Electronic Supplementary Information

Converting Bulk $MoSi_2$ Alloy to SiO_x Based Anode Material through Controlled Oxidation Induced Sublimation

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Experimental Section

Characterization. Scanning electron microscopy (SEM) images were obtained on a JEOL-7100F microscope. Transmission electron microscopy (TEM) images, high-resolution TEM (HRTEM) images, and Energy dispersive X-ray spectroscopy (EDX) elemental mappings were collected on a JEM-2100F microscope. X-ray diffraction

(XRD) patterns were recorded on a Bruker D8 Advance X-ray diffractometer with a non-monochromated Cu Kα X-ray source (λ = 1.5418 Å). X-ray photoelectron spectroscopy (XPS) spectra were obtained on a VG Multilab 2000 X-ray photoelectron instrument.

The Brunauer–Emmett–Teller (BET) surface areas were calculated from N_2 sorption results, which were measured on a Tristar-3020 instrument at 77 K. The thermogravimetry-differential scanning calorimetry (TG-DSC) was obtained on a TA SDT650 apparatus, and the samples were heated to 1000 ^{o}C in air with a heating rate of 10 ^{o}C min^{-1}.

Electrochemical Characterization. The active material (70 wt%), acetylene black (20 wt%), and sodium alginate (10 wt%) were dispersed in water to form a slurry. The slurry was spread onto copper foil by the doctor blade method. The mass loading of the active material was 1.0–1.5 mg cm^{-2}. The electrolyte was 1.0 M $LiPF_6$ in ethylene carbonate/dimethyl carbonate (1:1 by volume) containing 5 vol% fluoroethylene carbonate (FEC). A Whatman glass fiber membrane (GF/A) was used as the separator. Li foil was used as the reference electrode in half cells. Discharge/charge measurements were performed in a potential window of 0.01–3.0 V (*vs.* Li^+ /Li) using a Neware CT4008 battery tester. Cyclic voltammetry (CV) was performed with an Autolab PGSTAT 302N electrochemical workstation in the potential range of 0.01–3.0 V *vs.* Li^+ /Li at 0.1 mV s^{-1}.

The SiMoO-800//$LiFePO_4$ full cells were assembled with cathode material/anode material ratio of about 4:1. 1.0 M $LiPF_6$ in ethylene carbon/dimethyl carbonate/ethyl methyl carbonate (1:1:1 by volume) was used as the electrolyte and GF/A was used as the separator. Before full cell assembly, the SiMoO-800 hybrid was pre-lithiated in half cells. The SiMoO-800//$LiFePO_4$ full cells were cycled at 0.5 C and 1 C (1 C = 170 mA g^{-1}) in a voltage window of 2.2–3.8 V.

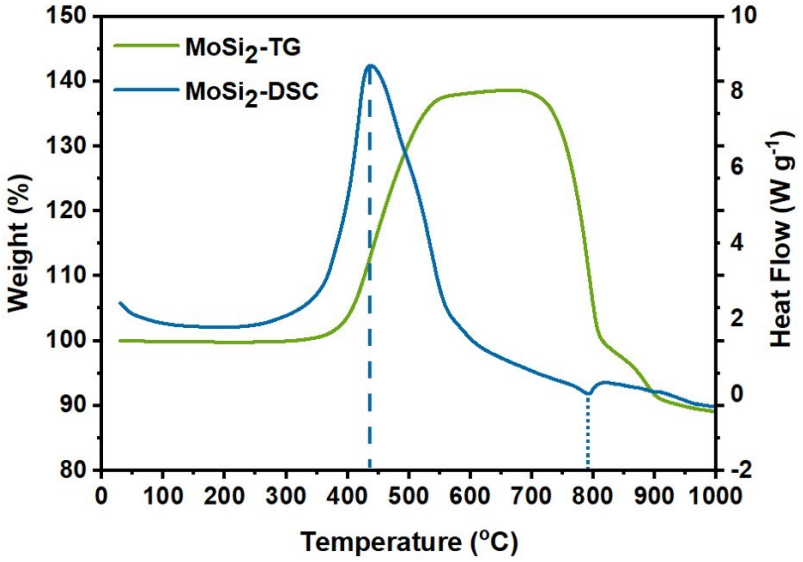

Figure S1. TG-DSC curves of $MoSi_2$ alloy.

