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Theoretical Insight on Anion Ordering, Strain and Doping Engineering on the Oxygen Evolution Reaction in BaTaO$_2$N

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Abstract

Oxynitride perovskites like BaTaO$_2$N are among the most promising materials to achieve efficient direct solar-to-chemical conversion. Albeit photoelectrochemical water splitting has been demonstrated, the required overpotentials remain prohibitively large compared with the theoretically accessible values, particularly for the oxygen evolution reactions (OER). Here, we apply Density Functional Theory (DFT) calculations to investigate the use of surface strain and cationic doping with Ca and Sr to optimize the OER theoretical overpotential. For the TaON-terminated BaTaO$_2$N (001) surfaces, 4% compressive uniaxial strain can lower the theoretical overpotential to $\eta = 0.59$ V. For the most stable TaO$_2$N-(100) termination, 1% tensile uniaxial strain, which is perfectly accessible by experiments, is enough to reduce the theoretical overpotential from $\eta = 0.43$ V to $\eta = 0.37$ V under (photo)electrochemical conditions. This value is close to the minimum predicted theoretical overpotential and points out how strain engineering could be efficiently used to improve electrocatalytic reactions.

Introduction
Over the last decade, oxynitrides have been investigated for multiple applications, ranging from ferroelectricity,\textsuperscript{1} over electrocatalysis\textsuperscript{2} to photocatalysis.\textsuperscript{3} In general, by combining oxygen and nitrogen as anions, oxynitrides show higher stabilities in air and moisture compared to pure nitrides, and the perovskite structured oxynitrides display smaller band gaps than those of pure oxides,\textsuperscript{4} which contribute to their attractive electronic and optical properties in photocatalysis or photoelectrocatalysis for water splitting devices. Among the identified compositions,\textsuperscript{5} BaTaO\textsubscript{2}N is one of the promising candidates as photoelectrocatalysts for water splitting, because of its optical band gap (approx. 1.9 eV, which is close to the minimum energy needed to split water once that the bare energy to split water and the reaction overpotentials are considered)\textsuperscript{6} and band edge position, which straddle the redox potentials of the hydrogen and oxygen evolution reactions.\textsuperscript{7,8,11–13} Although much effort has been carried out to improve the performance of BaTaO\textsubscript{2}N for water splitting, its photocatalytic activity is still far from practical applications.\textsuperscript{7,8,11–13} One of the strategies to improve the catalytic activity is to reduce the overpotentials required to split water into molecular oxygen and hydrogen. The lowest theoretical overpotentials for the oxygen evolution reaction (OER) on oxide and oxynitrides are predicted to be 0.2-0.4 V.\textsuperscript{14} Therefore, the surface reactions, especially for OER, is a critical bottleneck, which currently limits the efficiency of solar-to-chemical conversion and ultimately the use of oxynitrides as materials for water splitting.

The properties of perovskite oxynitrides are sensitive to surface local structure and oxygen/nitrogen ordering.\textsuperscript{15–17} The ordering of the O/N anions in oxynitrides is caused by the four coordinate ionic radii of O\textsuperscript{2−} (1.38 Å) and N\textsuperscript{3−} (1.46 Å) and the corresponding chemical bonding environment (valence) between O/N and neighboring high-valence metals (M-O or
M-N$^{18,19}$ Therefore, different exposed surface terminations show also different O/N anionic orderings, which affects the physicochemical properties and catalytic activity.$^{20}$ In addition to this, doping and strain engineering have been proved to be effective methods in tailoring the surface electronic structures and catalytic properties.$^{21-24}$ Substitution (or partial substitution) of the A site and/or B site by other elements with different radius or valences,$^{25}$ as well as strain manipulations, can easily alter the geometrical and electronic structure of the active sites.$^{26}$ A typical example is efficient electrochemical N$_2$ reduction could be achieved by doping strain induced bi-Ti$^{3+}$ pairs.$^{27}$ More specifically for perovskite oxynitrides, the changes in properties due to the applied strain have also been verified experimentally, starting from computational predictions, such as the change in anion arrangement in Ca$_{1-x}$Sr$_x$TaO$_2$N,$^{26}$ the 2D to 3D crossover on a cubic lattice of correlated disorder of O and N atoms within the Ba$_{1-x}$Sr$_x$TaO$_2$N series,$^{28}$ and the creation and switching of anion vacancy layers in SrVO$_{2.2}$N$_{0.6}$.$^{29}$ Another examples is epitaxial strain effects lead to a tetragonal distortion of the BaTaO$_2$N perovskite unit cell, with negligible volume change, which shows a unique combination of high dielectric permittivities and insensitivity to changes in temperature.$^{30}$ Furthermore, a ferroelectric response in tensile-strained SrTaO$_2$N films is observed due to a change of the anion ordering as a function of the applied strain.$^{31}$ On the electronic properties, a tuning of the bandgap has been achieved in Y-substituted LaTaO$_2$N from an orthorhombic strain.$^{32}$ From the perspective of photocatalysis, controlling the morphological and structural variations of LaTiO$_2$N and CoO$_x$ nanoparticles could influence the strain in the structure and hence promote the photocatalytic O$_2$ evolution.$^{33}$ It has also been reported that Au-SrTiO$_3$ with tensile strain, where the strain is induced by difference of thermal expansion coefficient between Au and SrTiO$_3$, shows 10.5
times higher photocatalytic activity for water splitting than the unstrained Au-SrTiO₃. The significant increase in the rate of H₂ and O₂ formation has also been reported for strained TiO₂, where the strain is obtained by Au dispersion.

