

Supplementary Information

Inhibit oxygen release and stabilize bulk structure of lithium-rich layered oxides by strong Mo-O covalent binding

Huinan Yu^a, Zhichen Xue^a, Zhiyuan Xue^a, Zhongyuan Luo^a, Chenxi Ding^a, Guorong Hu^{a,b,c}, Zhongdong Peng^{a,b,c}, Yanbing Cao^{a,b,c}, Ke Du^{a,b,c,*}

^a *School of Metallurgy and Environment, Central South University, Changsha, 410083, China*

^b *Engineering Research Center of the Ministry of Education for Advanced Battery Materials, Central South University, Changsha, 410083, China*

^c *Hunan Provincial Key Laboratory of Nonferrous Value-added Metallurgy, Central South University, Changsha, 410083, China*

*Corresponding author. Ke Du
E-mail address: dukecsu@163.com

1. Supplementary tables

Table S1. Rietveld Refinement Results of LRP and LR-Mo1.0.

| Sample | a=b (Å) | c (Å) | c/a | V (Å) ³ | Rwp | Rp | χ^2 |
|----------|---------|----------|--------|--------------------|-------|-------|----------|
| LRP | 2.85627 | 14.26103 | 4.9929 | 100.758 | 2.03% | 1.40% | 2.037 |
| LR-Mo1.0 | 2.85323 | 14.23955 | 4.9907 | 100.392 | 1.77% | 1.25% | 2.396 |

Table S2. Fitting Result of Equivalent Circuit from Nyquist Curves for LRP and LR-Mo1.0.

| Samples | R_s/Ω | R_{ct}/Ω | $\sigma/\Omega \text{ cm}^2 \text{ s}^{-1/2}$ | $D_{\text{Li}^+}/\text{cm}^2 \text{ s}^{-1}$ |
|----------|--------------|-----------------|---|--|
| LRP | 4.026 | 100.8 | 165.9 | 8.96×10^{-16} |
| LR-Mo1.0 | 2.777 | 65.1 | 78.7 | 3.98×10^{-15} |

