RuO$_2$ Monolayer: A Promising Bifunctional Catalytic Material for Nonaqueous Lithium–Oxygen Batteries

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Supporting Information

ABSTRACT: Rutile RuO$_2$ has been widely regarded as an excellent catalyst for the oxygen reduction reaction (ORR) and oxygen evolution reaction (OER) in nonaqueous lithium–oxygen batteries and achieved superior performance, but the catalytic activity of RuO$_2$’s polymorph, RuO$_2$ monolayer, has been less studied. In this work, we study the catalytic activities of both rutile RuO$_2$ and RuO$_2$ monolayer for ORR and OER in the battery using density functional theory method. Computational results show that the RuO$_2$ monolayer exhibits a higher catalytic activity than the rutile RuO$_2$ does. More interestingly, it is found that during discharge a similar lattice structure between RuO$_2$ monolayer and Li$_2$O$_2$ {0001} surface can induce the formation of crystallized Li$_2$O$_2$ with the conductive {0001} surface exposed, whereas during charge the RuO$_2$ monolayer can attract the remaining Li$_2$O$_2$ to its surface spontaneously, thus maintaining the solid–solid reaction interface. Our results suggest that the RuO$_2$ monolayer is a promising catalytic material for nonaqueous lithium–oxygen batteries.

1. INTRODUCTION

Nonaqueous lithium–oxygen batteries have attracted increasing attention because of their superhigh specific capacities; however, as an infant stage technology, this novel energy-storage system is still suffering from several severe issues, such as the high charge overpotential, sluggish reaction kinetics, and poor cycling stability, which seriously hindered its commercialization. A common strategy to solve these issues is using catalyst to lower the charge overpotential and accelerate the reactions, which could also alleviate the decomposition of electrolyte and cathode materials, thus enhancing cycling stability. Many possible catalysts have been tested among which rutile RuO$_2$ is a popular candidate for its superior catalytic activity and good chemical stability in the highly oxidative environment of nonaqueous lithium–oxygen batteries. As the polymorph of rutile RuO$_2$, RuO$_2$ monolayer exfoliated from lamellar ruthenates is also conductive and has been used as super capacitor and catalyst for the oxygen reduction reaction (ORR) in aqueous system. Being a 2D metal oxide, RuO$_2$ monolayer can achieve a large surface-to-mass ratio and exist stably during the operation of nonaqueous lithium–oxygen batteries. It is also expected to catalyze the reactions uniformly without the necessity to introduce defects or functional groups as carbon material does, making it a possible candidate for the catalyst or catalytic cathode of nonaqueous lithium–oxygen batteries. Recently, Liao et al. used lamellar ruthenate as a precursor to obtain RuO$_2$ nanosheet to be a catalytic cathode of nonaqueous lithium–oxygen batteries and achieved excellent performance. In their experiment, however, a considerable amount of exfoliated RuO$_2$ monolayer went through phase change and turned to rutile RuO$_2$ during the heat treatment process. Thus, whether RuO$_2$ monolayer contributed to the excellent performance is still unclear. Further detailed computational and experimental investigations are needed to identify whether RuO$_2$ monolayer is a promising effective catalytic material for nonaqueous lithium–oxygen batteries.

In this work, using density functional theory (DFT) method, we investigated the catalytic activities of both rutile RuO$_2$ and RuO$_2$ monolayer for the ORR and oxygen evolution reaction (OER) in nonaqueous lithium–oxygen batteries. The dominant surface of rutile RuO$_2$ was identified according to the Wulff construction to be representative in the study of the catalytic activity of rutile RuO$_2$. The adsorption behaviors of the lithium ion, intermediate discharge product Li$_2$O$_2$, and discharge product Li$_2$O$_2$ on both RuO$_2$ monolayer and the dominant surface of rutile RuO$_2$ were investigated to study the initial discharge process. The electronic properties of RuO$_2$ monolayer before and after the deposition of different layers of Li$_2$O$_2$ were obtained to study the following discharge process when Li$_2$O$_2$ accumulates after the initial deposition. Interfacial models among RuO$_2$ monolayer or the dominant surface of rutile RuO$_2$, Li$_2$O$_2$, and electrolyte were built to study the charge process.

