T	T	0.2657478238693072	0.2679453393588185	0.5438302640352721	T	T	T
0.7658451648386411	0.2654401833392372	0.5416865695875164	T	T	T	0.7657914898953119	0.2682585230920954	0.541642023263909	T	T	T
0.2658711888029055	0.765495940533680	0.5416748941331260	T	T	T	0.2656628438609874	0.7654524189928216	0.5418163884008526	T	T	T
0.7660092278782541	0.764176050559790	0.5410305639782302	T	T	T	0.7659058115195836	0.7657088195402594	0.5411099756695321	T	T	T
0.2693649927976825	0.2288793932664816	0.0955213458763485	T	T	T	0.2655487576612682	0.2288235599762472	0.095534949050816	T	T	T
0.7349424145877890	0.2724489386561055	0.0955827914045659	T	T	T	0.7325903024092308	0.2740848648058453	0.0955492556196027	T	T	T
0.2351725861768534	0.7721301590062427	0.0955837620758873	T	T	T	0.2327302808389238	0.7731569668795032	0.0955696279121453	T	T	T
0.7689745003700670	0.7283723448233744	0.0957258618101068	T	T	T	0.7657100448606483	0.7291228628546625	0.0957132790217909	T	T	T
0.2325679085296633	0.2708486141887466	0.1956048616051367	T	T	T	0.2317425683840676	0.2719920159906459	0.1955433118453106	T	T	T
0.7678193822009911	0.2251073410874490	0.1959247629132002	T	T	T	0.7656215851862586	0.2261362310553456	0.1958631198885909	T	T	T
0.2679320920575067	0.725704961199996	0.1959175590860313	T	T	T	0.2663328114145503	0.7268135616546361	0.1958819932156478	T	T	T
0.7324888590484357	0.7722436677772309	0.1959565998182551	T	T	T	0.7309974655403921	0.7735413378876493	0.1959384128237079	T	T	T
0.2757278781970201	0.2319585470196286	0.2951296039780284	T	T	T	0.2738619588998085	0.2341033380407801	0.2951808634287958	T	T	T
0.7385143244785350	0.2769808678359611	0.2946504274219497	T	T	T	0.7381235567871294	0.2788887553193005	0.2946481783968931	T	T	T
0.2392624307052822	0.7773453095212703	0.2946274260352165	T	T	T	0.2378130661626427	0.7790412043833602	0.294722282306612	T	T	T
0.7755798032974478	0.7308424285289977	0.2944815265032105	T	T	T	0.7748226830192536	0.7323186187251932	0.2944948400952221	T	T	T
0.2443664619411655	0.2821844826315358	0.3923056130162287	T	T	T	0.2442320103735965	0.2849456989063424	0.3925000476529585	T	T	T
0.7807583960577357	0.239171681838924	0.3911597693197740	T	T	T	0.7795111998361813	0.2409055959169717	0.3912031377239931	T	T	T
0.2782995872520977	0.77804556290101722	0.3911456690128743	T	T	T	0.2781684528755065	0.7392675338509217	0.3912012408898181	T	T	T
0.7474128444950080	0.7785872271694602	0.3909201329283861	T	T	T	0.7464862107809815	0.7809612782192819	0.3909508784575849	T	T	T
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0.5108295313402316	0.7262192606331370	0.3393066464923585	T	T	T	0.5086173663438680	0.7256422599202108	0.3401726526439195	T	T	T
0.0180029244367375	0.3073441137856140	0.4433613034299502	T	T	T	0.0163163250847745	0.3056067197335557	0.4432917564287005	T	T	T
0.5186898533276779	0.2333196712873070	0.4366947958943641	T	T	T	0.5152928874100420	0.2298544912641851	0.4373308786586080	T	T	T
0.0175306893855802	0.7317210065852818	0.4376746076023859	T	T	T	0.0150177960769779	0.7291083373877555	0.4387763530169953	T	T	T
0.5183195813684540	0.8073152933636575	0.4426725798581854	T	T	T	0.5155829785977315	0.8054595482472701	0.4416061242270181	T	T	T
0.0204885824090451	0.2625384153005155	0.5350853233389824	T	T	T	0.0180964239866689	0.2568399061002237	0.5344764880592467	T	T	T
0.5205637141832454	0.2698478367201605	0.5363789761890052	T	T	T	0.5154369190123845	0.2606012394838699	0.5374224718963904	T	T	T
0.0179072150849367	0.7722006918920873	0.5370177536854166	T	T	T	0.0180928571631319	0.7771178192571916	0.5358277269962667	T	T	T
0.5168807332968205	0.7598964775560135	0.5356169845053931	T	T	T	0.5150373252120455	0.7674489960539208	0.5359884603730813	T	T	T
0.2614046213576802	0.2719308497527588	0.5883920533374694	T	T	T	0.4024247322403940	0.0194039351938497	0.5609910933950606	T	T	T

O₂H adsorbed on the surface:

La Ni O H

1.0000000000000000

7.6462469100000003

0.0000000000000000

0.0000000000000000

0.0000000000000000

-0.1209078500000000

7.5973885000000001

0.0000000000000000

0.0000000000000000

0.0457189100000000

0.0378002900000000

39.8035000200000013

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Selective dynamics

Direct

0.0025902616567919

0.9867569376580221

0.1061697603070542

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0.4859829416230141

0.9999043589863987

0.1061742272221551

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0.9858529595540020

0.4996403361126482

0.1061716531799988

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0.5021553290749452

0.4866812512484202

0.1061443827276634

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0.0007983271637073

0.0002465753022136

0.1999562530855457

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0.5020918077255772

0.9992233202768119

0.1999316114876777

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0.0024802670798465

0.4987001349638547

0.1998928891977769

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0.5006319197906635

0.5001372513419682

0.1999549356403989

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0.0092412175700218

0.0046108832606677

0.2964787277008725

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0.5081978487320811

0.0052062344727659

0.2964634880258430

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0.0087937563698191

0.5053311707801882

0.2964300095340988

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0.5098578325337897

0.5042594168792007

0.2965350434043188

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0.0176914828675905

0.0112697503917474

0.3944847844681050

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0.5190545523233041

0.0114159363387145

0.3946220112857048

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0.0169426621893294

0.5119306776899748

0.3945602260725423

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0.5173376533616221

0.5123539608760410

0.3946263427735559

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0.0235899432718440

0.0173277084732746

0.4973301606126483

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0.5232092906638357

0.0162425950978005

0.4965471300463236

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0.0228199202778541

0.5158404495523143

0.4976195347853860

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0.5222444260257859

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0.4965595234673970

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0.2507575079072382

0.2509714818967979

0.1478723097502268

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0.7524023361830388

0.2484563250156953

0.1479172210584565

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0.2524778675129440

0.7484782380976469

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0.7508355921030656

0.7508200871811610

0.147916088065554

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0.2566469126003810

0.2535378490424236

0.2465034143348177

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0.7568247580761778

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0.2568627968063240

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0.7565810689232322

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0.7511011181136311

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0.7408163051305863	0.5147476816353773	0.4371812439460641	T	T	T	0.7349142017423523	0.5101390401013660	0.4362911210396113	T	T	T
0.2807941582058646	0.0160569896020775	0.5364856735856094	T	T	T	0.2813663244376862	0.0102489294053387	0.5347443408391516	T	T	T
0.7696808209427815	0.0161719270299727	0.53644961115706743	T	T	T	0.7590925868253007	0.0131952405203098	0.5336921179362646	T	T	T
0.2703911257438563	0.5167861951444266	0.5352556301922274	T	T	T	0.2566680381036966	0.5150551877772018	0.5355694021629737	T	T	T
0.7852797563826712	0.5155405774220441	0.5393382660150721	T	T	T	0.7897275919836861	0.5131113855350615	0.5400657197870312	T	T	T
0.0014919445897306	0.2249647097358505	0.1440466196270762	T	T	T	0.9981294750658303	0.2252064694456091	0.1438309806243157	T	T	T
0.5021360433414372	0.2741775789280325	0.1504722232334217	T	T	T	0.4988175206739034	0.2702281286445781	0.1495550449165720	T	T	T
0.0021053473811747	0.7742365047762121	0.1504994475746884	T	T	T	0.9987165529632772	0.7703068122149598	0.1495674118950679	T	T	T
0.5015771033493550	0.7247023924957219	0.1441214641844155	T	T	T	0.4983404800478314	0.7253278128794243	0.1438937074588722	T	T	T
0.0073000154579788	0.2868529365396881	0.2487679999908892	T	T	T	0.0038382988432059	0.2840639545875694	0.2479040555679134	T	T	T
0.5061499267910463	0.2232207804047306	0.2426524891727411	T	T	T	0.5030860297168013	0.2198647030035827	0.2421304306483979	T	T	T
0.0065300572906537	0.7236190623933538	0.2423971628277712	T	T	T	0.0032710519971011	0.7201329362220461	0.2421380650566456	T	T	T
0.5070343410577394	0.7869154646559195	0.2488406911872971	T	T	T	0.5036843844504673	0.7839782039374179	0.2480774197592364	T	T	T
0.0142266851248323	0.2267346543470978	0.3401712103156100	T	T	T	0.0100330441209555	0.2214250664710151	0.3400037360685298	T	T	T
0.5147771702289248	0.2951627783407389	0.3469862530410950	T	T	T	0.5098295533426536	0.2929158705661910	0.3461986568166933	T	T	T
0.0144814931099262	0.7952862998528474	0.3466135775378518	T	T	T	0.0100312420740663	0.7931223823995706	0.3460916411388812	T	T	T
0.5139062476893912	0.7272978705893394	0.3399964450961335	T	T	T	0.50924237551585858	0.7223849471947603	0.3398097394348121	T	T	T
0.0211922091981691	0.3095133695986263	0.4439258407836491	T	T	T	0.0160929378628737	0.3048861073343381	0.4445127195731817	T	T	T
0.5219449461150063	0.2342028261331492	0.4378119796177771	T	T	T	0.5156324511245649	0.2269627816098883	0.4371356278145327	T	T	T
0.0209095637580476	0.7336158753185842	0.4378978323803580	T	T	T	0.0149387669304221	0.7286619756636986	0.4377966384211632	T	T	T
0.5220478165763254	0.8064303091979141	0.4431539854842015	T	T	T	0.51581457774941924	0.8047303883569812	0.4425411951757331	T	T	T
0.0210504650819914	0.2610851898879858	0.5369568324073057	T	T	T	0.0161656358689236	0.2547392159534688	0.5322835666958201	T	T	T
0.5220536898044514	0.2722990067945403	0.5365819923112483	T	T	T	0.5217561392037112	0.2904175240418727	0.5434255603069604	T	T	T
0.0230932413921536	0.77533592178525039	0.5385674009696615	T	T	T	0.0177879177417064	0.7779608992235139	0.5370173408588458	T	T	T
0.5225309167280443	0.761103375733385	0.5358835877483727	T	T	T	0.517360711547589	0.7551944748681374	0.5360970953570769	T	T	T
0.2661909096871042	0.2808687432297035	0.5902719611683125	T	T	T	0.2897579079817580	0.2856162165095077	0.5889557521861841	T	T	T
0.1569411528988311	0.1527170240527553	0.6039650572704574	T	T	T	0.2517287651365764	0.4084176144238159	0.5899834198020820	T	T	T
0.0396032299205658	0.1897403974798024	0.5964803916730546	T	T	T	0.4183610336560351	0.2951033491716157	0.5833446946102721	T	T	T