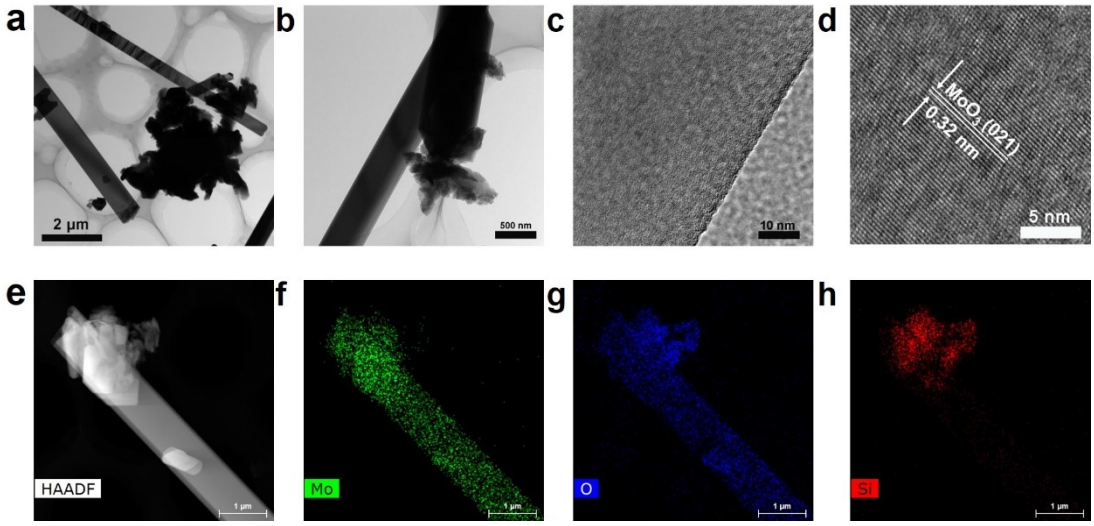

Figure S2. (a-b) TEM, (c-d) high-resolution TEM, (e) HAADF-STEM and (f-h) EDX elemental mappings of SiMoO-600.

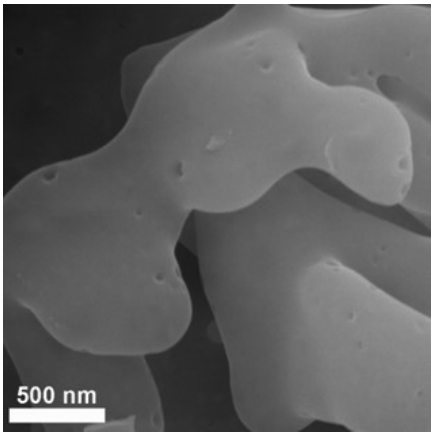

Figure S3. SEM images of SiMoO-800.