2. Supplementary figures



Fig. S1. Schematic diagram of material synthesis

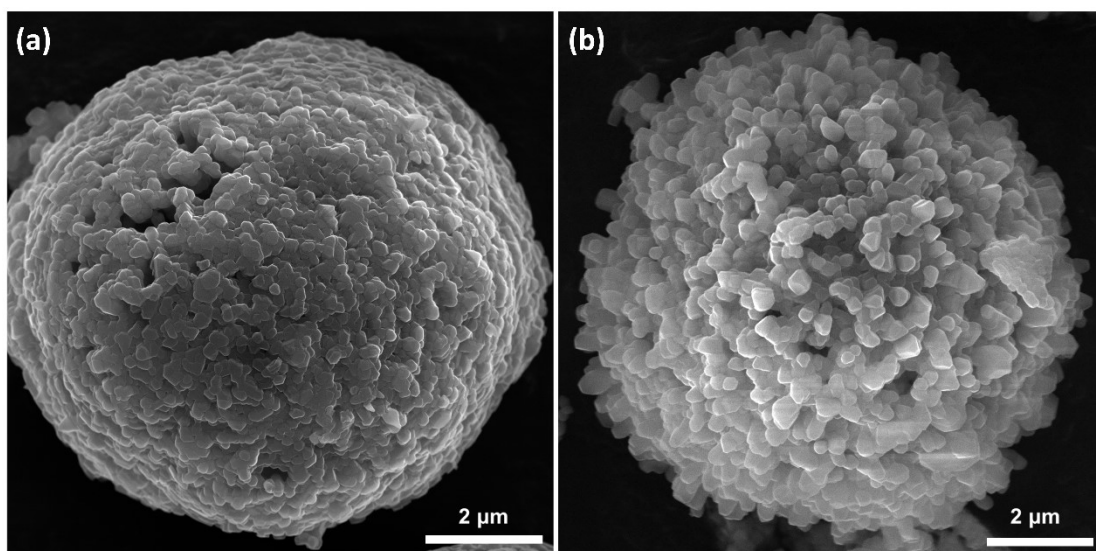


Fig. S2. SEM images of (a)LR-Mo0.5 and (b)LR-Mo1.5

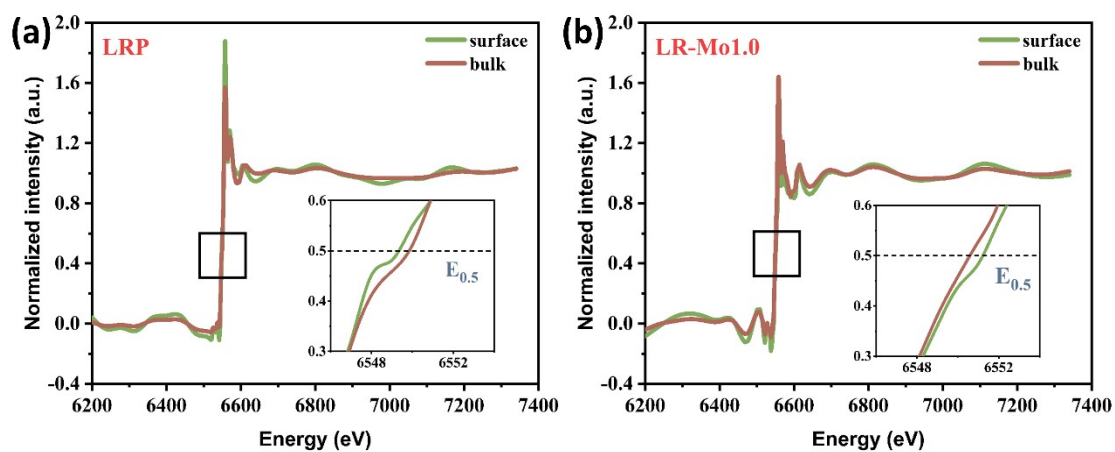


Fig. S3. Mn K-edge XANES of selected surface and bulk regions of (a)LRP and (b)LR-Mo1.0

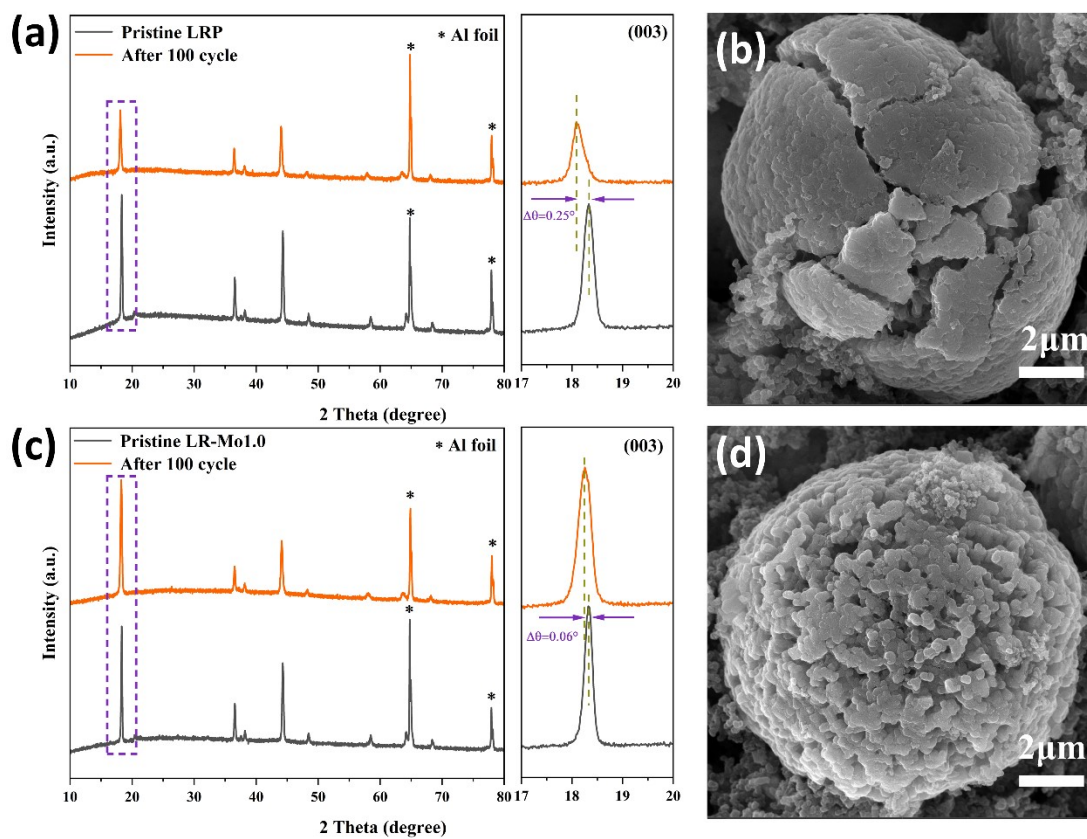


Fig.S4. XRD patterns and SEM images of (a, b) LRP and (c, d) LR-Mo1.0 after 100 cycles at 1C