2. COMPUTATIONAL DETAILS

DFT calculations were performed using the ABINIT software package with the projector-augmented-wave (PAW) method.
method\textsuperscript{26} and Perdew—Burke—Ernzerhof (PBE) generalized gradient approximation (GGA).\textsuperscript{27} The cutoff energy for the plane-wave basis was 20 Ha. Monkhorst—Pack scheme\textsuperscript{30} was used for the k-point sampling, and the spacing of the k-point mesh was set to be 0.05 Å\textsuperscript{-1}. All atoms were relaxed to a force tolerance of 0.02 eV Å\textsuperscript{-1} or less for the geometric optimization. The Bader charge partition analysis\textsuperscript{29,30} implemented in the ABINIT software was employed to study the related charge transfer. The density of states (DOS) were calculated using Heyd—Scuseria—Ernzerhof (HSE) hybrid density functional\textsuperscript{31,32} implemented in Quantum Espresso package.\textsuperscript{33} One-quarter (\(\alpha = 0.25\)) of the local DFT exchange was replaced by the unscreened and nonlocal Fock exchange.

The crystal structure of RuO\(_2\) montolayer was obtained by modifying the crystal structure of Na\(_x\)RuO\(_2\)-yH\(_2\)O.\textsuperscript{34} The optimized lattice parameters of RuO\(_2\) monolayer (listed in Table S1) agree well with experimental reports.\textsuperscript{19} The crystal structure of rutile RuO\(_2\) and Li\(_2\)O\(_2\) was taken from experimental results.\textsuperscript{35,36} Slab model adding vacuum layers was used to calculate the surface energies. All slabs are symmetrized and contain more than seven repeating layers with a vacuum layer thicker than 10 Å to achieve convergence within 1 meV Å\textsuperscript{-2} for the surface energies. The surface energies were calculated by

\[
\gamma = \frac{1}{2A} \left[ G_{\text{slab}} - N_{\text{Ru}} \mu_{\text{Ru}}^{\text{bulk}} - N_{\text{O}} \mu_{\text{O}}^{\text{bulk}} \right] \tag{1}
\]

where \(A\) is the slab surface area, \(G_{\text{slab}}\) is the total free energy of the slab supercell, \(N_{\text{Ru}}\) and \(N_{\text{O}}\) are the numbers of ruthenium and oxygen atoms, and \(\mu_{\text{Ru}}^{\text{bulk}}\) and \(\mu_{\text{O}}^{\text{bulk}}\) are the chemical potentials of ruthenium and oxygen atoms, respectively. The chemical potentials of RuO\(_2\) are correlated by

\[
\mu_{\text{O}_2}(T, P_{\text{O}_2}) = H_{\text{O}_2}(0 \text{ K}) + \Delta H_{\text{O}_2}(T) - T S_{\text{O}_2}^{\text{exptl}}(T) + k_B T \ln \left( \frac{P_{\text{O}_2}}{P_{\text{O}_2}^{\text{exptl}}} \right) \tag{7}
\]

where \(\Delta H_{\text{O}_2}(T)\) is the enthalpy energy change from 0 K to \(T\), for which we used diatomic ideal gas approximation as \(7/2k_B T\), and \(S_{\text{O}_2}^{\text{exptl}}(T)\) the entropy of oxygen at 1 atm and different temperatures obtained from experiments.\textsuperscript{39} \(P_{\text{O}_2}\) is set to be 1 atm.

The energy profiles of the ORR/OER process were calculated by adding/removing a lithium atom or an oxygen molecule at each step. The reaction free energy of intermediate steps was calculated by

\[
\Delta G = E - E_0 + \Delta N_{\text{Li}} (\mu_{\text{Li}} - eU) + \Delta N_{\text{O}_2} \mu_{\text{O}_2} \tag{8}
\]

where \(E\) is the total energy of the considered slab model, \(E_0\) is the total energy of the initial slab model, \(\Delta N_{\text{Li}}\) and \(\Delta N_{\text{O}_2}\) are the numbers of lithium atoms and oxygen molecules added/removed for each step, and \(\mu_{\text{Li}}\) and \(\mu_{\text{O}_2}\) are the chemical potentials of lithium bulk and oxygen, respectively. The \(eU\) term was added to account for the electronic energy under applied potential \(U\). The overpotential was defined by shifting all intermediates to \(\Delta G < 0\), which is consistent with previous works.\textsuperscript{40–42}