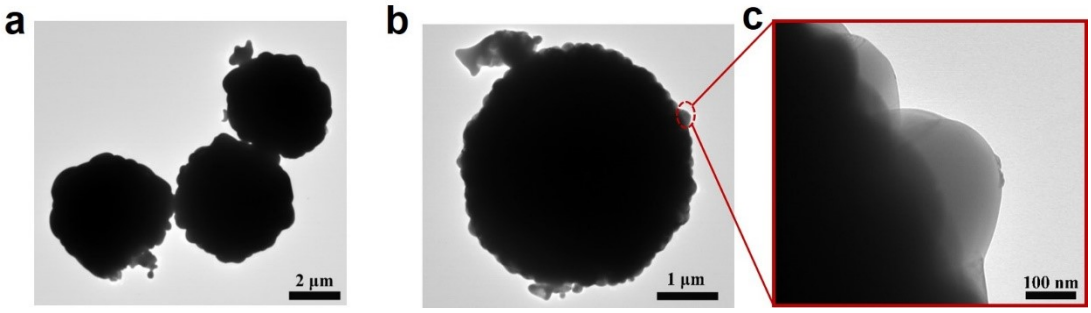

Figure S4. TEM images of SiMoO-1000.

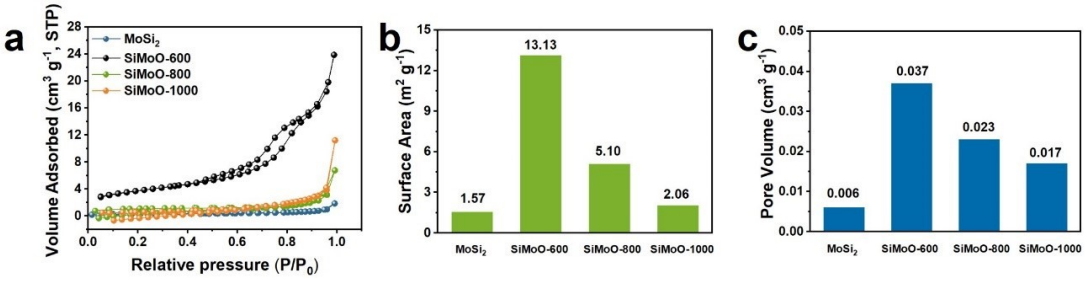

Figure S5. (a) N_2 adsorption/desorption isotherms, (b) BET surface area, and (c) pore volume of $MoSi_2$, SiMoO-600, SiMoO-800, and SiMoO-1000.

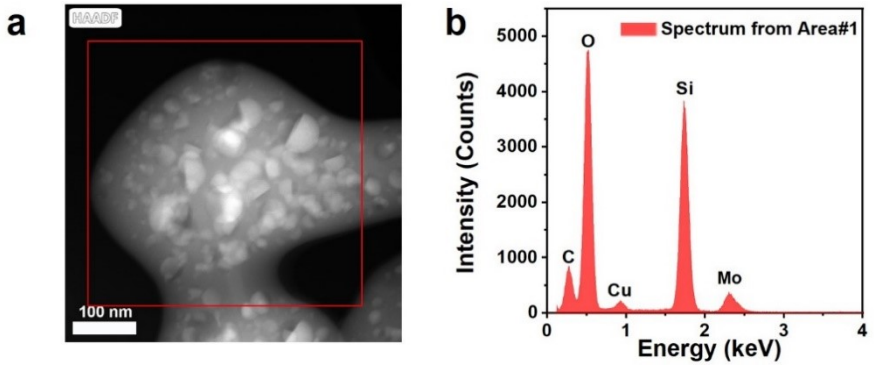

Figure S6. (a) HAADF-STEM images and (b) EDX spectrum.

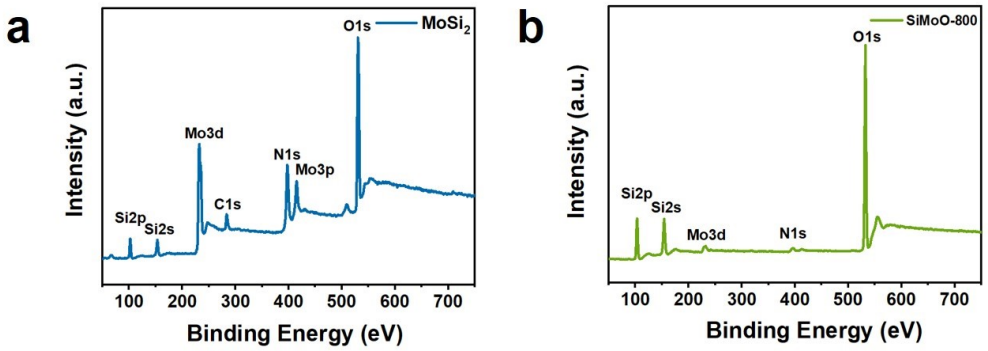

Figure S7. (a)XPS survey spectra of $MoSi_2$ and (b) SiMoO-800.