+1% Strain State:

O ₂ adsorbed on the surface:				OH adsorbed on the surface:			
La Ni O				La Ni O H			
1.000000000000000				1.000000000000000			
7.7227090000000000 0.000000000000000 0.000000000000000				7.7227090000000000 0.000000000000000 0.000000000000000			
-0.1209078500000000 7.673362000000000 0.000000000000000				-0.1209078500000000 7.673362000000000 0.000000000000000			
0.0457189100000000 0.0378002900000000 39.3615520099999969				0.0457189100000000 0.0378002900000000 39.3615520099999969			
20	20	62		20	20	61	1
Selective dynamics				Selective dynamics			
Direct				Direct			
0.0108378244049988	0.9934771219335746	0.1075847876848926	T T T	0.0110056670432947	0.9942058632678850	0.1074954290813060	T T T
0.4843609267207943	0.0038097197546253	0.1075771388585344	T T T	0.4847683250033640	0.0046924813822796	0.1074887239201015	T T T
0.9845160280957351	0.5036738862909547	0.1076042670755566	T T T	0.9848081334705087	0.5046842535116022	0.1075267628894708	T T T
0.5103888092387078	0.4932350329274875	0.1076034043877350	T T T	0.5104742152173479	0.4938504179259779	0.1075381550100601	T T T
0.9939915509665898	0.9977161725736164	0.2006344455190217	T T T	0.9938799121387527	0.9981875104540945	0.2005710599823944	T T T
0.497343067030023	0.9967156717538950	0.2006472471358785	T T T	0.4970543554581114	0.9971225657793933	0.2005598669692347	T T T
0.9979315606545166	0.4960019798377082	0.2006248239192301	T T T	0.9974794135672570	0.4965182974867627	0.2005898232537858	T T T
0.4938314308617901	0.4977232941836903	0.2006500735881663	T T T	0.4935328831716473	0.4982268711366414	0.2006130153131251	T T T
0.0024098901546729	0.0011963134935206	0.2966457406865786	T T T	0.0021801833334974	0.0019662174985360	0.2966175278476197	T T T
0.5007799970395164	0.0009845386025759	0.2965119686410755	T T T	0.5005224176143466	0.0017978630522528	0.2965078657798604	T T T
0.0009311318033338	0.5010324898657564	0.2965772349071965	T T T	0.0004363918310863	0.5020289338975019	0.2965745115594201	T T T
0.5025973460350533	0.5009099274460023	0.2967710520391760	T T T	0.5020703898340506	0.5017375407464381	0.2968267080567348	T T T
0.0088203429735156	0.0067635699487407	0.3946288959606923	T T T	0.0082731420565090	0.0078975462173553	0.3944741799532575	T T T
0.5112854826836171	0.0071516781933507	0.3945663963953021	T T T	0.5107194215737481	0.0082704191391101	0.3945718847218200	T T T
0.0083064541460561	0.5082203874704173	0.3947636227792737	T T T	0.0071232822021496	0.5093376507076213	0.3947757197307729	T T T
0.5082287637455140	0.5083560309522814	0.3946047915410961	T T T	0.5072667815861470	0.5095573679638942	0.3948275828403035	T T T
0.0176250777165393	0.0121851409684744	0.4967423495326384	T T T	0.0156379948054128	0.0129639976936663	0.4965978942540949	T T T
0.5149058071508292	0.0124251908209601	0.4966771457761381	T T T	0.5142085471570715	0.0126868670342781	0.4970583790160946	T T T
0.0133776579124181	0.51425560201835816	0.4971295796858033	T T T	0.0109154729007029	0.5172938282730375	0.4965613195217317	T T T
0.5118454223476759	0.5113084084643938	0.4964358138723116	T T T	0.5125643883237110	0.5125585186382250	0.4966772566504395	T T T
0.2480617450664777	0.2510303041522374	0.1481159719564105	T T T	0.2481170349115168	0.2517237993095153	0.1480548228818462	T T T
0.7496564974867153	0.2477461229970931	0.1481480667446873	T T T	0.7497830679236673	0.2485080211914900	0.1480818776340196	T T T
0.2496427730992269	0.7477508051338082	0.1481454557862417	T T T	0.2496975889968440	0.7484871468263283	0.1480796163981685	T T T
0.7480856023847775	0.7509470338326334	0.1481396038355872	T T T	0.7481364795380826	0.751671176351982	0.1480736782881025	T T T
0.2510027772887035	0.25114453605826548	0.2465568192868601	T T T	0.2508258992321524	0.2519046288151963	0.2463830830606622	T T T
0.7505121960626876	0.2508389130478033	0.2464539860502181	T T T	0.7502416206568382	0.2515651624073345	0.2464307256506950	T T T
0.2506704486152352	0.7509442943175968	0.2464478322484667	T T T	0.2504718597165103	0.7516608451025444	0.2464369414233118	T T T
0.7511260198293721	0.7508633602797846	0.2463837211177081	T T T	0.7508311779497689	0.7512298508486101	0.2463682786387018	T T T
0.2570551360241031	0.2547308324261758	0.3442455195461257	T T T	0.2565602358439414	0.2557760982709141	0.3443116389992467	T T T
0.7573286361932624	0.254980965053734	0.3441188630774906	T T T	0.7566703157187418	0.2560021556056298	0.3441162169247169	T T T
0.2566636825604902	0.7548882715935031	0.3440343993424954	T T T	0.2560648091818754	0.7556980372268018	0.3440638389494949	T T T
0.7565742228372714	0.7557740890661907	0.3439508793410177	T T T	0.7558263872474212	0.7565498478815300	0.3439300855304622	T T T
0.2627236381774767	0.2612450193890957	0.4423202743867393	T T T	0.2618196985167880	0.2624633049927809	0.44225044973932070	T T T
0.7640090574380607	0.2609881089622971	0.4427796011798387	T T T	0.7629325708184871	0.2616976803576859	0.4427797040524536	T T T
0.2634275979075429	0.7604044674693257	0.4426321089616975	T T T	0.2624256854380956	0.7619930119655706	0.4427012143172754	T T T
0.7627392524098233	0.7603350153871828	0.4428356710051744	T T T	0.7614732632749873	0.7621297711111745	0.4428168769724763	T T T
0.2600098439606434	0.2626156185838612	0.5437276493050527	T T T	0.2561763647615720	0.2648839547448992	0.5433255115699862	T T T
0.7601467089335487	0.2656209125357964	0.5409146610601826	T T T	0.7587413112919975	0.2663242762720930	0.5411580468819172	T T T
0.2605545027189782	0.7633018163726073	0.5415269100033046	T T T	0.2580493178143690	0.7627275006056157	0.54016213062034512	T T T
0.7599329073686288	0.7594940061774162	0.54058170438					

0.2373667808523706	0.2862683909113107	0.3925165151759160	T	T	T	0.2357266418559382	0.2873737974343637	0.3927337414394624	T	T	T
0.7783870991738140	0.23202723371871817	0.3916734183639005	T	T	T	0.7784949995917184	0.2320401134476621	0.3916396743518059	T	T	T
0.2745226206697187	0.7290095159980069	0.3915268304751447	T	T	T	0.2735877822942948	0.7297599554978812	0.3915908752840948	T	T	T
0.7422487624407608	0.78262723151489650	0.3914624570193344	T	T	T	0.7407659691285609	0.7823795275654412	0.3914064781646067	T	T	T
0.2781945263840792	0.2405072071713697	0.4888379936487988	T	T	T	0.2783656659373725	0.2387475818676948	0.4891433658251335	T	T	T
0.7522299448381995	0.2809752182904707	0.4903841917132720	T	T	T	0.7519202170935934	0.2788068737357928	0.4902847614975859	T	T	T
0.2544524287247356	0.7733570253146121	0.4898499791418271	T	T	T	0.2527667201292804	0.7765010066266930	0.4899287036249430	T	T	T
0.7698732427728736	0.7398900511668476	0.4903723588630661	T	T	T	0.7687232306338663	0.7457294145819271	0.4902453636072928	T	T	T
0.2542822790467694	0.9994183832200922	0.1527996576312818	T	T	T	0.2541067057033225	0.0001702486785094	0.1526898082721452	T	T	T
0.7440905117673495	0.09993469978988102	0.1415275240506160	T	T	T	0.7444705731948470	0.0000387682051425	0.1415397893222273	T	T	T
0.2439189280783506	0.4993057563993329	0.1415964342868360	T	T	T	0.2442257973343389	0.4999625237730543	0.1415929917424953	T	T	T
0.7543738252687024	0.4994309581274907	0.1529298305566296	T	T	T	0.7543310191111374	0.5002082608103497	0.1528064441454395	T	T	T
0.2334172583521107	0.0011985935720869	0.2401055712587171	T	T	T	0.2326615509778918	0.0018624905045907	0.2401445814516971	T	T	T
0.7717275730718376	0.0009632333703721	0.2515637445007136	T	T	T	0.7723525149182227	0.0017900858480129	0.2514509744715114	T	T	T
0.2719464503183542	0.5010392600058255	0.2515181669083185	T	T	T	0.2725799189195314	0.5018163463754746	0.2514142960702876	T	T	T
0.7338419700527505	0.5007582035070620	0.2398192235687535	T	T	T	0.7330321826860483	0.5016531419346382	0.2399155517337339	T	T	T
0.2864609304134711	0.0055108879865210	0.3491302664781794	T	T	T	0.2860263386259660	0.0065163866624177	0.3490898008022827	T	T	T
0.7334291420994630	0.0048823576119632	0.3375097998022581	T	T	T	0.7327876225551149	0.0058137965709848	0.3376167250252585	T	T	T
0.2342703692002535	0.5049077162467742	0.3374799846581047	T	T	T	0.2333157424408837	0.5058015077119380	0.3375608619065888	T	T	T
0.7864139489850664	0.5054748794202250	0.3485486912243657	T	T	T	0.7861671479911423	0.5063388836343896	0.3484095601156451	T	T	T
0.2392424282923487	0.0095503362101221	0.4357092365618651	T	T	T	0.2385068293348653	0.0107384479620787	0.4355805844711643	T	T	T
0.8030930448075770	0.0114367069733333	0.4452197044249002	T	T	T	0.8028094721392673	0.0126225803827711	0.4447220552500463	T	T	T
0.3040095875631028	0.5113695038619539	0.4452070500466921	T	T	T	0.3029669042637865	0.5124446733927340	0.4455522201037354	T	T	T
0.7389454659447038	0.5105729220357585	0.4357900416310998	T	T	T	0.7370075415575217	0.5120085436632847	0.4363271318456286	T	T	T
0.2742180313511854	0.0123585158243603	0.5375592412261467	T	T	T	0.2721621362265327	0.0138873218651764	0.538364101668070	T	T	T
0.7620577188752798	0.0117288494021979	0.5347404183075299	T	T	T	0.7621665190988915	0.0130834186966043	0.5353492354561323	T	T	T
0.2608703009055729	0.5133594842193122	0.5348449468156594	T	T	T	0.2585726279682481	0.5147429152506583	0.5341978317845352	T	T	T
0.7853990355447362	0.5119527417357149	0.5426027396728468	T	T	T	0.7813920655360521	0.5134273171058344	0.5408132017940902	T	T	T
0.9989681389646988	0.2440204116617119	0.1449149611196136	T	T	T	0.9989891342838083	0.2450799466497597	0.1447321191513834	T	T	T
0.4989647146614418	0.2548867747517494	0.1503443719781477	T	T	T	0.4991279318634951	0.2554672179464461	0.1503418880809222	T	T	T
0.9989791037593532	0.7548444356693018	0.1503777512624113	T	T	T	0.9990967490082769	0.7554527887451823	0.1503440231553910	T	T	T
0.4989896211642754	0.7438065454913348	0.1449210288471963	T	T	T	0.4989077483935466	0.7449202808945955	0.1447926085222579	T	T	T
0.0012180556783959	0.2718956104027475	0.2491733089228355	T	T	T	0.0009582834560332	0.2733178500430296	0.2492601353957444	T	T	T
0.5004481530408881	0.2328910694224871	0.2420949611591840	T	T	T	0.5002111483460268	0.2329155527003228	0.2418968724025923	T	T	T
0.0007834304418665	0.7328845058267182	0.2418546171080229	T	T	T	0.0005492448585894	0.7329801300986164	0.2418521145482570	T	T	T
0.5011025779951022	0.7718122024622007	0.2491634178074377	T	T	T	0.5008559054790103	0.7733409058649076	0.2491736498918168	T	T	T
0.0064246855903109	0.2314338015900777	0.3391768666058141	T	T	T	0.0059094630045705	0.2320256356729404	0.3391199985699618	T	T	T
0.5072108490825903	0.2842317499018863	0.3473805286789495	T	T	T	0.5065130579164734	0.2856548866611345	0.3476204921726084	T	T	T
0.0067073155016402	0.7850788782241731	0.3466736648724962	T	T	T	0.0061024387054994	0.7858870508403226	0.3466927000155507	T	T	T
0.5063418425054481	0.7318806544656468	0.3392818191085361	T	T	T	0.5056807344046271	0.7326916804586650	0.3392690833076692	T	T	T
0.0133943687216331	0.3002319849563698	0.4442582582188360	T	T	T	0.0123569401351863	0.3017097376239943	0.4444497574745235	T	T	T
0.5141466235251104	0.2359836116902472	0.4367536387494565	T	T	T	0.5132992844887984	0.2374241426299719	0.4366268964496781	T	T	T
0.0126141357975910	0.7353028763240211	0.4375773696782501	T	T	T	0.0115822845495599	0.7360502418132167	0.4377268568650084	T	T	T
0.5137002292827867	0.7982842351984616	0.4429787874941641	T	T	T	0.5125504723800439	0.8000968248705711	0.4430345562999343	T	T	T
0.015081800683892	0.25806727979336624	0.5347615530481851	T	T	T	0.0134688495641793	0.2604187700796233	0.5340415738578027	T	T	T
0.5159609388164224	0.2698937525293609	0.5366511531948757	T	T	T	0.5165885857241669	0.2694358509908513	0.5363537226907036	T	T	T
0.0157061047808829	0.7197907416296591	0.5377537531334999	T	T	T	0.0137798608851330	0.7740035723198685	0.5379378674765208	T	T	T
0.5149554365848178	0.7556928743092555	0.5354608063350204	T	T	T	0.5130669790759839	0.7577195656665000	0.5356981883079700	T	T	T
0.2635655737411636	0.2804364368379076	0.5904661826834250	T	T	T	0.2506408332757102	0.2654327794341682	0.5885004268856490	T	T	T
0.1652128612709725	0.1818511733361466	0.6074697637547463	T	T	T	0.2517738342224198	0.1406976896860815	0.5939991035125651	T	T	T