In this work, we show that doping and strain engineering in particular can be used to improve the catalytic OER performance of BaTaO₂N for water splitting. Using Density Functional Theory (DFT) calculations, we have investigated the role of the anion ordering, strain and doping modifications on the OER for the (100) TaO₂N-terminated and (001) TaON-terminated surfaces of BaTaO₂N. The theoretical overpotentials for OER on clean TaO₂N surface (η = 1.64 V) is much higher than that of clean TaON surface (η = 0.97 V). On the other side, under realistic (photo-) electrochemical conditions, the full oxygen covered TaO₂N surface shows the lowest theoretical overpotential of 0.37 V when 1% tensile uniaxial strain in [001] direction (Figure 1b) is applied, compared to 0.59 V that can be achieved by the TaON termination with full OH coverage and 4% compressive uniaxial strain in [010] direction. A possible strategy to achieve a lower theoretical overpotential closer to the theoretical limit is to combine strain with doping. The Ca-doped TaON-terminated BaTaO₂N (001) surface, with 4% tensile uniaxial strain in [010] direction, shows an theoretical overpotential of 0.53 V for the clean surface.

**Method**

*Computational Methodology*

The calculations were performed by using the projector augmented wave (PAW) potentials implemented in the VASP package in the framework of the generalized gradient approximation (GGA). The Perdew–Burke–Ernserhof revised for solids (PBEsol) exchange
correlation potential was used for optimizing the bulk structures, while for surface calculations we used the Perdew–Burke–Ernserhof (PBE). The Brillouin zone of the 40-atom bulk unit cells, which is the smallest cell allowing to represent the correct anion ordering, is sampled with a 6 x 6 x 6 Γ-centered Monkhorst–Pack k-point mesh and a 6 x 6 x 1 Γ-centered Monkhorst–Pack k-point mesh for the slabs. The slab model includes 8 atomic layers where the bottom 4 layers was fixed, and a vacuum thickness of 20 Å was added to separate the reciprocal images. For the doping modification, one Ba atom in the sublayer was replaced by Sr or Ca, and the corresponding doping concentration is 6.25%. Dipole correction was also included. Grimme’s D3-type method was carried out for van der Waals interactions corrections. A plane-wave energy cutoff of 550 eV was used. Cell and atomic positions were fully relaxed until the forces on the atoms were below 0.02 eV/Å. These structures were then used to build the surface models, for which only the atomic positions have been relaxed, keeping the cell frozen. The energy barrier for formation of N₂ on the (100) surface of BaTaO₂N was calculated using the climbing images nudged elastic band method (CI-NEB) and the structures were relaxed with force less than 0.05 eV/Å. A more sophisticated semi-local functional (GLLB-SC) was used to calculate the bandgap of bulk BaTaO₂N as implemented in the GPAW program package. All data are stored and freely available at the address: DTU DATA.