3. RESULTS AND DISCUSSION

3.1. Representative Surface of Rutile RuO\(_2\). To identify the stable surfaces of rutile RuO\(_2\) in the operation condition of nonaqueous lithium—oxygen batteries, we calculated the surface energies of \{001\}, \{100\}, \{101\}, \{110\}, and \{111\} surfaces with different terminations (as shown in Figure S1). The calculated surface energies under different oxygen chemical potentials are shown in Figure 1a. Because nonaqueous lithium—oxygen batteries operate in an oxygen-rich condition, here we take the surface energies when \(P_{\text{O}_2} = 1\) atm to construct the Wulff structure of rutile RuO\(_2\). From the Wulff shape shown in Figure 1b, it can be found that the \{001\} surface occupies most of the...
exposed surface area. Thus, in the following, we will take the (001) surface as a representative of rutile RuO₂ to study its catalytic activities toward the ORR and OER in nonaqueous lithium—oxygen batteries.

3.2. Initial Discharge Process on RuO₂ (001) and RuO₂ Monolayer. It is now widely agreed that the ORR in nonaqueous lithium—oxygen batteries goes through a two-step reaction. In the first step, the oxygen molecular will complex with a lithium ion and get an electron to form lithium superoxide as

\[
\text{Li}^+ + \text{O}_2 + e^- \rightarrow \text{LiO}_2
\]  

(step 1)

Then, the formed LiO₂ could either go through an electrochemical reaction route and be further reduced to Li₂O₂ as

\[
\text{LiO}_2 + \text{Li}^+ + e^- \rightarrow \text{Li}_2\text{O}_2
\]  

(step 2.1)

or go through a chemical disproportionation reaction route as

\[
2\text{LiO}_2 \rightarrow \text{Li}_2\text{O}_2 + \text{O}_2
\]  

(step 2.2)

The electrochemical reactions take place only on the catalytic surfaces, whereas the chemical disproportionation reaction can happen anywhere. It is commonly believed that the large compact toroid Li₂O₂ particles resulted from the chemical disproportionation reactions that happened in electrolyte. From our calculation results on the adsorption behaviors of Li⁺+e⁻, LiO₂, and Li₂O₂ onto both RuO₂ monolayer and rutile RuO₂ {001} surface, as listed in Table 1, it can be found that in the both cases the adsorption energies of LiO₂ are quite large. The large adsorption energies of LiO₂ could confine all reactions onto the surfaces in the initial stage of discharge process, rather than letting the LiO₂ dissolve into the electrolyte and disproportionate into Li₂O₂, thus effectively suppressing the formation of large compact toroid particles that are hard to be charged back. So, in this study, we only consider the disproportionation reactions that happened on the surfaces.

Table 1. Adsorption of Li⁺+e⁻, LiO₂, and Li₂O₂ onto the RuO₂ Monolayer and Rutile RuO₂ {001} Surface, Respectively

<table>
<thead>
<tr>
<th>adsorbate</th>
<th>RuO₂ monolayer</th>
<th>RuO₂{001}</th>
<th>RuO₂ monolayer</th>
<th>RuO₂{001}</th>
<th>RuO₂ monolayer</th>
<th>RuO₂{001}</th>
</tr>
</thead>
<tbody>
<tr>
<td>Li⁺+e⁻</td>
<td>−5.27</td>
<td>−3.67</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>LiO₂</td>
<td>−4.18</td>
<td>−2.21</td>
<td>1.27</td>
<td>1.24</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Li₂O₂</td>
<td>−5.02</td>
<td>−3.29</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The detailed reaction route for the disproportionation reaction occurring on the surfaces can be much more complex. Here we consider only the reaction enthalpy change for an initial evaluation by defining the formation heat following Geng et al.’s approach as

\[
E_{\text{dis}} = E_{\text{Li}_2\text{O}_2@\text{surf}} - 2E_{\text{LiO}_2@\text{surf}} + E_{\text{surf}} + E_{\text{O}_2}
\]  

(step 2.2)

where \(E_{\text{O}_2}, E_{\text{LiO}_2@\text{surf}}\) and \(E_{\text{Li}_2\text{O}_2@\text{surf}}\) represent the energy of oxygen molecule, considered surface, considered surface adsorbed with LiO₂ and considered surface adsorbed with Li₂O₂, respectively. The calculated \(E_{\text{dis}}\) for the disproportionation reactions that happened on the RuO₂ monolayer is +3.17 eV, and for the rutile RuO₂ {001} surface it is +0.953 eV, which means the disproportionation reactions on both surfaces are endothermic and can hardly be realized.