O adsorbed on the surface:						H adsorbed on the surface (O):					
La Ni O						La Ni O H					
1.000000000000000						1.000000000000000					
7.722709000000000		0.000000000000000		0.000000000000000		7.722709000000000		0.000000000000000		0.000000000000000	
-0.120907850000000		7.673362000000000		0.000000000000000		-0.120907850000000		7.673362000000000		0.000000000000000	
0.045718910000000		0.037800290000000		39.361552009999969		0.045718910000000		0.037800290000000		39.361552009999969	
20		20		61		20		20		61	
Selective dynamics						Selective dynamics					
Direct						Direct					
0.0076397484463048		0.9903243910213667		0.1074153439944739		T	T	T	T	T	T
0.482235561375323		0.0012670053656433		0.1073945027244060		T	T	T	T	T	T
0.9823121053815141		0.5012943720571199		0.1074124903233230		T	T	T	T	T	T
0.5071956401159572		0.4899570640327280		0.1074535423063771		T	T	T	T	T	T
0.9930856202841408		0.9964980500028593		0.2005199988620796		T	T	T	T	T	T
0.4967640575735951		0.9952729658682827		0.2005384211595608		T	T	T	T	T	T
0.9968688436796126		0.4949150726079893		0.2005578084143645		T	T	T	T	T	T
0.4929364951425847		0.4966111110731386		0.2005764645287509		T	T	T	T	T	T
0.0023269161285247		0.00052264179055343		0.2966445993503661		T	T	T	T	T	T
0.5008890404000960		0.0001971057426334		0.2965452591461590		T	T	T	T	T	T
0.000376363657197		0.5007463699327246		0.2965797097137589		T	T	T	T	T	T
0.5025608189170306		0.5002306857531249		0.2967908801632995		T	T	T	T	T	T
0.0089561677473836		0.0063068173320238		0.3946686893206314		T	T	T	T	T	T
0.5114094257732448		0.0055328337509746		0.3946110159610252		T	T	T	T	T	T
0.0084630229815349		0.5073916540788920		0.3947526386104912		T	T	T	T	T	T
0.5086039738082454		0.5067563996195469		0.3946294070353148		T	T	T	T	T	T
0.0189388116902545		0.0113112039891022		0.4964486274011703		T	T	T	T	T	T
0.5129761110410521		0.012815612179154		0.4973331751921327		T	T	T	T	T	T
0.0128440419018225		0.5152828046775853		0.4961635734399252		T	T	T	T	T	T
0.5104105644209425		0.5085888995309865		0.496232827657959		T	T	T	T	T	T
0.2468420620340193		0.249128534024887		0.1480581812711625		T	T	T	T	T	T
0.7485005261804216		0.2463168354864969		0.1480555617328924		T	T	T	T	T	T
0.2483350989509997		0.7461179730124600		0.1480692635059841		T	T	T	T	T	T
0.7468135277213745		0.7492144180540232		0.1480091148442568		T	T	T	T	T	T
0.2502841758868324		0.2501624933854947		0.246533574203048		T	T	T	T	T	T
0.7498104947348926		0.2499067925728043		0.2464450664833713		T	T	T	T	T	T
0.2500174151769968		0.7506060846025264		0.2464546438734042		T	T	T	T	T	T
0.7504018496114265		0.74983237815410449		0.246370821984224		T	T	T	T	T	T
0.2569518147970413		0.2538969607481491		0.246420876588959584		T	T	T	T	T	T
0.7569851378252563		0.2540110862350546		0.3441992977835547		T	T	T	T	T	T
0.2565707355119519		0.7539915895672746		0.3441054778933206		T	T	T	T	T	T
0.7565561317530806		0.7554954383896938		0.344030663102823		T	T	T	T	T	T
0.2640514767995920		0.25846696300164330		0.4421756182218453		T	T	T	T	T	T
0.7646754903197148		0.2591058611700614		0.4427358996124221		T	T	T	T	T	T
0.2645650834931607		0.7582505099827223		0.4426625335428566		T	T	T	T	T	T
0.7620140037750820		0.7594760325766780		0.44282535084035728		T	T	T	T	T	T

0.2438059041187184	0.2742349631219391	0.5477214795942381	T	T	T	0.2607395813633602	0.2662729408104908	0.5419202968893535	T	T	T
0.7587928068536387	0.2696026180337062	0.5403692048573608	T	T	T	0.7632721264891793	0.2611096483533171	0.541539646860110	T	T	T
0.2581452487536616	0.7658320055723794	0.5413261302432407	T	T	T	0.2609883824131668	0.7539336646241332	0.5421881404777598	T	T	T
0.7585237919450792	0.7606414607466376	0.5401170537210701	T	T	T	0.7639897036102585	0.7589683635151887	0.5416365147803374	T	T	T
0.2630699919695393	0.2191965629466394	0.0971114157013018	T	T	T	0.2616959411892409	0.2188759697115847	0.0973725929603699	T	T	T
0.7351996907655757	0.2784481207684003	0.0972852873234353	T	T	T	0.7364164096998317	0.2803068565062570	0.0973057647056472	T	T	T
0.2347940772218139	0.7780841029343858	0.0972849663522056	T	T	T	0.2367395786017683	0.7803087417503459	0.0972707244209995	T	T	T
0.7625150620211253	0.7195798997192377	0.0973356161828979	T	T	T	0.7615027279500960	0.7188748820750837	0.0973739573427172	T	T	T
0.2309203209515002	0.2806653278180479	0.1968555778202320	T	T	T	0.2317541844402826	0.2831762730079390	0.1969848791346397	T	T	T
0.7668020061882534	0.2165737072435243	0.1968357894998946	T	T	T	0.7661655829282543	0.2159595426094483	0.1970084442235338	T	T	T
0.2665195696344322	0.7166774108179393	0.1968918695822584	T	T	T	0.2648612216447165	0.7160929006063264	0.1969798013747119	T	T	T
0.7307757627755619	0.7811677557200288	0.1968329339729460	T	T	T	0.7326328807072456	0.7832787379029167	0.1969949597589571	T	T	T
0.2735769617042710	0.2205430968702875	0.2954099423980703	T	T	T	0.2719600484391317	0.2196866616430366	0.2949109003502990	T	T	T
0.7323968263125005	0.2816508271000046	0.2946874088279029	T	T	T	0.7312484238968590	0.2839035310100235	0.2948081810998996	T	T	T
0.2337046510574484	0.7834235725121035	0.2947265179197857	T	T	T	0.2338609036651377	0.7843076775563579	0.2949074848317162	T	T	T
0.7718815857575074	0.7208878208929633	0.2946371504529095	T	T	T	0.7696019310343577	0.7192047135425497	0.2947685979900428	T	T	T
0.2376085170594706	0.2852585441584812	0.3922168130588242	T	T	T	0.2379473538004474	0.2846800337638290	0.391819885653558	T	T	T
0.7778023427179885	0.2300078250158921	0.3919317822271152	T	T	T	0.7744750808289163	0.2278366667322799	0.3915240231168250	T	T	T
0.2740317971740016	0.7280503499456197	0.3917354039256519	T	T	T	0.2701135158467413	0.725705998295958	0.3917819337130612	T	T	T
0.7435708211602127	0.7812813154014837	0.3916834280249032	T	T	T	0.7409751351594789	0.7826299397515201	0.3914783687550577	T	T	T
0.2779806441195247	0.2390186896591306	0.4881519348155944	T	T	T	0.271993343235252	0.2277950022857055	0.4904260634153251	T	T	T
0.7574379549465969	0.2834731381589758	0.4910475768539603	T	T	T	0.7510792492912925	0.2713620074909042	0.4897091917656894	T	T	T
0.2558227901373891	0.7687564749589815	0.4905207028053931	T	T	T	0.2548572635446485	0.7896814200111689	0.4903406847680101	T	T	T
0.7683648563218128	0.7373430911997470	0.490522827876329	T	T	T	0.7644687034016802	0.7465563505064093	0.4896840898970733	T	T	T
0.2565456786938594	0.9976492686369034	0.1526360590035290	T	T	T	0.2533087707178773	0.9988035648045582	0.1529575322661798	T	T	T
0.7391123492914069	0.997843948523932	0.1416111103629879	T	T	T	0.7437177730317088	0.9988912516103198	0.1415290434582727	T	T	T
0.2389852894136209	0.4977336815263071	0.1416683631305562	T	T	T	0.2437289200372047	0.4988806934888089	0.1415100765521789	T	T	T
0.7567180471051369	0.4976579078397242	0.1526732619606339	T	T	T	0.7534831422789041	0.4988072641041635	0.152958339008166	T	T	T
0.2307964917618536	0.0000349766269727	0.2401099645849250	T	T	T	0.2335472020842128	1.0001198308986519	0.2399064645030378	T	T	T
0.7730532932122959	0.0000526653323025	0.2513534051665278	T	T	T	0.7695812968891534	0.0003991401949401	0.2517029214685076	T	T	T
0.2732335063686587	0.5001347405893175	0.2514577715029002	T	T	T	0.2698484844875860	0.5004765125604104	0.2516977246197343	T	T	T
0.7310143657653972	0.4996646961971001	0.2400296042142470	T	T	T	0.7336822237110754	0.4999593349413469	0.2397527484147164	T	T	T
0.2867280725720437	0.0044982584951871	0.3491576577847340	T	T	T	0.2828823447368150	0.0046469882473175	0.3490104613614622	T	T	T
0.7325568103740233	0.0040188281586639	0.3377713926954735	T	T	T	0.7315269873978580	0.0039877042458904	0.3374081232483393	T	T	T
0.2337210033040472	0.5041832936882583	0.3374460917482592	T	T	T	0.2314073445542383	0.5039513100240561	0.3372743727254601	T	T	T
0.7868306475790710	0.5046135346544031	0.3484908654704125	T	T	T	0.7847473034694741	0.5044978497456970	0.3488724101985858	T	T	T
0.2388081975119916	0.0080194419122285	0.4358129597090707	T	T	T	0.2353247892445200	0.0088307480393550	0.4351395814838769	T	T	T
0.8039127235540415	0.0103439305788526	0.4453304580614508	T	T	T	0.8000672655975092	0.0096033378718738	0.4454140296881084	T	T	T
0.3045850835836805	0.5094755411303733	0.4452016250615354	T	T	T	0.3017237408491714	0.5094463240859527	0.4466772358861716	T	T	T
0.7385469137684328	0.5094159691498616	0.4359622287614903	T	T	T	0.7350822804366743	0.5087260506630147	0.4363312978088308	T	T	T

