Supporting Information

Facet-Selective Deposition of FeO_x on α-MoO_3 Nanobelts for Lithium Storage

Yao Yao,[1] Nuo Xu,[2] Doudou Guan,[1] Jiantao Li,[1] Zechao Zhuang,[1] Liang Zhou,*[,1] Changwei Shi[1], Xue Liu[1], and Liqiang Mai*[,1]

[1]*State Key Laboratory of Advanced Technology for Materials Synthesis and Processing, Wuhan University of Technology, Hubei, Wuhan 430070, China*

[2]*School of Chemistry, Chemical Engineering and Life Sciences, Wuhan University of Technology, Hubei, Wuhan 430070, China*

**E-mail: liangzhou@whut.edu.cn; mlq518@whut.edu.cn*

Experimental Section

Materials synthesis: α-MoO_3 nanobelts are synthesized according to a reported hydrothermal method.[1] In a typical synthesis, 10 m mol of Mo powder was dissolved in a mixture of 20 mL of 30 wt. % H_2O_2 and 20 mL of H_2O under stirring at 25 ^oC. The resulting solution was stirred for 12 h at 25 ^oC. The solution was then transferred into a Teflon-lined stainless-steel autoclave, sealed, and hydrothermally treated at 180 ^oC for 24 h, after which a white suspension (α-MoO_3 nanobelts) was obtained.

For the fabrication of heterostructured α-MoO_3@FeO_x nanobelts, 0.686 g $(NH_4)_2Fe(SO_4)_2 \cdot 6H_2O$ was dissolved in 40 ml H_2O. Then, the as-synthesized α-MoO_3 nanobelts (2 ml) were added dropwise into the $(NH_4)_2Fe(SO_4)_2 \cdot 6H_2O$ solution under stirring at 70 ^oC for 4 h to obtain the α-MoO_3@FeO_x heterostructures.

Characterization: The morphology of the as-prepared products were investigated by field-emission scanning electron microscopy (JEOL JSM-7100 F) at an acceleration voltage of 20 kV. Transmission electron microscopy (TEM), selected area electron diffraction (SAED) pattern, and high-resolution TEM (HRTEM) images were collected by a JEOL JEM-2100F. An energy-dispersive X-ray spectroscopy (EDS) facility attached to the TEM was used to analyze the element distribution. The crystal phase of products was characterized by X-ray diffraction (XRD). XRD patterns of the products were recorded by a Rigaku D/MAX-III diffractometer with monochromatized Cu K_α radiation. The chemical composition of the products was analyzed by inductively coupled plasma-atomic emission spectrometry (ICP-AES, PerkinElmer Optima 4300DV). X-ray photoelectron spectroscopy (XPS) spectra were obtained on a ESCALAB 250 system with a monochromatic Al K_α source (1,486.6 eV). All XPS profiles were calibrated based on the C 1s peak at 284.6eV.

Electrochemical measurements: Electrochemical properties were measured in 2016 type coin cells. The coin cells were assembled in an argon-filled glovebox with lithium metal as the counter and reference electrodes. The working electrode was

fabricated by mixing 70 wt.% of the active material (α-MoO_3 and α-MoO_3@FeO_x), 20 wt.% of conductive carbon black (acetylene black), and 10 wt.% of carboxymethyl cellulose (CMC) binder in H_2O. The mass loading of the active material was ~1.5 mg cm^{-2}. The electrolyte used was a solution of 1 M $LiPF_6$ in ethylene carbonate, dimethyl carbonate, ethyl methyl carbonate (1:1:1 by volume). Galvanostatic discharge/charge experiments were performed in the potential range of 0.005 – 3 V with a battery testing system (LAND CT 2001A) at room temperature. Cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS) were conducted using an autolab potentiostat galvanostat.