We now discuss the electrochemical route. As for both the RuO₂ monolayer and rutile RuO₂ {001}, all ruthenium atoms are coordinatively saturated, making the initial adsorption of oxygen not preferred, which can be further confirmed by the bond lengths of adsorbed oxygen molecules onto the surfaces, as shown in Figures S3 and S4. Thus, we study the electrochemical ORR in nonaqueous lithium—oxygen batteries by taking the reaction route \(\text{Li} \rightarrow \text{LiO}_2 \rightarrow \text{Li}_2\text{O}_2\). The corresponding energy profiles for this process on different surfaces are shown in Figure 2. For both RuO₂ monolayer and rutile RuO₂ {001} surface, the ORR following the electrochemical reaction route are thermodynamically favored. Figure 2a shows the energy profiles of the ORR on the RuO₂ monolayer at an open-circuit potential \(U = 0\ V\), the highest voltage at which discharging is energetically downhill for all steps \(U = 2.51\ V\), the equilibrium voltage of bulk Li₂O₂ \(U = 2.96\ V\), and the equilibrium voltage for the initial discharge process, which could just keep all of the intermediates having a negative energy \(U = 3.95\ V\). Figure 2b presents the energy profiles of the ORR on the rutile RuO₂ {001} surface at an open-circuit potential \(U = 0\ V\), the equilibrium voltage of

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bulk Li2O2 (U = 2.96 V), and the equilibrium voltage for the initial discharge process, which could just keep all of the intermediates having a negative energy (U = 3.08 V). It can be found that the equilibrium voltage for the electrochemical ORR on RuO2 monolayer is as high as 3.95 V, much higher than that of the equilibrium voltage on rutile RuO2 {001} (3.08 V), indicating a higher catalytic activity of RuO2 monolayer toward the electrochemical ORR process. This result may also explain the experimental discharge curve of Liao et al., where an initial discharge voltage higher than 3.5 V was observed (corresponding to the equilibrium voltage as high as 3.95 V in the initial stage of the discharge process) and gradually drop down to a voltage plateau below 2.96 V (corresponding to the equilibrium voltage of the following discharge process that happened on Li2O2 surface after RuO2 monolayer surface was fully covered by discharge product). The reverse process of the initial discharge process is the charge process in its final stage, when there is only a very small number of Li2O2 molecules adsorbed onto the surfaces waiting to be removed, corresponding to a high ending charge voltage for RuO2 monolayer, which also agrees with the experimental observation. The geometry change along with the initial discharge process on the surfaces is shown in Figure 3.

Figure 3. Geometries for the initial discharge process happened on (a) the surface of RuO2 monolayer and (b) rutile RuO2 {001} surface.

### 3.3. Electronic Conductance of RuO2 Monolayer Deposited with Li2O2.

As the discharge goes on, the active surfaces will be covered by Li2O2 and show little influence toward the following discharge process (shown in Figures S5 and S6). From the results of our previous work, the surface of Li2O2 also has a strong adsorption ability toward Li2O2, and thus the following ORR reactions will mainly take place at the surfaces of Li2O2. Because Li2O2 bulk is insulator, the electronic conductivity of Li2O2 will become the main limiting factor for the following ORR.1–6 For rutile RuO2, its lattice structure and lattice parameters are quite different from those of Li2O2, which could induce the formation of amorphous Li2O2 and increase the electronic conductivity through the formation of grain boundaries.15,45

For RuO2 monolayer, it should be noted that the crystal structures of Li2O2 {0001} surface and RuO2 monolayer are similar, and their lattice parameters are quite close, as listed in Table S1. Considering that lithium atoms tend to adsorb onto the hcp hollows formed by the Ru atoms (shown in Figure 3a) and {0001} surface is the dominant surface of Li2O2 in its equilibrium Wulff structure,8,42,44 we propose that after the initial deposition process the formed Li2O2 is very likely to adsorb onto the surface of RuO2 monolayer in the way shown in Figure 4. In this way, the optimized lattice parameters of Li2O2 after adsorbed onto RuO2 monolayer are quite close to that of bulk Li2O2 (as shown in Figure S7).