0.7502892212383263	0.2489913133954144	0.1490601051657871	T	T	T	0.7477205991767674	0.2465663866220231	0.1481055632784042	T	T	T
0.2506712007006953	0.7491126579616992	0.1491039804263634	T	T	T	0.2477791198950454	0.7466118654035474	0.1481040875229775	T	T	T
0.7495099768382689	0.7527545581211950	0.1491318132514826	T	T	T	0.7463463698941530	0.7499652795022397	0.1481246765788868	T	T	T
0.2519028123243204	0.2514726396566553	0.2475042065397469	T	T	T	0.2490734960910611	0.2484593925836861	0.2465941251888887	T	T	T
0.7529467434420734	0.2512127472711453	0.2474297142162545	T	T	T	0.7483277015383935	0.2486320676530353	0.2465425753996341	T	T	T
0.2521148211877967	0.7516815964661383	0.2474341450954385	T	T	T	0.2484216498184393	0.7485409382563163	0.2465115539341022	T	T	T
0.7527509727700327	0.7520102312737228	0.2473947868880040	T	T	T	0.7488208867636783	0.7486622369515420	0.2465056275666550	T	T	T
0.2593553795584291	0.2523486982313301	0.3453585009850692	T	T	T	0.2542494437952844	0.2516952072589409	0.3446126301066872	T	T	T
0.7568948724530221	0.2533037780724084	0.3451574075722053	T	T	T	0.7548845143196089	0.2518009777907347	0.3443813525188729	T	T	T
0.2581871523560457	0.7536309672275118	0.3449696036482752	T	T	T	0.2541893210572631	0.7509413301199446	0.3443425610803570	T	T	T
0.7578941293721264	0.7546387251163083	0.3448753205637151	T	T	T	0.7539115885101729	0.7519713541484360	0.3441354872078268	T	T	T
0.2615455486713578	0.2564447659279784	0.4438714732917572	T	T	T	0.2596029007085803	0.2583506813178123	0.4429272137747528	T	T	T
0.7672532317815058	0.2554807376183803	0.4438613706157501	T	T	T	0.7599231962104486	0.2568058180896424	0.4428769473581001	T	T	T
0.2636477445852449	0.7536512388364244	0.4431679607163526	T	T	T	0.2619034766794538	0.7568507357719596	0.4426708057788113	T	T	T
0.7660206772612648	0.7534494780998592	0.4432412957879732	T	T	T	0.7595634899372423	0.7563112207459890	0.4426270318759959	T	T	T
0.2826046433890502	0.2540135343203641	0.5427029419335722	T	T	T	0.2587594701022065	0.25259509793450907	0.5392474847821610	T	T	T
0.7553510881161299	0.2562608606268185	0.5415276365676346	T	T	T	0.7624503103394685	0.2601387121519996	0.5399622071399894	T	T	T
0.2717986322030089	0.7533126790582212	0.5423241389019723	T	T	T	0.2583132921885838	0.7649884575253417	0.5399460037173887	T	T	T
0.7631039570953823	0.7512590094414670	0.5417385841403277	T	T	T	0.7616431851178228	0.7559477426573957	0.5406754103995012	T	T	T
0.2569200602834441	0.2174357450033443	0.0980431255588105	T	T	T	0.2594100957195325	0.2176305765117192	0.0972130305117252	T	T	T
0.7437860949327814	0.2847584661701589	0.0981599468686779	T	T	T	0.7358347456193751	0.2800531230051631	0.097253780358789	T	T	T
0.2406852121177282	0.7839704214475696	0.0982453404742856	T	T	T	0.2357696588351451	0.7798896102217133	0.0972581721870843	T	T	T
0.7604131423276951	0.7180421254691003	0.0983124732647424	T	T	T	0.7597038394571609	0.7178941648742634	0.0972929823489732	T	T	T
0.2442151764766454	0.2860216460480967	0.1975662395211410	T	T	T	0.2319162316775971	0.2815117686172660	0.1966111427907333	T	T	T
0.7575509114052806	0.2150563377501923	0.1978844456800180	T	T	T	0.7634686459680409	0.2149723137967430	0.196905742273867	T	T	T
0.2653581599231180	0.7157807704095511	0.1979157518280942	T	T	T	0.2639306946947496	0.7153908479844975	0.1969087227491789	T	T	T
0.7361713749624290	0.78881162272095418	0.1979718762021797	T	T	T	0.7314223475534304	0.7823096604348868	0.1969669036662077	T	T	T
0.2573463022411508	0.2199437009055563	0.2963427336213605	T	T	T	0.2687636863152096	0.2205916197844225	0.2950499858679926	T	T	T
0.7526067659459657	0.2876586354069566	0.2958857853659263	T	T	T	0.7324801599568802	0.2811948464359910	0.2949534547880449	T	T	T
0.2380103947932922	0.78714439323112	0.295888574409753	T	T	T	0.2325955255573748	0.7807625124886612	0.2949133537998134	T	T	T
0.7716628870452991	0.7171741029902404	0.2956881966510480	T	T	T	0.7695329145989318	0.7176713912558960	0.2948565145303690	T	T	T
0.2681022212327497	0.2841801725480353	0.3942559107492172	T	T	T	0.2371890953209576	0.2812371402176306	0.3935600488220641	T	T	T
0.7543192894043307	0.2245207352453493	0.3928724612835210	T	T	T	0.7752496789311619	0.2267627185423733	0.3921297939632660	T	T	T
0.2732377853748105	0.7237109681176587	0.3924775148702947	T	T	T	0.2711688301690445	0.7246101227829058	0.3920526142428769	T	T	T
0.7465593103641496	0.7839158379615987	0.3923530764819597	T	T	T	0.7398328037598459	0.7795046945219472	0.3917350416576720	T	T	T
0.2359833818364028	0.2378196881834375	0.4914969849055468	T	T	T	0.2852745040834716	0.2253586642314331	0.4918131161524500	T	T	T
0.7866320161826618	0.2741390805305352	0.4910754867645451	T	T	T	0.7399209009367694	0.2755784459289115	0.4907515509232945	T	T	T
0.2593231725901016	0.7665694578261613	0.4902618828757876	T	T	T	0.2550832512175968	0.778224022095733	0.4902806718523376	T	T	T
0.7717244799909046	0.73356417854344836	0.4906678945299118	T	T	T	0.7665013440593385	0.7388410174424516	0.49023101360847319	T	T	T
0.2552982123723005	0.700563060876593	0.1541207531763425	T	T	T	0.2513844087161174	0.9982283003367697	0.1529031506933140	T	T	T
0.7453227209970257	0.0008844104221590	0.1419348106055849	T	T	T	0.7434560565121595	0.9984460932553234	0.1414305747116119	T	T	T
0.2457282327730722	0.5007905877596678	0.1420307639509569	T	T	T	0.2434835327533552	0.4984846917840174	0.1414129223405797	T	T	T
0.7550293871392123	0.5008895002884780	0.1541872920559319	T	T	T	0.7514696183138680	0.4982496936371150	0.1529232770345158	T	T	T
0.2340043618235181	0.00117632283147756	0.2406977588623463	T	T	T	0.2299341028800201	0.9985971886392343	0.2401173503529035	T	T	T
0.7756171336961426	0.0017161499572151	0.2530394783097789	T	T	T	0.7710831297511196	0.9989669156835733	0.2517234544509307	T	T	T
0.2746611495071589	0.5015828691715319	0.2528098751884772	T	T	T	0.2713655550874243	0.4987706300954968	0.2515276254043552	T	T	T
0.7340166897230587	0.5014645689525739	0.2405285640495292	T	T	T	0.7299259705535689	0.4983814575831815	0.2399505753604661	T	T	T
0.2906294692486658	0.0038756675572895	0.3502879078583607	T	T	T	0.2848334409146679	0.0021253720830455	0.3490634811402057	T	T	T
0.7332036943176788	0.00306201229715590	0.3378743462115792	T	T	T	0.7294242595440263	0.0015493559899374	0.3377718705938260	T	T	T
0.2324933639253520	0.5036027209327734	0.3387897921258155	T	T	T	0.2293639967982184	0.5010144365171917	0.3380847164465399	T	T	T
0.7879546735058738	0.5040766283036500	0.3501671941425511	T	T	T	0.7855087163302640	0.5019600755443061	0.3489898341057447	T	T	T
0.2394302223039961	0.0035977694296134	0.4370644781207362	T	T	T	0.2333717206635063	0.0064079523430384	0.3460666180096576	T	T	T
0.8037371604711043	0.0045679399190757	0.4465147059819649	T	T	T	0.7999156880084816	0.0071910943584895	0.4453633832699317	T	T	T
0.3042503675597892	0.5045119388437708	0.4464987717420262	T	T	T	0.3011098474539438	0.5070938044310931	0.4468025040269337	T	T	T
0.7372654993173904	0.5044196059285049	0.4369605696910410	T	T	T	0.7356550491625875	0.5065207923657820	0.4361743911559514	T	T	T
0.2734651850121617	0.0023601854389242	0.5372200027760494	T	T	T	0.2971995250271980	0.0056570455779131	0.5420352809792791	T	T	T
0.7638843563303924	0.0048576425372096	0.5351592049249766	T	T	T	0.7594923325196837	0.0090482448290526	0.5343421622569020	T	T	T
0.2700008780252979	0.5048959100693893	0.5347514531235699	T	T	T	0.2545510360592164	0.5095112569878283	0.5338212095740499	T	T	T
0.7844720463559882	0.5028591897727223	0.5423968920270241	T	T	T	0.7926432548627702	0.5089436416829056	0.5422072729075001	T	T	T
0.9999316803994722	0.2459019826736616	0.1474101327731566	T	T	T	0.9970717751868259	0.2442897445781011	0.1450829893306144	T	T	T
0.5001745534664692	0.2565120793075534	0.1499143178781529	T	T	T	0.4970184839235274	0.2528470579291917	0.1500920115348042	T	T	T
0.0001294185648403	0.7560297865948047	0.1508815870611788	T	T	T	0.9970243834527046	0.7528740908016588	0.1501902716290684	T	T	T
0.5001051351105144	0.7451854167993552	0.1464645201730395	T	T	T	0.4972360420293033	0.7442327686807809	0.1450915292243357	T	T	T
0.0027599703250323	0.2736237567960185	0.2475562599526816	T	T	T	0.9989883262932042	0.2709382799610546	0.2488681529544081	T	T	T
0.5021151770926519	0.2309573370001095	0.2457298539503626	T	T	T	0.4982749933087217	0.2286217633270058	0.2424355770984288	T	T	T
0.0023471195742649	0.7308820360942020	0.2435671900829905	T	T	T	0.9984560253496497	0.7290002437374776	0.2423188947067473	T	T	T
0.5025775355620169	0.7743366777768997	0.2495946225618441	T	T	T	0.4988466201221169	0.7711671286919145	0.2490039121532665	T	T	T
0.0083908876023656	0.2252595097365364	0.3449671057124383	T	T	T	0.0043982663514152	0.225298773824501	0.340004738683160	T	T	T
0.5081896236482308	0.2843163348167634	0.3442306926279088	T	T	T	0.50429797969594628	0.2823393756475567	0.3473686445048423	T	T	T
0.0081777045761543	0.7849651237863383	0.3471366737772546	T	T	T	0.0042374044438106	0.7820081840480327	0.3467772465022892	T	T	T
0.5077886527911682	0.7265138501522733	0.3409364154311130	T	T	T	0.5037443115311191	0.7264409147370853	0.3398117252446316	T	T	T
0.0136155374488725	0.2858539740960204	0.4385610689517045	T</								