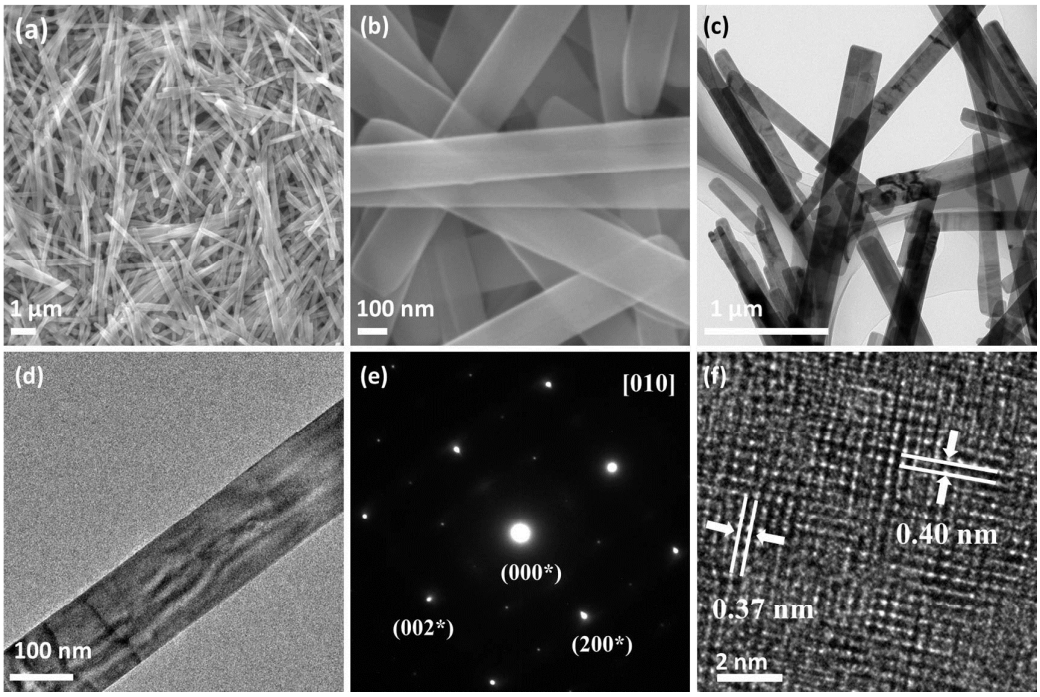

Figure S1. SEM images (a, b), TEM images (c, d), SAED pattern (e) and HRTEM image (f) of α-MoO_3 nanobelts.

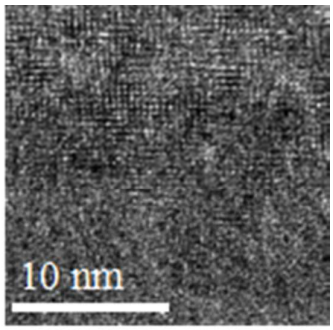

Figure S2. The HRTEM image of the interfacial region between FeO_x and MoO_3.

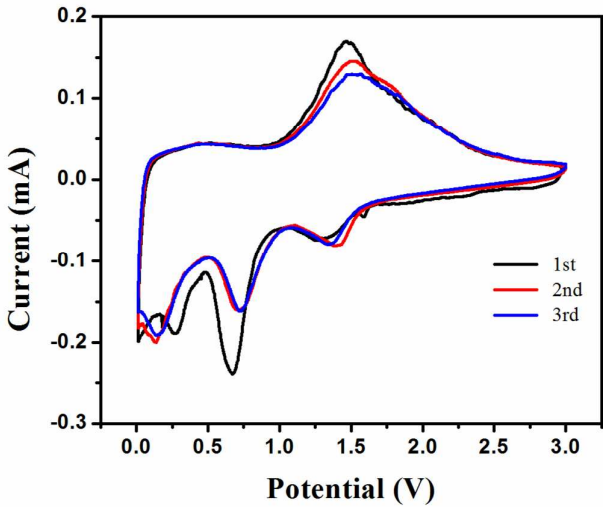

Figure S3. CV curves of α-MoO_3@FeO_x at a sweep rate of 0.1 mV s^{-1} in the potential range of 0.005 – 3.0 V *vs.* Li/Li^+.