We now present the study on electronic conductivity of RuO2 before and after the deposition of one, three, and five layers of Li2O2. HSE hybrid density functional was used to get accurate band information.31,32 The constructed models and calculated DOS maps are shown in Figure 4. According to the calculation results, RuO2 monolayer is a metallic material (Figure 4a), which is consistent with experimental observations.18–21 After the deposition of one layer of Li2O2, the RuO2 monolayer and the deposited Li2O2 are both conductive (Figure 4b). If we continue to increase the Li2O2 deposition (Figures 4c,d), the RuO2 monolayer will still be conductive, while the conductive Li2O2 layer will shift up to the top layer exposed, which will be further away from RuO2. At the same time, the Li2O2 layer in contact with the RuO2 monolayer will exhibit to be an insulator with a band gap larger than 4.0 V, which is similar to that of bulk Li2O2.48,49 This phenomenon is consistent with the previous result that the {0001} surface of Li2O2 is conductive.38 The surface conductivity would provide an electron pathway for the following discharge process.

Because a small lattice mismatch between Li2O2 and RuO2 monolayer exists, the strain caused by lattice mismatch will become larger as the adsorbed Li2O2 grows thicker.50 This strain may induce the generation of defects and grain boundaries, which could further enhance the electronic conductivity.49,51 The {111} surface of previously reported cathode material for nonaqueous lithium–oxygen batteries, TiC, also has s similar lattice structure and a small lattice mismatch compared with the Li2O2 {0001} surface.52 It is quite interesting to notice that the discharge product morphologies on TiC cathode53 and RuO2 nanosheet cathode22 are also similar; in both cases, a rare morphology of assembled thin discs was observed. We propose that this morphology may be caused by the stripping of Li2O2 along the {0001} surface to relieve the internal strain, as shown in Figure S8, just as those observed in heteroepitaxial growth experiments.50,54,55

### 3.4. Charge Process on Rutile RuO2 {001} and RuO2 Monolayer.

The involvement of solid-state discharge product makes the ORR and OER in nonaqueous lithium–oxygen...
batteries asymmetric. As previously mentioned, the adsorption models built above to study the initial discharge process could also be used to interpret the end stage of the charge process but obviously not the beginning and middle stages. To describe the charge process more accurately, while keep the computational efforts reasonable, we built solid–solid interface models following Zhu et al.’s approach. The same amount of nanoscale Li$_2$O$_2$ was put onto both RuO$_2$ monolayer and rutile RuO$_2$ {001} surface, with {0001} surface of Li$_2$O$_2$ in contact with them. After geometry optimization, for the rutile RuO$_2$ {001} surface, the adsorbed Li$_2$O$_2$ showed a tilt to fit the large lattice mismatch, as shown in Figure S9; for RuO$_2$ monolayer, one of the oxygen–oxygen bonds near the interface was cleaved due to the lithium-rich termination.

According to previous studies, the OER in nonaqueous lithium–oxygen batteries takes place at the three-phase interface of cathode/Li$_2$O$_2$/O$_2$. Thus, we chose a unit cell of Li$_2$O$_2$ near the RuO$_2$ monolayer or rutile RuO$_2$ {001} surface/Li$_2$O$_2$/electrolyte interface to study the OER mechanism. Two possible reaction routes, namely, Li$^+ \rightarrow$ Li$^+$ → O$_2$ (route 1) and Li$^+$ → O$_2$ → Li$^+$ (route 2) were considered accordingly. The energy profiles for these two different routes are shown in Figure S5. For RuO$_2$ monolayer, as shown in Figure S5a, the equilibrium voltage for route 1 is 2.82 V, much lower than that of 6.48 V for route 2. For rutile RuO$_2$ {001} surface, as shown in Figure S5b, the equilibrium voltage for route 1 is 3.08 V, which is quite close to the charge voltages reported in experiments and a bit lower than that of 3.30 V for route 2. Thus, route 1 will be the preferred reaction route in both situations. The equilibrium charge voltage for RuO$_2$ monolayer is lower than that of rutile RuO$_2$ {001} surface, indicating a higher catalytic activity during the initial and middle stages of the charge process.