Selective dynamics				Selective dynamics			
Direct				Direct			
0.0162820192749689	0.9941256938991999	0.1090678285303225	T T T	0.0168675902845785	0.9996678983969008	0.1091566350624339	T T T
0.4830099069562537	0.0014025479746866	0.1090676105473979	T T T	0.4836537521199680	0.0070293811488683	0.1091084024532252	T T T
0.9832754954815437	0.5012014887775005	0.1090947384928667	T T T	0.9837544826833253	0.5069416156088881	0.109148984673183	T T T
0.5162455896719619	0.4941292032622834	0.1090904602644821	T T T	0.5166748636600423	0.4995798954640642	0.1091816302808483	T T T
0.9944523688842120	0.996933988061882	0.2014537676297836	T T T	0.9953018235838695	0.0024532167662513	0.2015286084226407	T T T
0.5017720310308749	0.9959095247248063	0.2013993502687936	T T T	0.5026577426198634	0.0015514328092720	0.2014649426952873	T T T
0.0020378466027743	0.4955477692190721	0.2014058883674912	T T T	0.0031112741098086	0.5012100203205339	0.2014538222228612	T T T
0.4943553561779648	0.4967702151968184	0.2014598378734699	T T T	0.4952160421394081	0.5022421753106545	0.2015452348522849	T T T
0.0027283322603494	0.9978616685729834	0.2964449726293978	T T T	0.0026825822529972	0.0024366628798665	0.2964246479129892	T T T
0.4995403396433429	0.9965437220355687	0.2962082950060745	T T T	0.4993771044654515	0.0010793790822470	0.2962219626543212	T T T
0.9989513151743065	0.4971474124082371	0.29626447040083897	T T T	0.9988795412281783	0.5015695347573768	0.2963043773594514	T T T
0.5031281904576893	0.4973365432683488	0.2964906426823984	T T T	0.5028651112012972	0.5019884911103664	0.2965359463103167	T T T
0.0064417214374050	0.0022677250775775	0.3935475348314037	T T T	0.0056488417659809	0.0054667406810890	0.3933733825871208	T T T
0.5106859966337897	0.0034248522647534	0.3935284220394374	T T T	0.5098636426631077	0.0066478054398515	0.3934712714198174	T T T
0.0082055095653003	0.5041574650795093	0.3935689420418739	T T T	0.0074337945929548	0.5069596782052981	0.3934619309964461	T T T
0.5060299407350003	0.5038301882634022	0.393345904510981	T T T	0.5049510824536294	0.5069615449400744	0.3933795076264565	T T T
0.0186792348472024	0.0070579256558086	0.4947086849838413	T T T	0.0175631857302698	0.0079705782238660	0.4937789202251743	T T T
0.5138779935853709	0.0094123071762383	0.4945140831535669	T T T	0.5133216786833332	0.0094027472096950	0.4947498670964141	T T T
0.0133405124065040	0.511210010964571	0.4944469415222372	T T T	0.0110299172103936	0.5146260041967862	0.4935271347838881	T T T
0.5118121909760831	0.5084101065388505	0.4935740627001492	T T T	0.5100794906795719	0.5090107048379462	0.4937469630415953	T T T
0.2494687102810288	0.2494577480252160	0.1489764070960851	T T T	0.2500555501249943	0.2549982559643910	0.1490557690671636	T T T
0.7505226983366522	0.2457699619627822	0.1489802872432462	T T T	0.7510770195428091	0.2512958004080645	0.1490563653849960	T T T
0.2505373480439174	0.7457366862759612	0.1490049038410128	T T T	0.2510925709613254	0.7512811265544669	0.1490727079896020	T T T
0.7495397367490165	0.7495099871574947	0.1489841815611514	T T T	0.7500898689837540	0.7551060897654563	0.1490303175788516	T T T
0.2518104819807353	0.248448980409476	0.2465811323515886	T T T	0.2520562419664924	0.2534325830247515	0.2466192536770263	T T T
0.7509258277779620	0.2482583104695330	0.2464444893593676	T T T	0.7512641482008365	0.253330754136102	0.2464781608044852	T T T
0.2509977618757152	0.7483426358814022	0.24645113747603046	T T T	0.2513787423347706	0.7533540748977196	0.2464764699727209	T T T
0.7518730423534946	0.7481102711546123	0.2463899814458442	T T T	0.7521437330347497	0.7529943752053047	0.2463934898246977	T T T
0.2564316126757961	0.250850895229385	0.3433388596503411	T T T	0.2560358248292202	0.2546701925220005	0.3433621998409426	T T T
0.756272261985639	0.2509770319597276	0.3432491025908255	T T T	0.7561304940921744	0.2549524205417597	0.3432113798757220	T T T
0.2562231708198909	0.7507987673869568	0.3430918149174086	T T T	0.2556589200244319	0.7546880794892415	0.3430886204461679	T T T
0.7559097521631826	0.7521574322303723	0.3430871781366200	T T T	0.7554312535933102	0.7560156541738510	0.3430186826079968	T T T
0.2618345419611231	0.2567329258437036	0.4404507155922832	T T T	0.2613865715899956	0.2592074760261665	0.4405365557123738	T T T
0.7634300972923739	0.2568865199797606	0.4407316637179121	T T T	0.7624311312976572	0.2588530667173364	0.4405732433467741	T T T
0.2625959108333799	0.7567092050395093	0.4404983402876533	T T T	0.2619680075846823	0.7594520668062680	0.4403911447494352	T T T
0.7617412971798408	0.7567039479500922	0.4407162823835890	T T T	0.7602040356230139	0.7589704473738796	0.4404952286119697	T T T
0.2585153876249462	0.2633365469185120	0.5399666014173258	T T T	0.2509803862493766	0.2625345405176022	0.5395690416331080	T T T
0.7597217914187722	0.2664625142268311	0.5374856294949851	T T T	0.7589130372517235	0.2679514913247416	0.537105347753627	T T T
0.2594334251998067	0.7606452208754367	0.5382796408667655	T T T	0.2555875354966449	0.7599514990291351	0.5380801365839680	T T T
0.7588247493011467	0.7551375996046545	0.5371775798708909	T T T	0.7575679176882242	0.7550554183875460	0.536999885160974	T T T
0.2587064994244180	0.2094628619994098	0.0986653406697476	T T T	0.2600222078682962	0.2156467062760712	0.09879222591106947	T T T
0.7413334742189479	0.2852848501921524	0.0988904525684856	T T T	0.7418331995909506	0.2910784469516067	0.0989923596541292	T T T
0.2412432383706618	0.7849714410948777	0.0989206167693457	T T T	0.2418813940721568	0.7907140866186183	0.0990242203141329	T T T
0.7591709242529922	0.7016157057451167	0.0988687445865937	T T T	0.7602526709640280	0.7161915763468071	0.0989631899160818	T T T
0.2378716377781833	0.2889059076452699	0.1974625248252423	T T T	0.2384506810769214	0.2942015381539093	0.1973505003187919	T T T
0.7631787254190417	0.2062094859291908	0.1974341749535564	T T T	0.7633797753870639	0.2108718166325888	0.1974887051250705	T T T
0.2633444233575089	0.7062083480127547	0.1974866710247146	T T T	0.2634468535778219	0.7109411392908092	0.1975326599490882	T T T
0.7376948843911360	0.7897770655578691	0.1974199551178014	T T T	0.7381349689955805	0.7953955864495398	0.1974411900986871	T T T
0.2717669892175263	0.2102773131572687	0.2948665079139901	T T T	0.2709169796274332	0.2144725080954211	0.2948741844337376	T T T
0.7364499587757340	0.2880172306866397	0.2942928561301679	T T T	0.7371870541491276	0.2935300774468247	0.2942855141319424	T T T
0.2367744240484737	0.7894534224509734	0.2942882588362629	T T T	0.2377318121187057	0.7945402387448153	0.2942944701229923	T T T
0.7704058321786660	0.710808436337325	0.2941950217355300	T T T	0.7696595903726723	0.7143125387356655	0.2941578077438592	T T T
0.2394993003337038	0.2902444645450375	0.3911152961839295	T T T	0.2395274340097102	0.2935695008711523	0.3912173692512844	T T T
0.7765558135215722	0.219316924448718	0.3906105533725560	T T T	0.7757104010858155	0.2222938322854469	0.3905661099728850	T T T
0.2731818094550603	0.7180844863012523	0.3902678841685895	T T T	0.2713038981942305	0.7205732356812787	0.3902845664231750	T T T
0.7425777771052587	0.7864233383656256	0.3904230615210457	T T T	0.7427742811594331	0.7905459648531886	0.3902987948063179	T T T
0.2765315814364402	0.2288541223949175	0.4870035839033618	T T T	0.2782216169114495	0.2291488059217010	0.4872253941226065	T T T
0.7520601689944010	0.2879460218049612	0.4882086861916806	T T T	0.7540277814853151	0.2911888724063587	0.4881301993341651	T T T
0.2533524987797708	0.7754834325850007	0.4876470293470544	T T T	0.2540666053978247	0.7797907049231593	0.487635578485143	T T T
0.7717011189373074	0.7271184176166521	0.4881281497376915	T T T	0.7685678420066612	0.7287333962200299	0.4879161590859429	T T T
0.2523411597671039	0.9974718852654891	0.1547390921207735	T T T	0.2525188267676524	0.0030971392720983	0.1548413396139838	T T T
0.7482404817792635	0.9976966283402429	0.141176370712404	T T T	0.7488485598809960	0.0032952767157235	0.1411748286262629	T T T
0.2482783726557494	0.4975273211223183	0.1412198112380546	T T T	0.2488267688756625	0.5030864084062101	0.1412736365341160	T T T
0.7523214626908991	0.497531864627928	0.1547589886408637	T T T	0.7525455534123694	0.5031635306729301	0.1548552499719999	T T T
0.2417387856888169	0.9983685529740673	0.2391594698920421	T T T	0.2435406358173733	0.0035423745824263	0.2391260115312685	T T T
0.7633281707260964	0.9982348011935932	0.2526718723644362	T T T	0.7616134035280501	0.0031727943357682	0.2528154139518812	T T T
0.2633635861240666	0.4982417254920070	0.2527335922049314	T T T	0.2617207096855960	0.5032493826298231	0.2528489781832581	T T T
0.7418541732034497	0.4980791241223251	0.2390223299920402	T T T	0.7439343059755013	0.5031536926229203	0.2388950581855646	T T T
0.2795007320633990	0.0016686874651956	0.3493960774528039	T T T	0.2775162531516533	0.0055045639268667	0.3495057256609165	T T T
0.7375279124867647	0.0011642240248471	0.3358670674359351	T T T	0.7382181992153320	0.0052103781903807	0.3357501675010731	T T T
0.2383932686784852	0.5011163069367157	0.3356495055444940	T T T	0.2388167498584268	0.5050853783358454	0.3357228877873423	T T T
0.7792512263430148	0.5016398341610822	0.3488603687175507	T T T	0.7776114349383287	0.5054486783147450	0.3489771342928535	T T T
0.2424840341994778	0.0059463567257531	0.4331039238663060	T T T	0.2415608103119483	0.0080825005394453	0.4330313915991287	T T T
0.7966407640695848	0.0074736405505848	0.4448626490665851	T T T	0.7946955700672077	0.0098447322035613	0.4448137486015412	T T T
0.2964201180655548	0.5066532292860716	0.4446209714757717	T T T	0.2942612148372480	0.5087785747632144	0.4449239168890573	T T T
0.7415761499753994	0.5069666283402429	0.4331782521023217	T T T	0.7413819845304837	0.5092164508545350	0.4330504118675961	T T T
0.2754077999348510	0.0066170970672111	0.5358599515882186	T T T	0.2755363504177155	0.0095750243950142	0.5371193271512460	T T T
0.7624440981168601	0.0077693239432016	0.5312403981050617	T T T	0.7629054058115082	0		