Surface energy

In BaTaO₂N, each exposed facet has two possible terminated surface. To determine the most stable surface, which is more likely to form experimentally, we have calculated the surface energy (γ).
\[ E_{\text{surf}}^{\text{unr}}(X) = \frac{1}{4} \left[ E_{\text{slab}}^{\text{unr}}(\text{A-termination}) + E_{\text{slab}}^{\text{unr}}(\text{B-termination}) - nE_{\text{bulk}} \right], \]  

where \( X \) is the specific termination, \( E_{\text{slab}}^{\text{unr}}(\text{A-termination}) \) and \( E_{\text{slab}}^{\text{unr}}(\text{B-termination}) \) are the unrelaxed A- and B-terminated slab energies, \( E_{\text{bulk}} \) is the energy of BaTaO\(_2\)N unit cell with 40 atoms.

The relaxation energy for each termination can be computed from the corresponding slab alone using:

\[ \Delta E_{\text{surf}}^{\text{rel}}(X) = \frac{1}{2} \left[ E_{\text{slab}}(X) - E_{\text{slab}}^{\text{unr}}(X) \right], \]  

Where \( E_{\text{slab}}(X) \) is the slab energy after relaxation. The relaxed surface energy it then

\[ E_{\text{surf}}(X) = E_{\text{slab}}^{\text{unr}}(X) + \Delta E_{\text{surf}}^{\text{rel}}(X). \]  

\textit{OER mechanism}

The OER is regarded as a key reaction as well as bottleneck in the water splitting process.

Various mechanism have been proposed for the OER, which depends on many factors from material to the reaction environment.\textsuperscript{49,50} In this study, we adopted a widely used mechanism for the OER that considers a process in which oxygen molecules are formed via a surface OOH intermediate, at standard conditions (\( T = 298.15 \, \text{K}, \, P = 1 \, \text{bar}, \, \text{pH} = 0 \)), the computational standard hydrogen electrode (SHE) approach.\textsuperscript{50} In this model, it is assumed a four proton-coupled electron-transfer (PCET) process:

A: \( \ast + \text{H}_2\text{O} \rightarrow \text{OH}\ast + \text{H}^\ast + e^- \),  

B: \( \text{OH}\ast \rightarrow \text{O}\ast + \text{H}^\ast + e^- \),  

C: \( \text{O}\ast + \text{H}_2\text{O} \rightarrow \text{OOH}\ast + \text{H}^\ast + e^- \),  

D: \( \text{OOH}\ast \rightarrow \ast + \text{O}_2 + \text{H}^\ast + e^- \),

where the symbol \( \ast \) represents a surface reaction site and \( \text{O}\ast, \text{OH}\ast \) and \( \text{OOH}\ast \) are adsorbed
oxygen, hydroxyl and hydroperoxy groups, respectively.

While the kinetic overpotential cannot be directly determined from DFT-level calculations, we here introduce the theoretically thermodynamic overpotential (theoretical overpotential, $\eta$), which is defined as the lowest overpotential for which all the electrochemical steps are downhill in free energy. The potential of the water splitting reaction is 1.23 V per proton–electron pair transfer and the entire process has an energy change of 4.92 eV. The step with maximum Gibbs free energy change ($\Delta G$) of these four steps is the potential determining step. To estimate the potential determining step, Gibbs free energy change ($\Delta G$) of each chemical reaction is calculated by:

$$\Delta G(U, pH, T) = \Delta E + \Delta ZPE - T\Delta S + \Delta G_U + \Delta G_{pH} \quad (8)$$

where, $\Delta E$ is the reaction energy determined from the DFT total energies and $\Delta ZPE$ is the difference in zero-point energies due to the reaction between the adsorbed and gas phase species by setting $H_2O$ and $H_2$ in the gas phase as reference states. $\Delta S$ is the change in entropy, which was computed using DFT calculations of the vibrational frequencies and standard tables for gas phase molecules. The computed values of $\Delta ZPE$ and $T\Delta S$ are reported in Table S2. $\Delta G_U = -eU$ is the free energy change due to electrode potential $U$, and $\Delta G_{pH} = k_B T \ln[H^+] = -k_B T \ln10 pH$ is the free energy change due to the change in $pH$. Since Gibbs free energy change ($\Delta G$) of each chemical reaction is affected by the same value of $k_B T \ln10 pH$ at $pH \neq 0$ and the theoretical overpotential, $\eta$, is independent of pH. All values of $\Delta G$ were computed at $T = 298.15$ K and $pH = 0$. Due to the universal scaling relations between the adsorption energies of OOH and OH (a constant difference of 3.2 eV), the theoretical minimum overpotential for the OER, proceeding via these four PCET steps, is 0.37 V = (3.2 eV – 2 x 1.23 eV) / 2e.$^{14}$
**Result and discussion**

