Supporting Information Elucidating the Mechanism Underlying the Augmented Capacity of MoO₂ as an Anode Material in Li-Ion Batteries

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Fig. S1. Atomic structure of crystalline MoO₂. The purple and red balls represent Mo, and O atoms, respectively.



Fig. S2. In situ XRD of a fresh MoO_2 cell cycled at 1 C rate.



Fig. S3. a)The height, b)FWHM and d-spacing of $Li_{0.98}MoO_2$ peak (011) shown in Fig. 2. From the variation of height and FWHM, $Li_{0.98}MoO_2$ was not obviously disappeared to form Mo and Li_2O , and its d-spacing kept consistent.



Fig. S4. In situ XAS analysis of a fresh MoO₂ cell.



Fig. S5. EELS of a partially lithiated MoO₂ electrode. No traces of metallic lithium were detected.

b

Fig. S6. SEM images comparison: a) electrode without exposure to air; b) electrode exposed to air with gel-coating like fusion.

1µm LED

5.0kV

JEOL



Fig. S7. a) Ex-situ SEM of an MoO_2 electrode at point (1) after lithiation.



Fig. S8. a) SEI thickness at point (1) and b) SEI thickness at point (3).