0.5122065455552182	0.7887844552736412	0.4411925065820802	T	T	T	0.5108823684659027	0.7902462410547145	0.4406773452849522	T	T	T
0.0148234945555485	0.2555150866039930	0.5316491696629703	T	T	T	0.0139052815393759	0.2563647746238515	0.5302430761195537	T	T	T
0.5173739580113365	0.2671834175297596	0.5335865756046203	T	T	T	0.5215759154020400	0.2670661180729211	0.5332149204175433	T	T	T
0.0169792257437793	0.7656704921793429	0.5350381851156126	T	T	T	0.0148347221148918	0.7690271511325718	0.5340903980377261	T	T	T
0.5164537252547174	0.7519109637810981	0.5321876403714841	T	T	T	0.5147989246788562	0.7528854284649932	0.5323092316851055	T	T	T
0.2625346993660138	0.2613084962477152	0.5868765511812613	T	T	T	0.2466649081102333	0.2671877699744858	0.5847560357937447	T	T	T
0.1618884851237687	0.3568588037362633	0.6028425594303991	T	T	T	0.2502945801033918	0.1440041379176504	0.59054613977084624	T	T	T

O adsorbed on the surface:					H adsorbed on the surface (O):				
La Ni O					La Ni O H				
1.000000000000000					1.000000000000000				
7.7991720000000004					7.7991720000000004				
-0.1209078500000000					-0.1209078500000000				
0.0457189100000000					0.0457189100000000				
20	20	61			20	20	60	1	
Selective dynamics					Selective dynamics				
Direct					Direct				
0.0185852709951022	0.9973572248549786	0.1088463068250574	T	T	0.0169880843466174	0.9952389888265977	0.1091420535188399	T	T
0.4846226141974264	0.0027317276431253	0.1087162364383124	T	T	0.4836386556283738	0.0016885196706743	0.1091516075565219	T	T
0.9862904763193358	0.5027747265261117	0.1087061903263560	T	T	0.9834596183688638	0.5018373506073471	0.1091711478759801	T	T
0.5201112428915516	0.4973272952916594	0.1085464096300391	T	T	0.5167841788042371	0.4951367572201594	0.1092120281383524	T	T
0.9944334904063896	0.0008016516187416	0.2012301138704374	T	T	0.9950507063226542	0.9984774954958784	0.2015020498565026	T	T
0.5032813142420496	0.9999161616387300	0.2013427648025905	T	T	0.5026818284846537	0.9972734973972711	0.2014235463178531	T	T
0.0071683999497685	0.4988200250278882	0.2007541462526631	T	T	0.0021693249048242	0.4974124557724738	0.2015369676879082	T	T
0.4994604729029057	0.5003764236395249	0.2009051540999450	T	T	0.4941327116004299	0.4984271127803401	0.2015708388842174	T	T
0.0004062376055137	0.0012984188568792	0.2968105233396383	T	T	0.0033052966506480	0.9990318023543739	0.2963412823299132	T	T
0.4965323444817574	0.0008627256645998	0.2961717024284642	T	T	0.4985635435037565	0.9981971776059877	0.2960297009969367	T	T
0.0046905315340099	0.5011818956862703	0.2953456696906217	T	T	0.9970600677232122	0.4985647879817340	0.2962861427852341	T	T
0.5107726594131291	0.4997764140845005	0.2952992351789036	T	T	0.5012412733353079	0.4993109677737607	0.2967703554775045	T	T
0.0006239221683475	0.0019781668966992	0.3938430003516266	T	T	0.0047992644811846	0.0021202778813788	0.3929487115046210	T	T
0.5040765471106061	0.0030185465751129	0.3947325938083830	T	T	0.5087979275216986	0.0033140609435437	0.3927560090870420	T	T
0.0173942300753341	0.5017960059853890	0.3913713274425280	T	T	0.0067820983563797	0.5033776351880571	0.3938215479902976	T	T
0.5113800707135421	0.5037234521902673	0.3914429745470742	T	T	0.5019865317927342	0.5039243593931210	0.3940651799233419	T	T
0.0240382945569432	0.0105406413862482	0.4954896762233179	T	T	0.0078290096293201	0.0070298505537924	0.4935402286071205	T	T
0.5023380298092601	0.0046471500546981	0.4961963411664376	T	T	0.5211078897271115	0.0051935906745715	0.4927042670750411	T	T
0.0211580470132308	0.5095416731436162	0.4904194601474958	T	T	0.0061580498362989	0.5092176395793976	0.4942417507901999	T	T
0.5046237159167092	0.4954455696594685	0.4919175145668307	T	T	0.5178175283365951	0.5046247391355391	0.4957345716538141	T	T
0.2528939749783461	0.2518641855220056	0.1486234953682943	T	T	0.2501402646263714	0.2505035738120616	0.1490432161170941	T	T
0.7529960116698368	0.2481974740334332	0.1485849538932051	T	T	0.7511657693333763	0.2468144720545158	0.1490494354787233	T	T
0.2532807117472181	0.7480637832659772	0.1486881517888874	T	T	0.2510281746407938	0.7468042899324582	0.1490271146079213	T	T
0.7523990766937276	0.7521506965569602	0.1486242314635760	T	T	0.7501427810824696	0.7505338105342721	0.1490383564792117	T	T
0.2533946070424364	0.2509479563451692	0.2461278975195150	T	T	0.2516539385787668	0.2495366912362442	0.2465360476486204	T	T
0.7545013126239938	0.2508835948443221	0.2461180296298128	T	T	0.7506385134774946	0.2496236277058364	0.2464883706405363	T	T
0.2532789500454549	0.7513049651909279	0.2460374360337571	T	T	0.2508826153953220	0.7494240953005803	0.2464807605415782	T	T
0.7542588375893792	0.7509966083725782	0.2460678602209513	T	T	0.7513844507671271	0.7493490307063306	0.2464522848648840	T	T
0.2590140167105075	0.2496213007285867	0.3427375901038633	T	T	0.2543461490813018				

0.8004171811796833	0.5053629426478916	0.5413842515135263	T	T	T	0.7682074215902075	0.5061208799818004	0.5364573532414874	T	T	T
0.0031507007632334	0.2474076044492698	0.1476562649713747	T	T	T	0.0006999976765429	0.2459458777443302	0.1468419968072968	T	T	T
0.5029567130395733	0.2531781269785369	0.1491122447996198	T	T	T	0.5007545707653177	0.2516792651219005	0.1506379453478221	T	T	T
0.0027269514554221	0.7526982315450012	0.1502958411954543	T	T	T	0.0007977988817175	0.7516449011252484	0.150458595796888	T	T	T
0.5030463912774690	0.7462923900102912	0.1464365347223344	T	T	T	0.5006045473687896	0.7461055555351549	0.1470406262025732	T	T	T
0.0040491350159939	0.2629450201292546	0.2454936755703811	T	T	T	0.0011642571375660	0.2607315081118433	0.2484584705306214	T	T	T
0.5038878342524656	0.2402798560841152	0.2450611130951645	T	T	T	0.5011600341905875	0.2394374662643478	0.2427587201011487	T	T	T
0.0037324482587219	0.7396759703338651	0.2424891213042954	T	T	T	0.0012916546026955	0.7395854457986968	0.2431787573872778	T	T	T
0.5038139247363402	0.7627596126782968	0.2478560284100474	T	T	T	0.5011416777415586	0.7607797411877062	0.2480490320027113	T	T	T
0.007280502061292	0.2289150386687608	0.3433912481067902	T	T	T	0.0045017967145188	0.2331078918668653	0.3386899428853641	T	T	T
0.5083412178055506	0.2747120095303249	0.3406305224259839	T	T	T	0.5046432948632474	0.2756385607697065	0.3459310581327352	T	T	T
0.0072180880353536	0.7752064069529172	0.3447718680649226	T	T	T	0.0045844037648187	0.7753475015063593	0.3448778328411218	T	T	T
0.5072402863649413	0.72978737005173912	0.3386722797095728	T	T	T	0.5040697623551227	0.7337651607192884	0.3395231384702568	T	T	T
0.0119338651814322	0.2777731980621149	0.4346269577222578	T	T	T	0.0108712091904438	0.2880934059730020	0.4420287511197183	T	T	T
0.5133691428561374	0.2197684920033257	0.4423496713644996	T	T	T	0.5103678107237851	0.2320812423416991	0.4354776202322977	T	T	T
0.0123239516449084	0.7207035151272005	0.4365420967726180	T	T	T	0.0097814261937344	0.7325850419597939	0.4369801776771677	T	T	T
0.5113772576860186	0.78644482286303378	0.4406378911705203	T	T	T	0.5101848660208482	0.7873891242935974	0.4400025373452222	T	T	T
0.0034415796874533	0.2427308285127889	0.5414982841173643	T	T	T	0.0136438061257259	0.2516831691421328	0.5319322024385468	T	T	T
0.5421598786589626	0.2655647657120560	0.5299500250740917	T	T	T	0.5105222726067349	0.2516365563779928	0.5357776686532575	T	T	T
0.0118736992527925	0.7541673958601227	0.5306102731913724	T	T	T	0.0133262740726857	0.7648747728345182	0.5335752237886647	T	T	T
0.5168194670280259	0.7337648957653228	0.5314629121996446	T	T	T	0.5100064380074799	0.7590888184268825	0.53382858477443589	T	T	T
0.1984537816014266	0.3283835797429671	0.6022886471650556	T	T	T	0.3887430039928630	0.0118100184403761	0.5600170283188233	T	T	T