The perovskite structure of BaTaO$_2$N exists two possible N/O orderings in the TaO$_2$N$_2$ octahedral structures: one is “cis-type” TaO$_2$N$_2$ octahedra corresponding to N-Ta-N bonds with 90° angles and the other one is “trans-type” octahedra with 180° N-Ta-N bonds drawn in Figure 1a. Here, we consider different configurations with various 2D O/N orderings (see Supporting Information, Figure S1 and Table S1) and the cis-ordered structure shown in 1b, is thermodynamically most stable among all the structures considered. The 40-atom bulk supercell is the smallest cell allowing representing the correct anion ordering as well as possible octahedral distortions. The corresponding lattice parameters are $a = b = 8.287$ Å and $c = 8.095$ Å. The band gap of bulk BaTaO$_2$N is 2.49 eV, which is narrow enough to absorb visible light. To study photo-oxidation, it is essential to determine the position of valence-band edge versus SHE at pH=0 as the driving force for OER is provided by holes at the upper edge of the valence band. We calculate that the VBM positions is 2.20 eV vs SHE, which could provide an additional potential of 0.97 V with respect to the OER potential. The details of the calculation can be seen in the supporting information.

The two most commonly exposed (100) and (001) facets have been studied. As reported in Figure 1c-d, each facet has two terminations: for the (100) facet TaO$_2$N and BaON-terminated surface; and for the (001) facet, TaON and BaO$_2$-terminated surface. As indicated by the surface energies in Table 1, the Ta-exposed surfaces have the lowest energies, for both the (100) and (001) facets, for which we now investigate their catalytic properties. For TaO$_2$N terminated (100) surfaces, there are 1/3 N atoms within anions and the two N atoms are in the symmetric
sites, while for TaON terminated (001) surface, there are 1/2 N atoms within anions and each two N atoms connected to Ta atom forms N-Ta-N bonds with 90° angles.

**Figure 1.** (a) Schematic representation of the anion ordering in a TaO$_2$N$_2$ mixed-anion octahedron. Structure of (b) bulk BaTaO$_2$N, (c) (100) surface of BaTaO$_2$N with TaO$_2$N termination on top and (d) (001) surface of BaTaO$_2$N with TaON termination on top.

**Table 1.** The calculated surface energies of different surfaces

<table>
<thead>
<tr>
<th>Facet</th>
<th>Termination</th>
<th>Surface energy (eV/Å$^2$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(100)</td>
<td>TaO$_2$N</td>
<td>0.032</td>
</tr>
<tr>
<td></td>
<td>BaON</td>
<td>0.056</td>
</tr>
<tr>
<td>(001)</td>
<td>TaON</td>
<td>0.081</td>
</tr>
<tr>
<td></td>
<td>BaO$_2$</td>
<td>0.086</td>
</tr>
</tbody>
</table>

*(100) facet TaO$_2$N-terminated*
As shown in Figure 2 a-d, the OH and OOH fragments prefer to adsorb on top of one of the Ta atom on the surface. The situation is different for O. When there is only one O, it adsorbs on the bridge site between Ta and N, while for full O coverage, half O are adsorbed on the bridge site and half O are located on top of Ta atom. To predict the most relevant surface coverage under (photo)-electrocatalytic operating conditions, surface Pourbaix diagrams are computed at pH = 0, as shown in Figure 2e. The clean surface is stable only at low potential (below 0.47 V). At operating conditions, where the potential is higher than 1.23 V, the full O coverage is the energetically most stable.

Figure 2. Structure of (100) surface of TaO$_2$N-terminated BaTaO$_2$N with (a) 1/4 OH, (b) 1/4 O, (c) 1/4 OOH and (d) 1 O adsorbates. The purple ball and white ball represent adsorbate O and H atom. (e) Surface Pourbaix diagram of the TaO$_2$N-terminated (100) surface at pH = 0.

