Supporting Information

## α-MoO3-*x* by Plasma Etching with Improved Capacity and Stabilized Structure for Lithium Storage

Guobin Zhang,a,# Tengfei Xiong,a,# Mengyu Yan,b Liang He,a,c Xiaobin Liao,a Chunqing He,d Chongshan Yin,d Haining Zhang,e and Liqiang Mai\*a

a State Key Laboratory of Advanced Technology for Materials Synthesis and Processing & International School of Materials Science and Engineering, Wuhan University of Technology, Wuhan 430070, China. E-mail: mlq518@whut.edu.cn

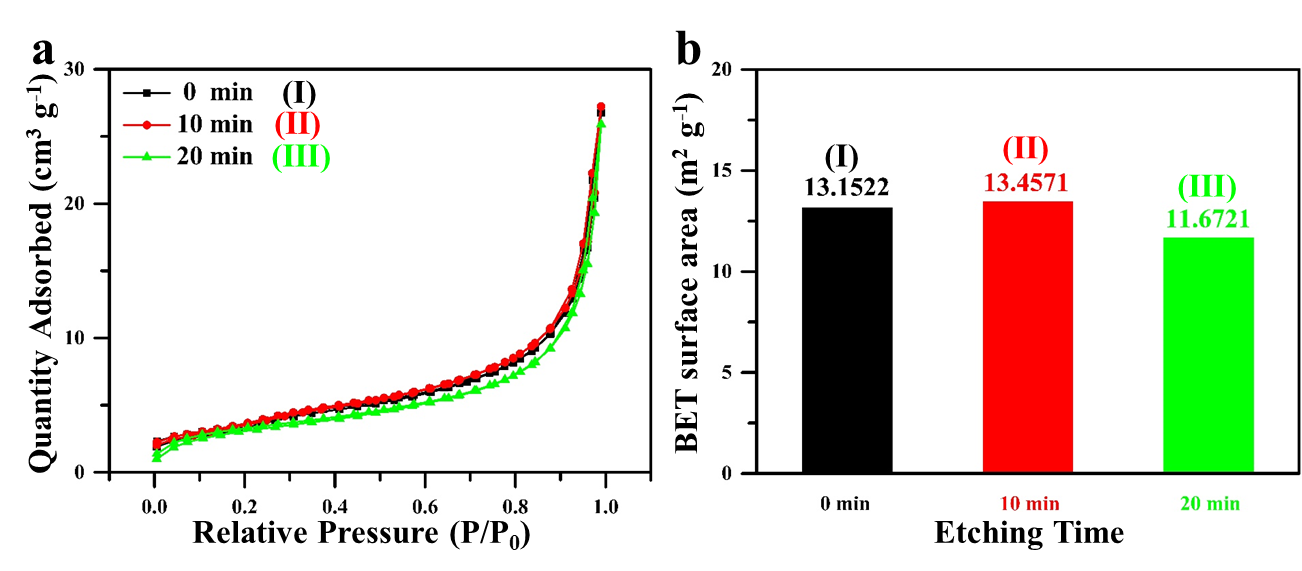
b Department of Materials Science and Engineering, University of Washington, Seattle, WA 98195, USA

c Department of Materials Science and NanoEngineering, Rice University, Houston, TX 77005, USA

d Key Laboratory of Nuclear Solid State Physics Hubei Province, School of Physics and Technology, Wuhan University, Wuhan 430072, China

e State Key Laboratory of Advanced Technology for Materials Synthesis and Processing & School of Materials Science and Engineering, Wuhan University of Technology, Wuhan 430070, China