O ₂ H adsorbed on the surface:						H ₂ O adsorbed on the surface:					
La Ni O H						La Ni O H					
1.0000000000000000						1.0000000000000000					
7.7991720000000004	0.0000000000000000	0.0000000000000000				7.7991720000000004	0.0000000000000000	0.0000000000000000			
-0.1209078500000000	7.7493359999999996	0.0000000000000000				-0.1209078500000000	7.7493359999999996	0.0000000000000000			
0.0457189100000000	0.0378002900000000	39.2802489700000024				0.0457189100000000	0.0378002900000000	39.2802489700000024			
20	20	62	1			20	20	61	2		
Selective dynamics						Selective dynamics					
Direct						Direct					
0.0194887491030456	0.9985555972414174	0.1103011899572942	T	T	T	0.0146788645057639	0.9964869652325132	0.1092815957955288	T	T	T
0.4854881745207131	0.0043863885992057	0.1101741200438822	T	T	T	0.4811300880147527	0.0032518416016275	0.1093044113603675	T	T	T
0.9872242740389030	0.5042012440405388	0.1102309082533584	T	T	T	0.9812844801603838	0.5031524671776129	0.1093412115714439	T	T	T
0.5208273631972916	0.4985529154313107	0.1100463259165845	T	T	T	0.5145471330916492	0.4963563026317633	0.1093201835510387	T	T	T
0.9955802119684209	0.0019911609843402	0.2027001996886736	T	T	T	0.9929836421684519	0.9989657405689228	0.2016528425720668	T	T	T
0.5036102199677509	0.0008359212071257	0.2027762194791916	T	T	T	0.5002884370055023	0.9978253578843636	0.2016329583695536	T	T	T
0.0082192690633254	0.4999761994171658	0.2022826437296517	T	T	T	0.0008456501876997	0.4974284000293918	0.2016661273810847	T	T	T
0.5000018454170042	0.50110742585587024	0.2024106476148990	T	T	T	0.4926109417984423	0.4985096911129948	0.2017077852446874	T	T	T
0.0024116155745234	0.0028936706089721	0.2981879226344703	T	T	T	0.0013474073530856	0.9985156161430995	0.2965104715014019	T	T	T
0.4974087539124878	0.0024800625453149	0.2975295054196420	T	T	T	0.4974227893169231	0.9976247875569786	0.2964323719540325	T	T	T
0.0057511794284412	0.5017048403474832	0.2969477017244853	T	T	T	0.9974588031416762	0.4977211820896559	0.2965154192050625	T	T	T
0.5108366191962889	0.5010513166301033	0.2969180832485478	T	T	T	0.5007861238998415	0.4979994073396785	0.2967895421585647	T	T	T
0.0011628372058100	0.0060417409968025	0.3950199743974935	T	T	T	0.0042419295393109	0.0008016137660708	0.3930543639564318	T	T	T
0.5062058316319646	0.0060993790116858	0.3954654738829473	T	T	T	0.5086311446416425	0.0029115684934189	0.3935154375084640	T	T	T
0.0170260472258720	0.5047506620322008	0.39313111172758591	T	T	T	0.0048058680916904	0.5030182820916655	0.3938910745287511	T	T	T
0.5124489506207691	0.5055706368413123	0.3933497570172320	T	T	T	0.5034394551840412	0.5027459325646092	0.3938189052359732	T	T	T
0.0126642883125282	0.9984592087322345	0.4971544119183429	T	T	T	0.0133894045219979	0.0034512905509145	0.4923621237491664	T	T	T
0.5103206268885851	0.9994701251266210	0.4933824825039885	T	T	T	0.5182602212432779	0.0028297559467905	0.4946464067941890	T	T	T
0.0210076087964402	0.5110103825540989	0.4959384250793281	T	T	T	0.0083594493339135	0.5140228519614232	0.4936093937602787	T	T	T
0.5210752407102890	0.5110196740909095	0.4916568775038856	T	T	T	0.5132024415337196	0.5077333571444164	0.4949237112315598	T	T	T
0.2535691837387451	0.2533469872298378	0.1500537138629712	T	T	T	0.2476688357219531	0.2516022027439100	0.1491647588645288	T	T	T
0.7537869387153484	0.2495327680637163	0.1500592342056500	T	T	T	0.7487212809937310	0.2477148097102704	0.1492107896258380	T	T	T
0.2542380252988883	0.7495846007063498	0.1501418812104571	T	T	T	0.2486876803653977	0.7477239313025414	0.1491989086285801	T	T	T
0.7532917768262016	0.7534700019251640	0.1501239234346969	T	T	T	0.7477273185425155	0.7515237999614477	0.1492106730004589	T	T	T
0.2541727488099821	0.251999956300258	0.2476012194336907	T	T	T	0.2501669099955099	0.2494504693210660	0.2468047662170259	T	T	T
0.7551405172945647	0.2518610674466961	0.2475193258950003	T	T	T	0.7491385135959953	0.2496292808465340	0.2467046561615021	T	T	T
0.2541700918446415	0.7523543938276398	0.2475162379033580	T	T	T	0.2493159560014030	0.7497045404647477	0.2466915130314313	T	T	T
0.7551473663329522	0.7522039479043231	0.2474843043135751	T	T	T	0.7499817141226581	0.7493588818288318	0.2466271446610442	T	T	T
0.25296271315416714	0.2520909599152755	0.3443887503355424	T	T	T	0.2543910199029626	0.2509224691566127	0.3437526682320139	T	T	T
0.7567544745836389	0.2522891498480949	0.3442277678646603	T	T	T	0.7549784864965901	0.2513773611843697	0.3434060389128609	T	T	T
0.2585868404216433	0.75343109133968456	0.3439462353128724	T	T	T	0.2541952862927273	0.7502518026490557	0.3434166772579251	T	T	T
0.7574369657485913	0.7548444978228845	0.3439516347285320	T	T	T	0.7538018433564410	0.7517636328212504	0.3431771844639803	T	T	T
0.2593173745164515	0.2564184862333438	0.4417686050726349	T	T	T	0.2590413179154303	0.2571874054720087	0.4409140666189530	T	T	T
0.7660428062972090	0.2560406165437654	0.4416681141480779	T	T	T	0.7598601996626668	0.2555444958377871	0.4407451674535661	T	T	T
0.2609010492434338	0.7544985759822385	0.4409121926233874	T	T	T	0.2613773958335421	0.7556466510542487	0.4405152687616251	T	T	T
0.7650231496380271	0.7540736881028633	0.4410600647242163	T	T	T	0.7587978368121703	0.7551576382623499	0.4405421202075944	T	T	T
0.2820865572168236	0.2567239192289993	0.5391609749360978	T	T	T	0.2567073031843577	0.2527472427114765	0.5358355730795665	T	T	T
0.7518248664471161	0.2601679305548583	0.5379053518128106	T	T	T	0.7632995964319800	0.2607094021269092	0.5368057645830507	T	T	T
0.2705137893783406	0.7539341920521810	0.5390838774805213	T	T	T	0.2574762600400131	0.7652671404851030	0.5368360665409492	T	T	T
0.7592705188564816	0.7499287419187609	0.5384865208296424	T	T	T	0.7609750377975462	0.7549936886942276	0.5377394722116601	T	T	T
0.2586606955269907	0.2125835001525149	0.0997716195615830	T	T	T	0.2564874862360518	0.2116559565952766	0.0988752560628422	T	T	T
0.7488957838776896	0.2902247306178387	0.099048209550123	T	T	T	0.7400782552979338	0.2875684477821824	0.0990673627987789	T	T	T

+3% Strain State:

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0.7457693856091009	0.2911431763085918	0.0993396873572682	T	T	T	0.7462090197704988	0.2968889979292271	0.0993551356887687	T	T	T
0.2455757043555540	0.7910687086018227	0.0993608848321709	T	T	T	0.2461435525398982	0.7966584228021460	0.0993713450596721	T	T	T
0.7593949241813959	0.7062843073252102	0.0993730310494941	T	T	T	0.7581210949463165	0.7115294504213415	0.0993777678234155	T	T	T
0.2435433626637342	0.2966990173681170	0.1972991724764933	T	T	T	0.2440383132528381	0.3020037384024611	0.1973229554835235	T	T	T
0.7604617983322952	0.2014693870252770	0.1972240865887622	T	T	T	0.7603977281903742	0.2059617202213827	0.1972500950409847	T	T	T
0.2614783263024737	0.7014219787449879	0.1972389584696729	T	T	T	0.2603986497831179	0.7058885871741437	0.1972883133431654	T	T	T
0.7421445664985329	0.7969342225417303	0.1972333923064866	T	T	T	0.7440679016787694	0.8024399305362544	0.1972206444419784	T	T	T
0.2639798355544317	0.2036553631592279	0.2937763484941727	T	T	T	0.2634443276846783	0.2070137220432912	0.2938384716010904	T	T	T
0.7439044591761921	0.2970163050088535	0.2934146651105661	T	T	T	0.7441664550900317	0.3012415602540163	0.2934575092090028	T	T	T
0.2415279036533308	0.7971148193918756	0.2933718062949269	T	T	T	0.2442926259436776	0.8022760364754000	0.2934338887008925	T	T	T
0.7659935692776881	0.7044352932506319	0.2934582745618168	T	T	T	0.7629864664849004	0.7071263012510339	0.2934846501564052	T	T	T
0.2473741105248518	0.2972851957085510	0.3892795682513534	T	T	T	0.2471104422649448	0.3005609463170394	0.3894657175551552	T	T	T
0.7670203449027521	0.2082239795645259	0.3889850202812207	T	T	T	0.7669642037527123	0.2102506809906559	0.3896050392325113	T	T	T
0.2683448858418636	0.7084900702218835	0.3886622360504649	T	T	T	0.2628462493265167	0.7106272678270885	0.3886958911742541	T	T	T
0.7459685344753375	0.7962534048520521	0.3889658300205336	T	T	T	0.7491532383185043	0.8011178297041384	0.3889953811737354	T	T	T
0.2697576553830232	0.2180189152210041	0.4847663560831836	T	T	T	0.2760504264906768	0.2235220085760069	0.4852539329167430	T	T	T
0.7548560492361868	0.2966099154351812	0.4851581595655652	T	T	T	0.7565097229295650	0.3008694186991253	0.4852024236449309	T	T	T
0.2553022866339162	0.7861624741450972	0.4846956508289518	T	T	T	0.2586358015582604	0.7897083135451750	0.4846645830821974	T	T	T
0.7669599831677947	0.7071530415179638	0.4847207706615114	T	T	T	0.7607761173910962	0.7046745779545542	0.4844143624377740	T	T	T
0.2532376115025957	0.9987560802341303	0.1554030734326633	T	T	T	0.2525720672354548	0.0039345892937585	0.1554473404252974	T	T	T
0.7513673163504470	0.9987264991796064	0.1403239830615060	T	T	T	0.7519826700511095	0.0041477839608150	0.1402580207573977	T	T	T
0.2512974631188022	0.4986140930789504	0.1403426760480328	T	T	T	0.2518817876229695	0.5040229477580531	0.1403265384687466	T	T	T
0.7531266994327944	0.4988238159449358	0.1553889039100035	T	T	T	0.7525712223979362	0.5039886532039924	0.1554493215420932	T	T	T
0.24674070980418557	-0.0000115905950441	0.2379306795016846	T	T	T	0.2483041349788802	0.0043354983758849	0.2378978039644325	T	T	T
0.7592985111821244	0.9997993543873973	0.2528196123229442	T	T	T	0.7577583404920362	0.0041185691569007	0.2525983374968582	T	T	T
0.2592754235452359	0.4997121381677942	0.2528549982046252	T	T	T	0.2578253756945501	0.5042271655075624	0.2530469758214738	T	T	T
0.7468002583094173	0.4998447376569019	0.2378731941283904	T	T	T	0.7484111380066213	0.5041083823179342	0.2378124352955322	T	T	T
0.2698809926346418	0.00148377725861496	0.3490001695527230	T	T	T	0.2676726585283246	0.0048645476733155	0.3492470846009076	T	T	T
0.7439614027373868	0.0014398										