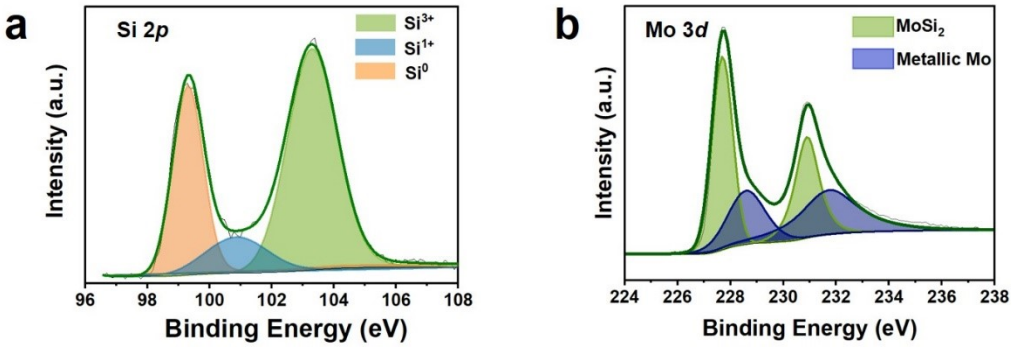

Figure S8. (a) High-resolution Si2p and (b) Mo3d XPS spectra of $MoSi_2$.

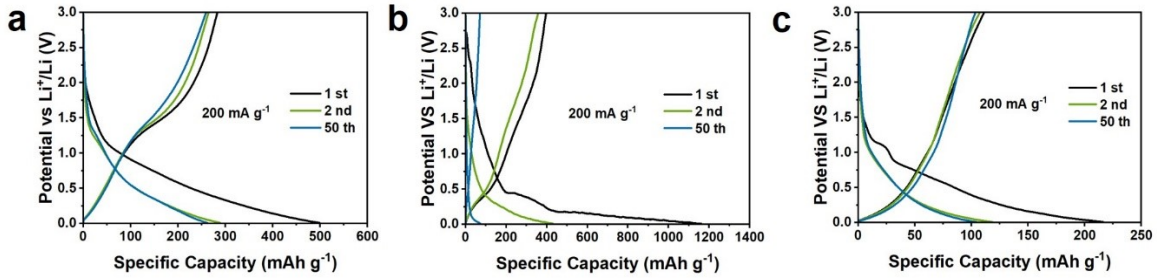

Figure S9. Representative GCD profiles of (a)$MoSi_2$; (b)SiMoO-600; (c)SiMoO-1000 at 200 mA g^{-1}.

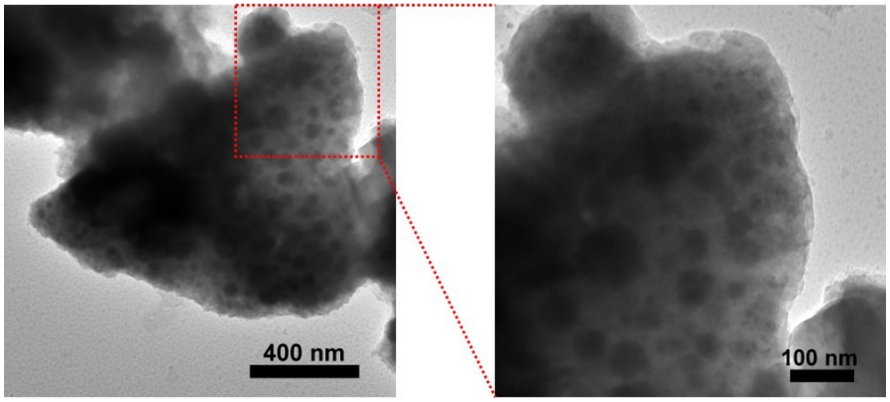

Figure S10. TEM images of SiMoO-800 after 100 cycles at 200 mA g^{-1}.

