Supporting Information

Atomic Layer Deposition of TiO$_2$ Shells on MoO$_3$ Nanobelts Allowing Enhanced Lithium Storage Performance

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Experimental Section

Material synthesis.

Synthesis of MoO$_3$ nanobelts. MoO$_3$ nanobelts were synthesized via hydrothermal method. In a typical synthesis, 2.0 g ammonium molybdate powder was first dissolved in 30 mL deionized water under magnetic stirring to form a clear solution. Afterwards, 10 mL nitrogen acid was added into by drop-by-drop under continuous stirring for 2 h. The mixture was then transferred to a Teflon lined stainless steel autoclave, which was kept at 180 °C for 24 h. After naturally cooling down to room temperature, MoO$_3$ nanobelts were obtained after washing with distilled water and ethanol for several times, which were then dried at 80 °C for 12 h in the oven.

Atomic layer deposition (ALD) of TiO$_2$ layers on MoO$_3$ nanobelts. A home-made ALD system (Figure S1) was used for the deposition of TiO$_2$ layers on MoO$_3$ nanobelts. In a typical ALD cycle, MoO$_3$ nanobelts in vacuum were alternately exposed into the TiCl$_4$ and H$_2$O gases, thus the atomic layer adsorption of TiCl$_4$ and H$_2$O can react on the surface of MoO$_3$, producing an atomic layer of TiO$_2$. Desired thickness of TiO$_2$ shells can be obtained by repeating the ALD cycle (Figure S2).

Materials Characterization.

Powder X-ray diffraction (XRD) patterns of the products were obtained on a Bruker D2 PHASER X-ray diffractometer using Cu Kα radiation (λ = 1.5418 A) with an operating voltage of 30 kV and a current of 10 mA. Scanning electron microscope (SEM) was performed on an FEI Quanta 250 SEM. Transmission electron microscope (TEM) and high-resolution TEM (HRTEM) were carried out on a JEOL JEM2100 TEM operated at 200 kV. Energy-dispersive X-ray spectroscopy (EDS) was performed on JEM-F200 Field Emission TEM instrument. X-ray photoelectron spectroscopy (XPS) was performed on a Thermo Fisher ESCALAB 250Xi instrument. All the binding energies were calibrated by referring to the C 1s peak at 284.6 eV.

Electrochemical Measurements.
Electrochemical properties were examined using CR2025 coin-type cells assembled in an Ar-filled glovebox with both H₂O and O₂ content less than 1.0 ppm. The working electrode was prepared by casting aqueous slurry consisted of active material, acetylene black and polyacrylic acid (PAA) binder with a weight ratio of 80:10:10, followed by drying at 120 °C under vacuum overnight. Lithium foil was used as the counter electrode, and microporous membrane (Celgard 2400) was used as the separator. An electrolyte containing 1 M LiPF₆ dissolved in a mixture of ethylene carbonate/dimethyl carbonate with a volume ratio of 1:1. Galvanostatic discharge/charge tests of the cells were carried out on a battery test system (NEWARE BTS, Neware Technology Co., Ltd., China) in the range of 0.01-3.0 V (vs. Li/Li⁺) at room temperature (25 °C). Cyclic voltammetry (CV) was carried out on an electrochemical station (Autolab PGSTAT 302 N) in the range of 0.01-3.0 V at a scan rate of 0.2 mV/s. Electrochemical impedance spectroscopy (EIS) was performed in the frequency range of 10 MHz-0.01 Hz with a voltage amplitude of 5 mV using CHI600E electrochemical station. The specific capacities were based on the mass of the active materials with average loading amount of approximately 1.0 mg/cm².

Figure S1. Schematic illustration of the home-made ALD setup and the ALD cycling process.

Figure S2. (a) Relationship of TiO₂ thickness along with ALD cycle numbers, and (b) the effect of ALD cycles on the electrochemical properties of TiO₂@MoO₃.
Figure S3. XRD patterns of the MoO$_3$ and TiO$_2$@MoO$_3$ nanobelts.

Figure S4. EDS spectrum of TiO$_2$@MoO$_3$ nanobelts.

Figure S5. CV curves of the commercial MoO$_3$ (Macklin, AR, 99.5%).
Figure S6. Cycle performance of the MoO₃ and TiO₂@MoO₃ at a high-rate of 1 A g⁻¹. For MoO₃ electrode, a lower current density was applied in the first five cycles.

Figure S7. Nyquist plots of the MoO₃ and TiO₂@MoO₃ electrodes before cycling.