0.756596688990123	0.2497940521322323	0.2453444032115943	T	T	T	0.7530261901817378	0.2501421451727419	0.2459030833536346	T	T	T
0.2525479224087360	0.7505238605668448	0.2451992549889787	T	T	T	0.25306696141882313	0.7499227912705494	0.245925559024486	T	T	T
0.7561689842157521	0.7501554775774744	0.2452825530757228	T	T	T	0.7534248718411284	0.7495908012719553	0.2459031481992776	T	T	T
0.2591488259143301	0.2473108517335997	0.3411612240978974	T	T	T	0.2543427211193602	0.2520572066539868	0.3418952041634056	T	T	T
0.7561210035511761	0.248273270089791481	0.3415857340634100	T	T	T	0.7545324239466670	0.2509840066305629	0.3417895255260355	T	T	T
0.2580357087895666	0.7508956876210962	0.3409038709024424	T	T	T	0.2541641007123850	0.7511916559822530	0.3419106264192154	T	T	T
0.7569930996915917	0.7502660679034167	0.3414158254648102	T	T	T	0.7544137145742945	0.7523006816554451	0.3417672722835542	T	T	T
0.2566678481827181	0.2481956964725842	0.4371682606865514	T	T	T	0.2568283067775146	0.2515619061124371	0.4383222248546338	T	T	T
0.7606627046608038	0.2478341507871552	0.4380049408113988	T	T	T	0.7576360582801800	0.2535904762200421	0.4378944180632333	T	T	T
0.2597767878705701	0.75002277013526060	0.4367444604769691	T	T	T	0.2573830220433860	0.7556564935928700	0.4383130639168090	T	T	T
0.7580779267203159	0.7476752382447054	0.4375912285166666	T	T	T	0.7568163076195024	0.7532096806247764	0.4378357445925904	T	T	T
0.1527529283417821	0.3630237731904095	0.5603960996026345	T	T	T	0.2565200237374858	0.2645003946072070	0.5332818593721157	T	T	T
0.7597710652203464	0.3006629055318210	0.5327646177215541	T	T	T	0.7543225331115049	0.2632999099754457	0.5340225224158018	T	T	T
0.2483921656915048	0.7498970971965613	0.5332069988552097	T	T	T	0.2567371606428854	0.7441712845927007	0.5332576590415253	T	T	T
0.7557960569071815	0.7376509145656733	0.5291544194910464	T	T	T	0.7552536303724878	0.7462304532466173	0.5336446501105703	T	T	T
0.2584623067615227	0.2065804466511620	0.0986517113330254	T	T	T	0.2606159954753168	0.2065770462199582	0.0993623837048610	T	T	T
0.7542545059858334	0.2933577993100820	0.0986714330585436	T	T	T	0.7469970134007996	0.2913000025908677	0.0993289920046062	T	T	T
0.2478555331414079	0.7914491135555384	0.0988583786645440	T	T	T	0.2471276152003166	0.7913737051165239	0.0992975525107990	T	T	T
0.7636585382839747	0.7066624842285794	0.0987313338451256	T	T	T	0.7606081530675870	0.7066774951846277	0.0993818164571300	T	T	T
0.2574997554039796	0.2981612632567133	0.1967120260554249	T	T	T	0.2440884976403359	0.2969401066911493	0.1972800277468346	T	T	T
0.7540902898860182	0.2017949804426143	0.1965488799396726	T	T	T	0.7623255073275689	0.2016758784569138	0.1972680651474624	T	T	T
0.2682903927736184	0.7016111092626212	0.1965979118038780	T	T	T	0.2620816630037528	0.7018712128669530	0.1972819287801007	T	T	T
0.7426531285780816	0.7972010403918443	0.1965625367778724	T	T	T	0.7443281062476618	0.7971320792096364	0.1972669024360352	T	T	T
0.2479531239491352	0.2015680714057809	0.2931274104305567	T	T	T	0.2648904911579977	0.2040958921439890	0.2936031773490975	T	T	T
0.7652052270264482	0.2948867266535619	0.2930237667657161	T	T	T	0.7428606965071881	0.2979786726549927	0.2934603035434725	T	T	T
0.2394198333990908	0.7960540575258091	0.2926011461399100	T	T	T	0.2433047300473027	0.7972855363050567	0.2935907788846011	T	T	T
0.7728693239657386	0.7054570438247911	0.2930151273683830	T	T	T	0.7640747931530404	0.7038139715668930	0.2934885833469680	T	T	T
0.2778044743236606	0.2870570139911123	0.3881106841007887	T	T	T	0.2442362957809955	0.2965431525126892	0.3892064520632472	T	T	T
0.7433366826367217	0.2045324583826369	0.3893505740348972	T	T	T	0.7661889843521080	0.2078411701097641	0.3888465866218154	T	T	T
0.274134755202697	0.7136426625795287	0.3879020013707856	T	T	T	0.2640966338346213	0.7076711826198350	0.3892309718830673	T	T	T
0.7422213897764470	0.7935778316336272	0.3892054544690128	T	T	T	0.7458635029304385	0.7968404114473253	0.3888396713017389	T	T	T
0.2417559092393647	0.2477561712826062	0.4831334793340847	T	T	T	0.2666388774599590	0.2066696265110238	0.4850942256127388	T	T	T
0.8047792434095608	0.2818789467227159	0.4859328900012526	T	T	T	0.7489615454382365	0.2890589751835989	0.485077258212903	T	T	T
0.2615268017295589	0.7370861498929822	0.4844734269635795	T	T	T	0.2542718747559658	0.8020979403461294	0.4850513762571789	T	T	T
0.7586599358181376	0.6745258451952149	0.4835389569945496	T	T	T	0.7603721619228293	0.7143479627844066	0.4848432747130161	T	T	T
0.2581778939046144	0.9994548463355999	0.1547819299870692	T	T	T	0.2549161696959509	0.998987420360089	0.1554084429171402	T	T	T
0.7540799210471274	0.9996248857461242	0.1395919346584602	T	T	T	0.7526815288285962	0.9989275030088893	0.1404154944745714	T	T	T
0.2545590830461518	0.49994948531042762	0.1397620865695607	T	T	T	0.2526886993162091	0.4989315552075739	0.1404180959854954	T	T	T
0.7570928520287107	0.2495719452969072	0.1548756415354271	T	T	T	0.7549192032198515	0.4989893706784796	0.1554066494080074	T	T	T
0.24997856363523312	1.000935499630292	0.2370872154721809	T	T	T	0.2484370721588138	0.9998514656168662	0.2379592308718161	T	T	T
0.7633699058771022	0.9998455102723062	0.2521513437234568	T	T	T	0.7591720932152600	0.9998475480706416	0.2528505352706807	T	T	T
0.262422844464352	0.4998167152227528	0.2523751024725599	T	T	T	0.2592768661489709	0.4997896215953854	0.2528766350870340	T	T	T
0.7505256002100680	0.5000160748764980	0.2376321372414545	T	T	T	0.7483644796226432	0.4998811829188566	0.2378147333242057	T	T	T
0.2766626780220584	0.9992945284498038	0.3481482246484747	T	T	T	0.2674875825748996	0.0017088224883798	0.3490073732843249	T	T	T
0.7430835352148318	0.9994498453141526	0.3335548052403424	T	T	T	0.7432782038164393	0.0017065210996630	0.3335583700477109	T	T	T
0.2439677629243596	0.4996984831952561	0.3338764396373130	T	T	T	0.2435074772675206	0.5016001110507023	0.3338011039941782	T	T	T
0.7718674492523312	0.4992031504139477	0.3481296768466232	T	T	T	0.7680511379174819	0.5016721566638379	0.3490222626074113	T	T	T
0.2377943461004209	0.9990824551552150	0.432610582984601	T	T	T	0.2454682733925723	0.0036046482362961	0.4294126659954556	T	T	T
0.7913737168382012	0.9970306869021359	0.4442773613298674	T	T	T	0.7748325180827063	0.0035690185423137	0.4449532173146121	T	T	T
0.2766023648395206	0.49912240843663511	0.4393343885744522	T	T	T	0.2757307492056680	0.5037096906561439	0.4449436187542992	T	T	T
0.7456411727651445	0.4967862616722328	0.4288057911647571	T	T	T	0.7443749118300483	0.5035701516952813	0.4301324304997192	T	T	T
0.2591087808851125	0.97475111684258416	0.5312883910260051	T	T	T	0.2734850559681177	0.0029366523589232	0.5427622804168030	T	T	T
0.7572845513046987	0.9694576897792155	0.5247354873570554	T	T	T	0.7558244490185247	0.0009733959067074	0.5283359938748800	T	T	T
0.2551660737799969	0.5113544979954264	0.5354324619895722	T	T	T	0.2560630267471986	0.5040500668658128	0.5255758125422845	T	T	T
0.7773220327283054	0.5173184464303828	0.545114013265159	T	T	T	0.7795530296198916	0.5032635841548543	0.5393714660585940	T	T	T
0.0058639705075345	0.24746648173511146	0.1481364402434163	T	T	T	0.0036376747043111	0.2476146745686019	0.1474019066104995	T	T	T
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