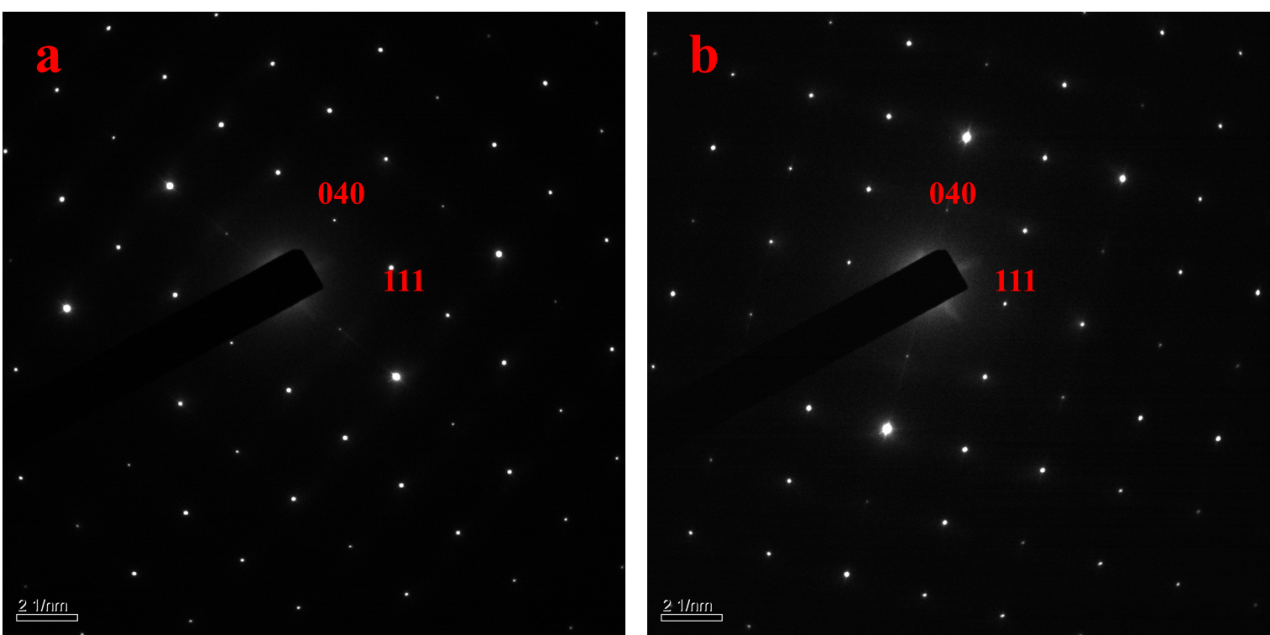
# Guobin Zhang and Tengfei Xiong contributed equally to this work.



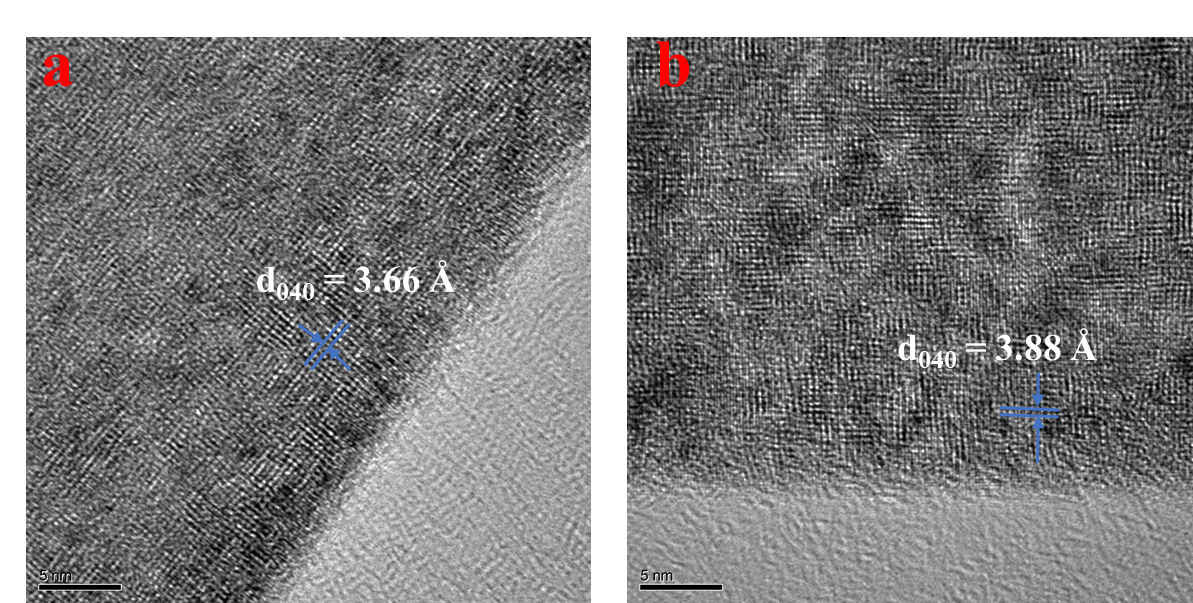
**Figure S1** (a) Nitrogen adsorption-desorption isotherms and (b) BET specific surface areas.