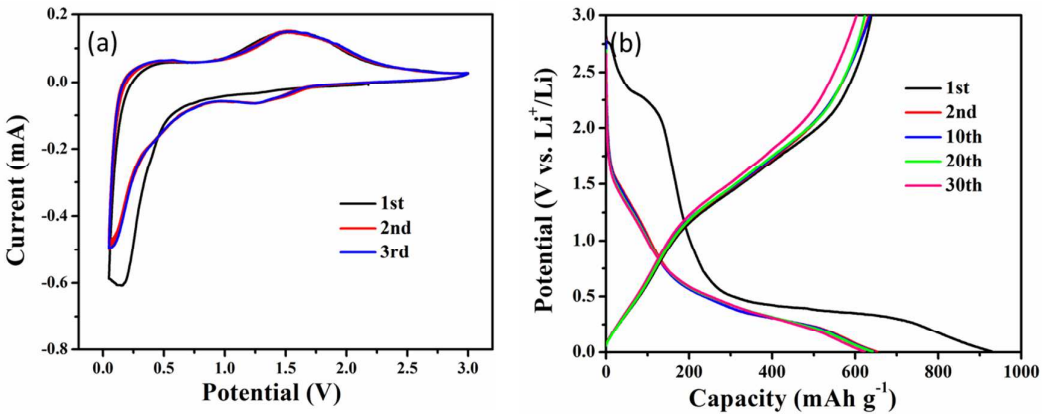

Figure S4. CV curves of α-MoO_3 at a sweep rate of 0.1 mV s^{-1} in the potential range of 0.005 – 3.0 V *vs.* Li/Li^+ (a); galvanostatic discharge-charge voltage profiles of the α-MoO_3 nanobelts at 200 mA g^{-1} (b).

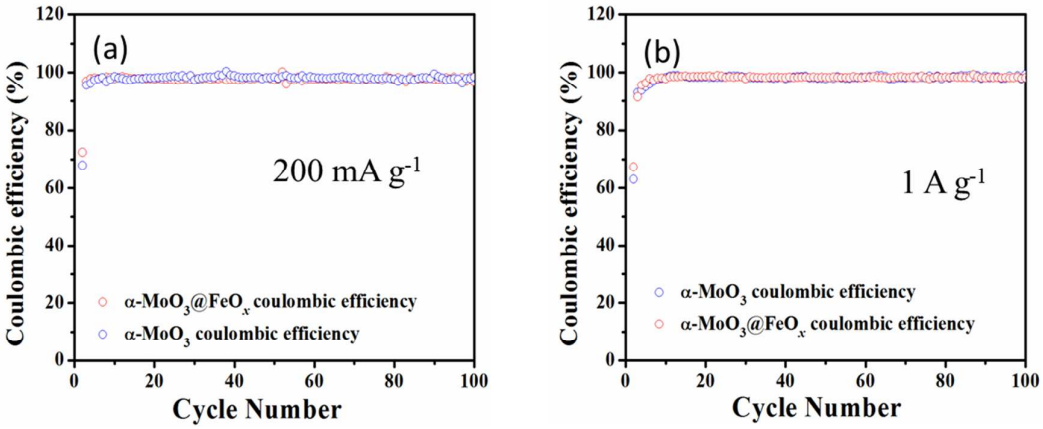

Figure S5. Coulombic efficiency of α-MoO_3 and α-MoO_3@FeO_x at 200 mA g^{-1} (a) and 1 A g^{-1} (b).