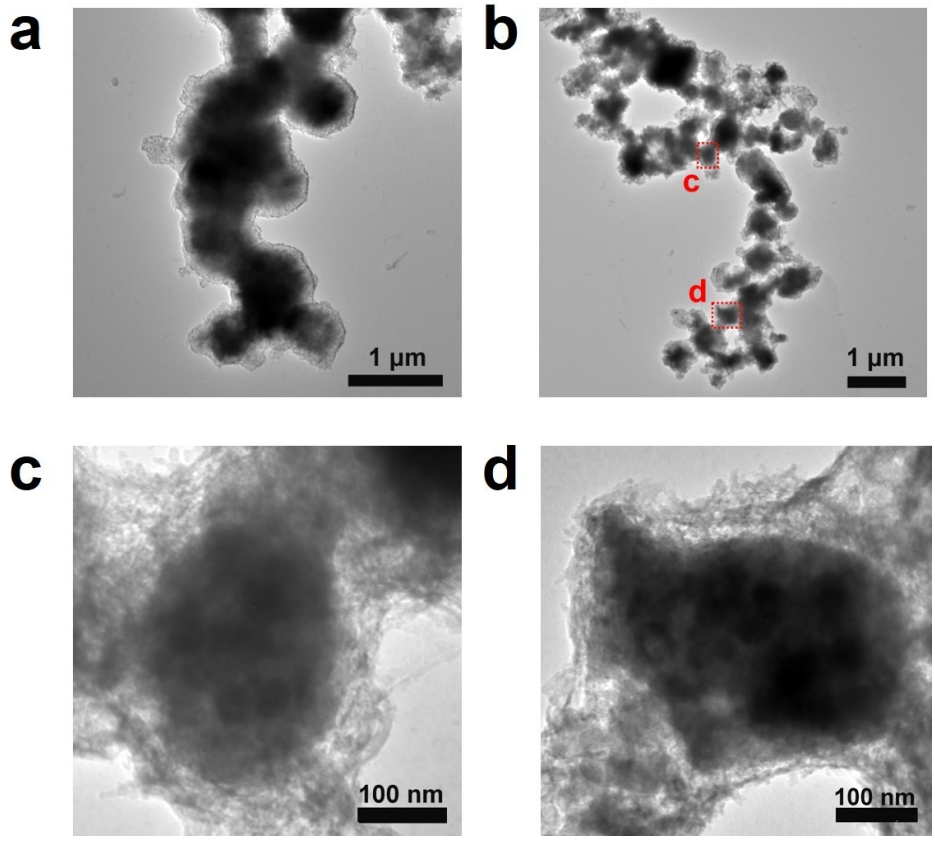

Figure S11. TEM images of SiMoO-800 after 100 cycles at 200 mA g^{-1}.