**Table S1** Assignment of vibrational modes of the Raman spectra (unit: cm-1).

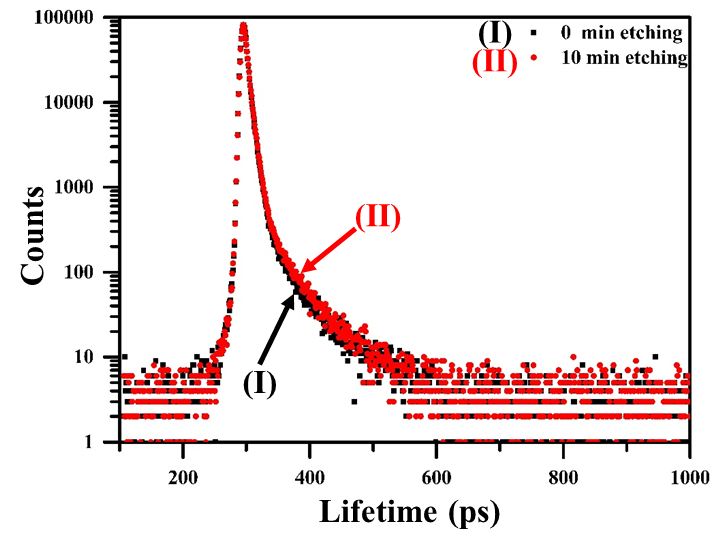
|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| This work | | | Others  [30-33] | Assignment |
| (I) | (II) | (III) |
| 83.5 | 85.0 | 84.2 | 89 | Ag, translational rigid MoO4 chain mode, Ta |
| 98.4 | 99.2 | 100.0 | 100 | B2g, translational rigid MoO4 chain mode, Ta |
| 117.1 | 118.1 | 117.3 | 116 | B2g, translational rigid MoO4 chain mode, Tc |
| 128.6 | 129.9 | 129.1 | 129 | B3g, translational rigid MoO4 chain mode, Tc |
| 159.7 | 158.9 | 158.9 | 159 | Ag/B1g, translational rigid MoO4 chain mode, Tb |
| 197.0 | 198.7 | 198.7 | 197 | B2g, *τ* O=Mo=O twist |
| 218.8 | 219.7 | 219.7 | 216 | Ag, rotational rigid MoO4 chain mode, Rc |
| 245.4 | 245.3 | 246.8 | 247 | B3g, *τ* O=Mo=O twist |
| 291.8 | 292.3 | 291.5 | 293 | B3g, *δ* O=M=O wagging |
| 338.5 | 339.8 | 339.8 | 334 | Ag, B1g, *δ* O–M–O bend |
| 379.6 | 380.1 | 379.4 | 380 | B1g, *δ* O–M–O scissor |
| 430.6 | 431.6 | 430.8 | 441 | Mo–O–Mo deformation |
| 665.4 | 666.8 | 666.8 | 667 | B2g, B3g, *ν*as O–M–O stretch |
| 707.1 | 709.0 | 709.8 | 698 | Unknown |
| 819.5 | 821.4 | 820.7 | 823 | Ag, *ν*s M=O stretch |
| 995.7 | 997.1 | 997.1 | 996 | Ag, *ν*as M=O stretch |
|  | 1007.6 | 1008.3 | 1008 | Bg, *ν*as M=O stretch |