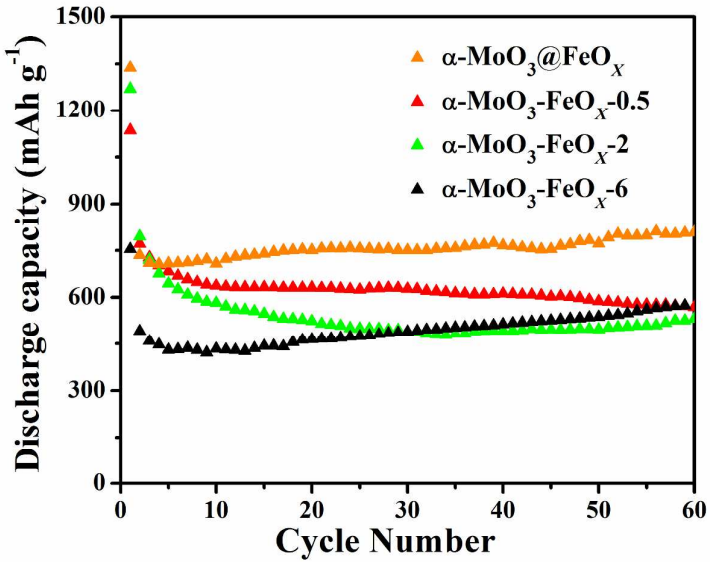

Figure S6. Comparison of cycling performances of the α-MoO_3-FeO_x-0.5, α-MoO_3-FeO_x-2.0, α-MoO_3-FeO_x-6.0 and α-MoO_3@FeO_x nanobelts at 200 mA g^{-1}.

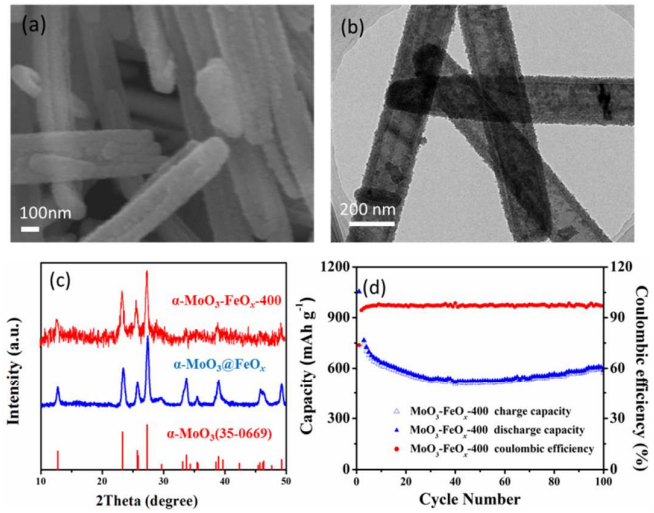

Figure S7. SEM image (a) and TEM image (b) of α-MoO_3-FeO_x-400; XRD patterns of α-MoO_3-FeO_x-400 and α-MoO_3@FeO_x (c); cycling performance of α-MoO_3-FeO_x-400 at 200 mA g^{-1}.

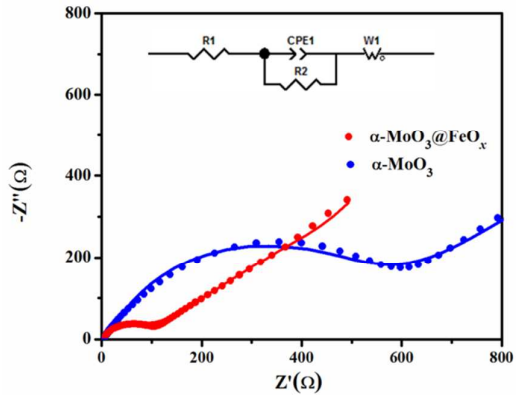

Figure S8. Nyquist plots of the α-MoO_3 and α-MoO_3@FeO_x electrodes. The inset shows the equivalent circuit. In the equivalent circuit, R1 is the total resistance of the electrolyte, separator, and electrical contacts; R2 is the Faradic charge-transfer resistance; CPE1 is the constant phase-angle element; W1 represents the Warburg impedance.

References

1.Zhou, L.; Yang, L.; Yuan, P.; Zou, J.; Wu, Y.; Yu, C., α-MoO_3 Nanobelts: A High Performance Cathode Material for Lithium Ion Batteries. *J. Phys. Chem. C* 2010, 114, 21868-21872.