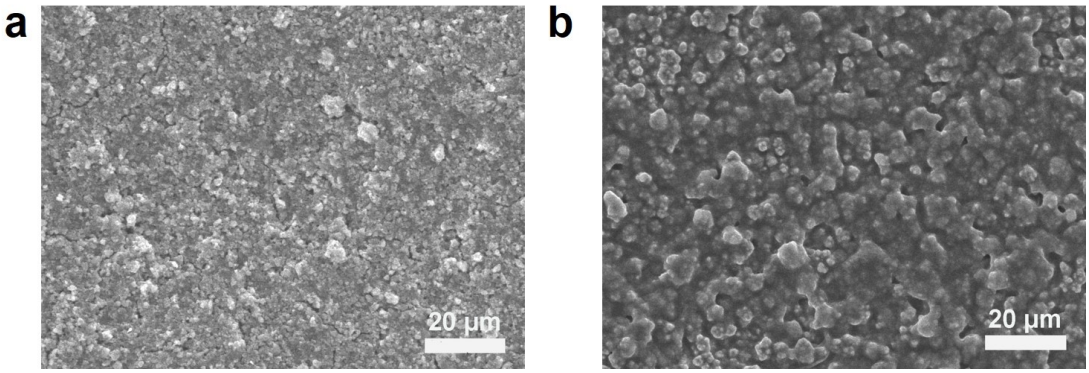

Figure S12. Top-view SEM images of SiMoO-800 (a) before and (b) after 100 cycles at 200 mA g^{-1}.

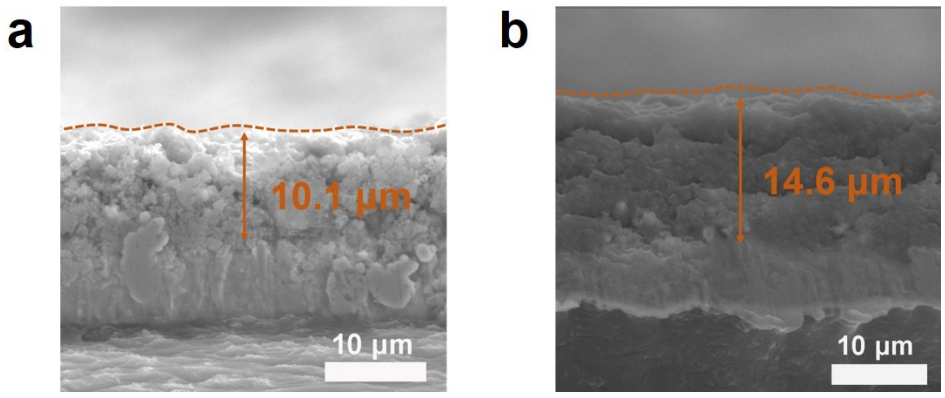

Figure S13. Cross-sectional SEM images of SiMoO-800 (a) before and (b) after 100 cycles at 200 mA g^{-1}.

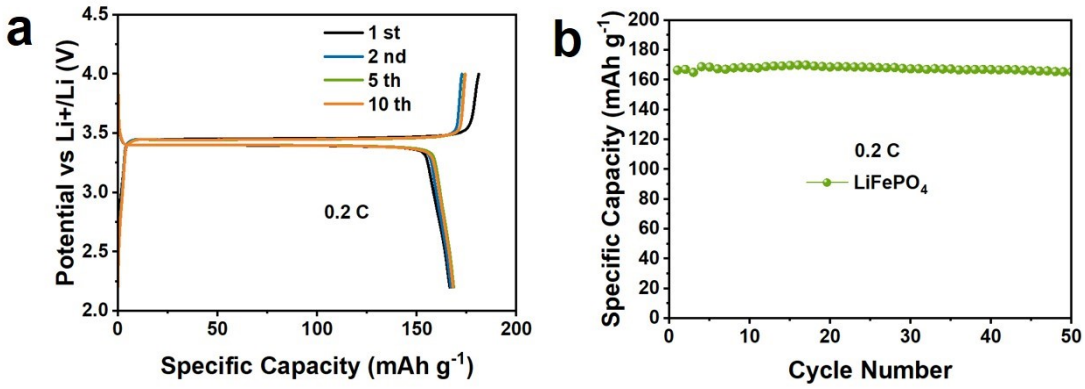

Figure S14. (a) Representative GCD profiles and (b) cycling performance of $LiFePO_4$ at 0.2 C (1 C = 170 mA g^{-1}).