**Figure S2** Selected area electron diffraction of the pristine (a) and the MoO3 (II) (b).



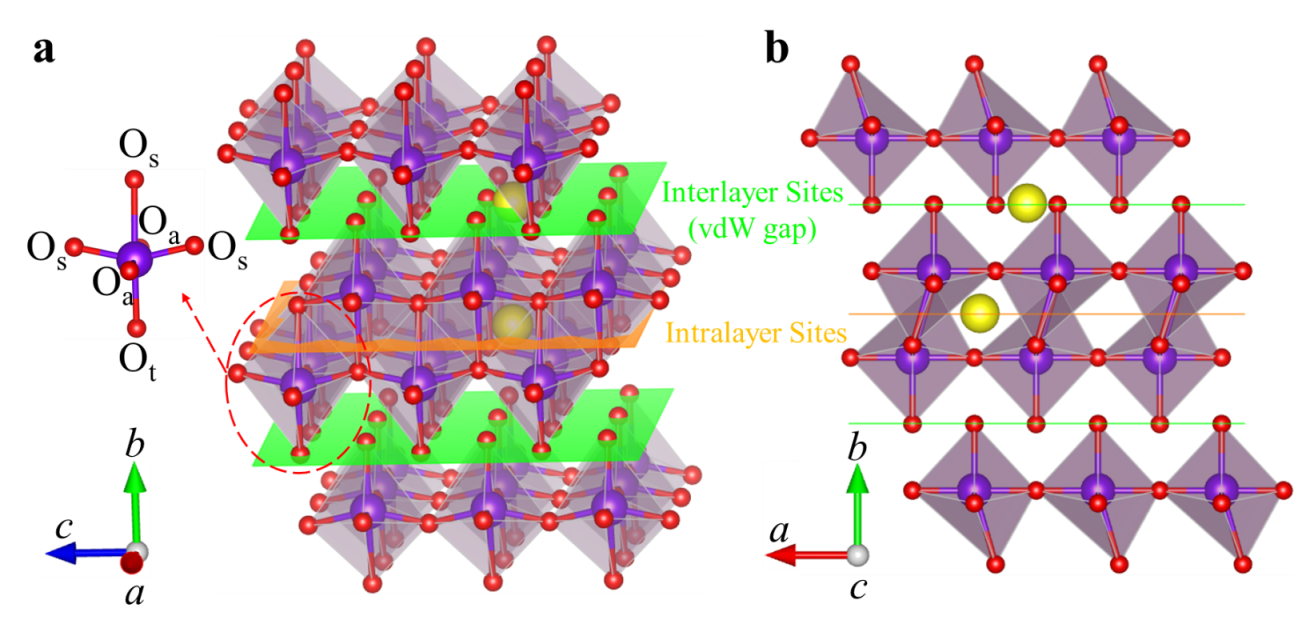
**Figure S3** High resolution transmission electron microscopy of the pristine (a) and the MoO3 (II) (b).



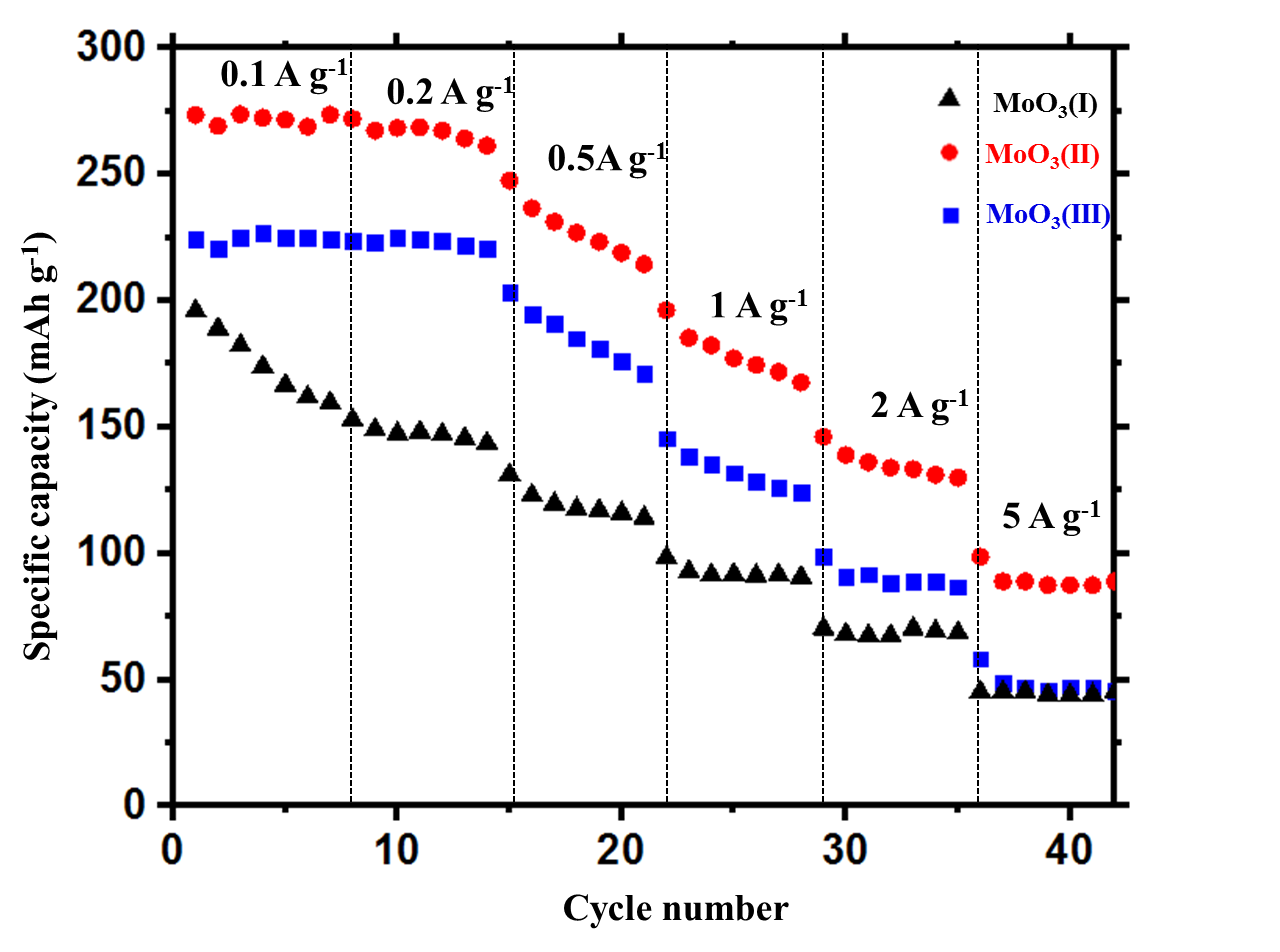
**Figure S4** Positron annihilation lifetime spectra of MoO3 (I) and MoO3 (II).