The geometry changes of the adsorbed Li$_2$O$_2$ along with the charge process following the route 1 are shown in Figure 6. It is quite interesting to find that for RuO$_2$ monolayer, as shown in Figure 6a, after the removal of one unit cell of Li$_2$O$_2$, the remaining Li$_2$O$_2$ will be attracted to move toward the RuO$_2$ monolayer spontaneously (the center of mass of the adsorbed Li$_2$O$_2$ moves toward the RuO$_2$ layer about 0.2 Å), while similar behavior cannot be observed for the rutile RuO$_2$ {001} surface, as shown in Figure 6b (the center of mass of the adsorbed Li$_2$O$_2$ moves away from the RuO$_2$ {001} surface about 0.4 Å).

**4. CONCLUSIONS**

In summary, we comparatively investigated the ORR and OER in nonaqueous lithium–oxygen batteries occurring on both the surface of RuO$_2$ monolayer and rutile RuO$_2$. The calculation results show that in nonaqueous lithium–oxygen batteries, RuO$_2$ monolayer exhibits higher catalytic activity in both ORR and OER than rutile RuO$_2$ does. In addition, during discharge, the similar lattice structure between RuO$_2$ monolayer and Li$_2$O$_2$ {001} can induce the conductive Li$_2$O$_2$ {001} surface to expose, and the small lattice misfit can facilitate the electron transportation through the formation of defects or grain boundaries due to the internal strain, whereas during charge the RuO$_2$ monolayer can attract the adsorbed Li$_2$O$_2$ to move toward its surface to maintain the solid–solid reaction interface.

We propose that this attraction effect could help maintain the solid–solid reaction interface until all adsorbed Li$_2$O$_2$ is decomposed. Gittleson et al. observed that for the gold cathode, after the beginning stage of the charge process when the first layer of Li$_2$O$_2$ was consumed, the remaining Li$_2$O$_2$ would be in poor contact with the cathode and can hardly be charged back. Our calculation results show that the vanishing of the reaction interface along with the charge process is unlikely to happen when the reactions take place on the surface of RuO$_2$ monolayer.

Figure 5. Energy profiles for the charge process of Li$_2$O$_2$ happened on (a) the surface of RuO$_2$ monolayer and (b) rutile RuO$_2$ {001} surface following two possible reaction routes.

Figure 6. Geometries for the charge process following route 1 happened on (a) the surface of RuO$_2$ monolayer and (b) rutile RuO$_2$ {001} surface.
promising catalytic material for nonaqueous lithium–oxygen batteries. Further experimental and computational explorations on the application of RuO$_2$ monolayer as well as other cheaper 2D metal oxide materials in nonaqueous lithium–oxygen batteries are expected.

**ASSOCIATED CONTENT**

*Supporting Information*

The Supporting Information is available free of charge on the ACS Publications website at DOI: 10.1021/acs.jpcc.6b00014.

Optimized lattice parameters of Li$_2$O$_2$, RuO$_2$ monolayer, and rutile RuO$_2$. The orientations and terminations of rutile RuO$_2$ considered for the Wulff construction. Surface energies of different orientations and terminations of rutile RuO$_2$ under different oxygen chemical potentials. Optimized geometry for oxygen molecular adsorbed onto the surface of RuO$_2$ monolayer. Optimized geometry for oxygen molecular adsorbed onto rutile RuO$_2$ {001} surface. Optimized geometry of discharge process happened on Li$_2$O$_2$ {0001} surface with and without RuO$_2$ monolayer. Energy profile for the discharge process happened on the Li$_2$O$_2$ {0001} surface with and without RuO$_2$ monolayer. Optimized lattice parameters of Li$_2$O$_2$ before and after adsorption onto RuO$_2$ monolayer. Illustration for proposed formation mechanism for the assembled thin disc morphology of Li$_2$O$_2$. The geometries of the interfacial model of rutile RuO$_2$ {001} surface and Li$_2$O$_2$ {0001} surface before and after optimization. (PDF)

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Notes

The authors declare no competing financial interest.

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