## Supplementary Information

## Bismuth oxyiodide nanosheets: a novel high-energy anode material for lithium-ion batteries

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## Experimental

**Synthesis of BiOI nanosheets:** Typically, 1 g of  $BiI_3$  powder was placed in a corundum boat covered with a ceramic chip. Then the corundum boat was moved into a box furnace and annealed at 300 °C for 8 h. The product was collected by washing with ethanol and DI water for several times, and dried at 80 °C for 24 h.

**Characterization:** The morphology and structure of the products were measured by SEM (SIRION200), TEM (JEOL JEM-2010F), and XRD (PANalytical B.V., Holland).

**Electrochemical Measurements:** Electrochemical tests were carried out in 2032 coin type cells. The working electrodes were prepared by mixing the active material, super P and polyvinylidene fluoride (PVDF) dissolved in N-methyl-2-pyrrolidone solvent in a mass ratio of 7:2:1, and then coated onto a Cu foil. Lithium metal was used as the counter and reference electrodes, Celgard 2300 as the separator, and 1 M LiPF<sub>6</sub> in a mixture of ethylene carbonate (EC) and dimethyl carbonate (DMC) (1:1 by volume) as the electrolyte. Galvanostatic charge-discharge measurements were performed on a Land Battery Measurement System (Land, China) at various current densities with a cutoff voltage of 0.05–3 V or 0.5–2.5 V at room temperature. Cyclic voltammetry (CV) was measured on a PARSTAT 2273 potentiostat.

**Ex-situ Characterization of the BiOI electrodes:** The ex-situ XRD, Raman spectroscopy and XPS measurements were performed with a Cu foil supported electrode. Coin cells were cycled galvanostatically against lithium at a constant current density of 15 mA g<sup>-1</sup> (ex-situ XRD and Raman spectroscopy) or 30 mA g<sup>-1</sup> (ex-situ XPS), in a voltage range of 0.05–3.0 V. Electrodes with various lithiation states were obtained by disassembling the coin cells and washed with EC and ethanol for several times. XPS spectra were measured on a VG MultiLab 2000 system with a monochromatic A1 K $\alpha$  X-ray source (Thermo VG Scientific). Raman spectroscopy measurements were performed on a Renishaw Invia spectrometer with an Ar+ laser of 514.5 nm at room temperature.



Fig. S1 High-resolution TEM image of the BiOI product.



Fig. S2 Ex-situ Raman spectra of the BiOI electrode at various states of discharge in the first cycle at a current density of 15 mA  $g^{-1}$ .



**Fig. S3** Ex-situ survey XPS spectra of the BiOI electrode at various states of discharge then charge in the first cycle at a current density of 30 mA  $g^{-1}$ .



Fig. S4 TEM images of the BiOI electrode after discharging to 0.05 V.