To investigate the role of the surface, we firstly study the OER on the clean surface. The surface configurations are shown in Figure 3a: the deprotonation of H$_2$O molecule forms OH in step 1; then in step 2, OH is deprotonated to form an adsorbed oxygen O, when it comes in contact with another deprotonated H$_2$O molecule forming OOH (step 3); and finally, in step 4, O$_2$
molecule forms from the deprotonation of OOH and eventually leaves the surface. From the free energy diagrams (Figure 3a), we can see that the rate determining step (RDS) is the formation of OOH with a free-energy difference of 2.87 eV, which results in an theoretical overpotential of 1.64 V.

For the full O coverage, half of the O-atoms are adsorbed on the bridge sites and half O on top of Ta, therefore there are three kinds of possible reaction sites resulting in three possible OER paths. First the reaction could continue from an O on the bridge site. While we find that OOH cannot be formed from the bridge O, which is similar to the surface reaction on Sr$_2$TaO$_3$N.$^{52}$ Then, we consider the reaction occurring from the O atom on top of Ta atom (Ta$_1$), which shows an theoretical overpotential of $\eta = 0.74$ V in Figure 4b. Surprisingly, when the reaction happens on the Ta atom without O on the top sites (Ta$_2$), the theoretical overpotential is only 0.43 V (Figure 4c). For all OER processes, the RDS are the formation of OOH. To understand the reasons for the much lower theoretical overpotential of the latter mechanism, we calculate the Bader charges and the charge transfer q from the Ta. These values (Table 2) indicates that the Ta with adsorbed O on the bridge site is more oxidized, which weakens the Ta and O double bond, that breaks more easily on formation of the Ta-OOH intermediate (RDS) leading to a lower theoretical overpotential (0.43 V).
Figure 3. OER steps and Gibbs free energy diagrams for the TaO$_2$N-terminated (100) (a) clean surface, surface covered with full O (b) Ta$_1$ site and (c) Ta$_2$ site.

Table 2. A Bader charge analysis of the Ta in the TaO$_2$N-terminated (100) surface layer of BaTaO$_2$N with full O coverage. Positive value q indicates the electron is removed from Ta.

<table>
<thead>
<tr>
<th></th>
<th>Average Bader charge</th>
<th>Charge transfer q (e)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ta$_1$</td>
<td>8.44</td>
<td>+2.51</td>
</tr>
<tr>
<td>Ta$_2$</td>
<td>8.49</td>
<td>+2.56</td>
</tr>
</tbody>
</table>

Strain can be used to control the structure of the surface, with its electronic and catalytic properties. Therefore, to tune and improve the OER activity, we apply compressive and tensile uniaxial strain in both [010] and [001] directions, where the negative value means the compressive strain and the positive represents the tensile strain. As indicated by the volcano...
plot in Figure 4a, under uniaxial strain in [010] direction the theoretical overpotential increases. This can be seen for both compressive and tensile strain, however the effect is more pronounced for tensile strain. This can be explained as a combination of a change in the electronic properties of the surface, in particular the hybridization of the O-2p and Ta-d orbitals, and a structural modification of the geometry of the surface and adsorbate under different strain conditions. The response to the uniaxial strain in [001] direction is however different. The change of the $\Delta G_{\text{O}^*-\text{OH}^*}$ in figure 4a is linear with the strain. Under 4% compressive strain, the theoretical overpotential increases from 0.43 to 0.77 V, while under tensile strain, the theoretical overpotential firstly decreases, reaching the top of the volcano and afterward increases, on the other branch of the volcano. The lowest theoretical overpotential is reached at 1% tensile strain and it is equal to 0.37 V. On the left leg of the volcano, the RDS is the formation of OOH (Figure 4a,b and S2a-c), while on the right branch, we find that the formation of O is the RDS (Figure 4d and S2d). At 1% tensile strain, which is found at the top of the volcano, the RDS is shared between the formation of OOH and O (Figure 4c). Hence, the uniaxial strain in [001] direction can be used to modulate the RDS and tune the OER theoretical overpotential, by changing the adsorption energies of OOH and O on the surface.