**Table S2** Positron annihilation lifetime results of MoO3 (I) and MoO3 (II).

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | *τ*1 (ns) | *I*1 (%) | *τ*2 (ns) | *I*2 (%) | *τ* (ns) |
| MoO3 (I) | 0.209 | 49.11 | 0.381 | 50.89 | 0.2965 |
| MoO3 (II) | 0.226 | 51.76 | 0.399 | 48.24 | 0.3095 |



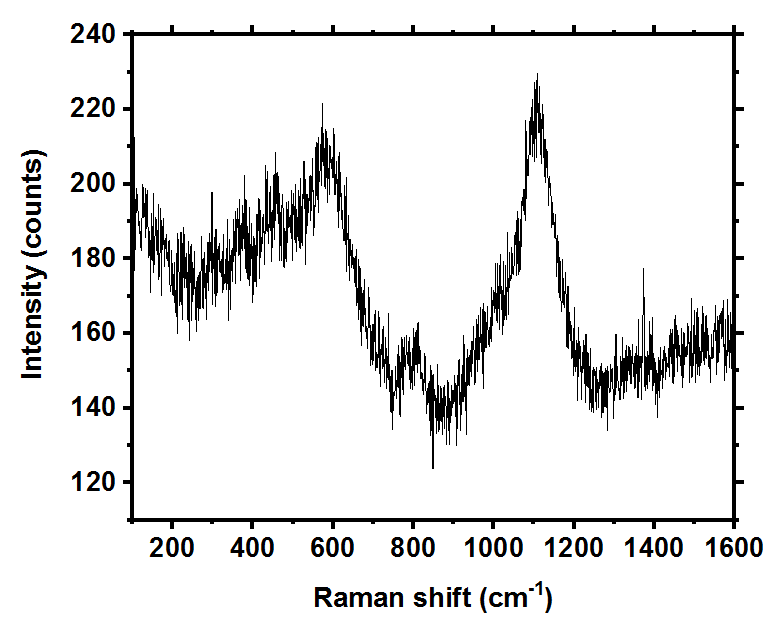
**Figure S5** Crystal structure of α-MoO3 and the two types of Li+ storage sites. (red: O; purple: Mo; yellow: Li)



**Figure S6** Rate capability of the pristine, MoO3 (II) and MoO3 (III).



**Figure S7** XPS spectrum of the MoO3 (II) after the first cycle.



**Figure S8** Raman spectrum of the MoO