Supporting Information for

Coulomb Explosion Strategy to Tailor Nano-architecture of α-MoO₃ Nanobelts and Insight of its Intrinsic Mechanism

Junli Zhang¹, Liu Zhu¹, Yu Yang², Huadong Yong², Junwei Zhang¹, Yong Peng¹*, Jiecai Fu¹*

¹Key Laboratory of Magnetism and Magnetic Materials of the Ministry of Education, School of Physical Science and Technology, Lanzhou University, Lanzhou 730000, P. R. China

²Key Laboratory of Mechanics on Disaster and Environment in Western China attached to the Ministry of Education of China, Department of Mechanics and Engineering Sciences, College of Civil Engineering and Mechanics, Lanzhou University, Lanzhou, 730000, China

* Corresponding authors

Key Laboratory of Magnetism and Magnetic Materials of the Ministry of Education, Lanzhou University, Lanzhou 730000, P. R. China

E-mail: pengy@lzu.edu.cn (Yong Peng) and fujc@lzu.edu.cn (Jiecai Fu)
Figure S1. Bandgap analysis of the $\alpha$-MoO$_3$ nanobelts. UV-visible diffuse absorbance spectra of the $\alpha$-MoO$_3$ nanobelts. The bandgap of the $\alpha$-MoO$_3$ nanobelts can be estimated by the UV-visible adsorption results,$^{[1]}$ which shows that the bandgap value is about 3.1 eV. It demonstrates the semiconductor properties of $\alpha$-MoO$_3$ nanobelts with high resistivity, and it is possible to be engineered by the Coulomb explosion.

Figure S2. Nanopattern tailored on the $\alpha$-MoO$_3$ NB by EBI. (a) Representative TEM image of an ultrathin $\alpha$-MoO$_3$ NB; (b) TEM image of three gaps tailored on the NB with 100 nm lateral size.
Figure S3. Thickness and chemical analysis of the peeled-off $\alpha$-MoO$_3$. (a) EELS low loss spectra of the peeled-off layers, which thickness can be calculated from the ratio of zero-loss peak and plasmonic peak; (b) EELS core loss spectra of the peeled-off layers recorded with a energy dispersion of 0.25 eV/pixel to highlight the peak position and shape of the Mo-M$_{4,5}$, Mo-M$_{2,3}$ and O-K edges; The energy-loss near-edge structures (ELNES) of the Mo-M$_{2,3}$ edges (c) and O-K edges (d).

**Thickness and chemical analysis of the peeled-off $\alpha$-MoO$_3$**

**Thickness calculation.** The thickness of TEM specimen (e.g., the thickness of the peeled-off layer, $t$) can be calculated by a straightforward integration of the EELS low loss spectrum. The local thickness $t$ calculation based on the log-ratio formula is expressed as:[2]

$$t = \lambda \ln(I_t / I_0)$$  \hspace{1cm} (1)

where, $I_t$ and $I_0$ are the total and zero-loss areas in the low-loss region of EELS spectrum, respectively. $\lambda$ is the total inelastic mean free path, which can be formulated as:

$$\lambda = 106F(E_0 / E_\alpha) / \ln(2\beta E_0 / E_\alpha)$$  \hspace{1cm} (2)

It is noted that $F = (1 + E_0 / 1022) / (1 + E_0 / 511)^2$, $E_0$ is the incident energy of electron beam, $\beta$ is
the spectrum collection semi-angle, \( E_m = 7.6Z^{0.36} \) and \( Z \) is the atomic number. According to the above equations and the collected parameters from the EELS spectrum in Figure S3a, the thickness of the peeled-off \( \alpha\)-MoO\(_3\) structure can be calculated to be about 2.1 nm, well matching a mono-layer thickness of \( \alpha\)-MoO\(_3\).

**Table S1.** Comparison of Mo-M\(_3\) edge, the peak difference (i.e., M\(_3\)---M\(_2\)) between the Mo-M\(_3\) edge and the Mo-M\(_2\) edge, and the peak difference (Mo-M\(_3\)---O-K) between the Mo-M\(_3\) edge and the O-K edge with the references of stoichiometric MoO\(_3\) and MoO\(_2\).

<table>
<thead>
<tr>
<th>Chemical compositions</th>
<th>Mo-M(_3) (eV)</th>
<th>M(_3)---M(_2) (eV)</th>
<th>Mo-M(_3)---O-K (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Peeled-off MoO(_x)</td>
<td>397.5</td>
<td>16.6</td>
<td>131.8</td>
</tr>
<tr>
<td>MoO(_3)[4]</td>
<td>397.8</td>
<td>16.8</td>
<td>131.6</td>
</tr>
<tr>
<td>MoO(_2)[4]</td>
<td>397.7</td>
<td>16.5</td>
<td>132.2</td>
</tr>
</tbody>
</table>

**Chemical composition analysis.** The chemical compositions of the molybdenum oxides can be determined from the analysis of O-K and Mo-M edges of EELS spectra.[3] Figure S3b shows the EELS core-loss spectrum collected from the peeled-off materials, in which the peak positions and shapes of the Mo-M\(_{4,5}\), Mo-M\(_{2,3}\) and O-K edges demonstrating the chemical composition of the molybdenum oxide. Herein, we select the Mo-M\(_{2,3}\) edge to quantify the element and valence because it is shaper than the Mo-M\(_{4,5}\) edge and closer to the O-K edge. The ELNES spectrum of the Mo-M\(_{2,3}\) edge in Figure S3c shows two peaks at 397.5 eV and 414.1 eV, corresponding to the M\(_3\), M\(_2\) edges of Mo element, respectively. The energy difference between the Mo-M\(_3\) edge and Mo-M\(_2\) edge is the criteria to judge the oxidation state of Mo element, which is calculated to be 16.6 eV. Besides, the peak difference between the Mo-M\(_3\) edge and the O-K edge (peak at 529.3 eV in Figure S3d) is another criteria, which is 131.8 eV. It is clear to find that the peeled-off layer is a sub-stoichiometric molybdenum oxide (i.e. MoO\(_x\), 2<x<3) with low oxygen vacancy concentration based on the references of stoichiometric MoO\(_3\) and MoO\(_2\) in Table S1[4]. Thus, this result proves that the oxygen can be knocked from the \( \alpha\)-MoO\(_3\) NB by electron beam but with a low vacancy concentration.
REFERENCE