It should be noted that the oxidation of the $\text{N}^3$ ions forming $\text{N}_2$ has been put forward for oxynitrides and perovskite oxynitrides by photo-generated holes during the photocatalytic reaction, which have been confirmed by an obvious decrease in nitrogen content indicated by XPS. Therefore, we perform NEB calculations to investigate the migration of the surface N atoms to form $\text{N}_2$. As shown in Figure S3, the energy barrier is 1.05 eV, and the process is therefore kinetically hindered compared to OER.
Figure 4. (a) Volcano plot of the free-energy difference of $(\Delta G_{O^*} - \Delta G_{OH^*})$ and the OER theoretical overpotential (\(\eta\)) for TaO\(_2\)N-terminated (100) full O covered surfaces. Gibbs free energy diagrams for the full O covered TaO\(_2\)N-terminated (100) surface with (b) 4\% compressive uniaxial strain in [010] direction, (c) 1\% tensile uniaxial strain in [001] direction and (d) 2\% tensile uniaxial strain in [001] direction.

(001) facet TaON-terminated

Compared to perovskite oxides where all anions are oxygen, the N/O ordering differs from facet to facet. As shown in figure 1c-d, TaON-terminated (001) surface shows an obviously different N/O order compared to TaO\(_2\)N-terminated (100) surface. On the TaON-terminated
(001) surface, the two N atoms connected to Ta atom forms N–Ta–N bonds with 90° angles. The difference of the N distribution on the surface then will influence the adsorption of the fragments. The photocatalytic properties of the different facets can thus change significantly. As shown in Figure S4a, for the clean (001) surface, the RDS is the formation of OOH resulting in an theoretical overpotential of 0.97 V, which is lower than the theoretical overpotential of corresponding (100) surface (1.64 V). This is caused by a change in the adsorption of O. On the (001) surface the O would like to be adsorbed on top of Ta, while on the (100) surface the O prefers on the bridge site with a strong bond with N, which is hard to break to form OOH.

As shown in Figure 5, under 4% tensile uniaxial strain, the theoretical overpotential decreases from 0.97 to 0.69 V for the clean surface, while when 4% compressive uniaxial strain is applied, the theoretical overpotential change from 0.78 to 0.59 V for the full OH covered surface (most stable under operating condition shown in Figure S4b). Doping can be a valuable alternative to strain to modulate the theoretical overpotentials. Since for clean (001) TaON surface, tensile uniaxial strain could reduce the theoretical overpotential to only 0.69 V, we attempt to further decrease the theoretical overpotential, by combining the substitution of Ba with isovalent elements with smaller radii and strain. We thus replace a sublayer Ba with Ca and Sr. It should be noted that doping alone only has a small effect on the OER activities. Sr-doping slightly reduces the theoretical overpotential from 0.97 V to 0.90 V, and Ca-doping further reduces it to 0.88 V. Moreover, combing with 4% tensile uniaxial strain, the smallest theoretical overpotential is reached for the Ca-doping on the clean surface (0.53 V), which results from $\Delta G_{O^*} - \Delta G_{OH^*}$ increasing with doping and strain. All structures with full OH coverage surface are already on the right branch of the volcano and 4% compressive strain is not enough to reach
the top of the volcano. In general, this facet requires larger strain compared to the (100) facet, which might be hard to achieve experimentally.

**Figure 5.** Volcano plot of the free-energy difference of \( \Delta G_{O^*} - \Delta G_{OH^*} \) and the OER theoretical overpotential \( \eta \) for both TaON-terminated (001) clean and full OH\(^*\) covered surfaces. The uniaxial strain is in [010] direction.

**Conclusions**

In this work, we have investigated the effect that doping and strain engineering have on the oxygen evolution reaction for different terminations of the perovskite oxynitride BaTaO\(_2\)N. For the (100) facet TaO\(_2\)N-terminated, under (photo)electrochemical conditions, we have discovered that 1\% tensile uniaxial strain in the [001] direction can lower the theoretical
overpotential to 0.37 V, from 0.43 V calculated for the structure without any applied strain. The (001) facet shows larger theoretical overpotentials compared to the (100). As an attempt to reduce them, we apply stain, reaching an theoretical overpotential of 0.59 V, under operational conditions, which however is still larger than what we can achieve for the (100) facet. The reason of the difference between the (100) and (001) facets is related with the different anion orderings on the surface. By applying a small strain of 1%, which can be easily reached in experiments, this work provides the guidelines to experimentalists on how we can tune surface chemistry and optimize the OER catalytic properties of the material only by controlling anion ordering, strain, and doping.

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**Notes**

The authors declare no competing financial interest.
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Promoting OER activity

Strain
Doping
Anion ordering