Electronic supplementary information for

Amorphous Vanadium Oxide with Graphene by Atomic Layer Deposition for Stable High Energy Lithium Ion Anodes

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Experimental

Materials Synthesis

Graphene sheets were produced by thermal exfoliation of the graphite oxide powders, as described previously.1,2

\( \text{V}_2\text{O}_5 \) ALD was deposited utilizing vanadyl oxytriisopropoxide (VOTP) and \( \text{H}_2\text{O} \) as precursors. For the \( \text{V}_2\text{O}_5 \) ALD, VOTP and HPLC (high performance liquid chromatography) grade \( \text{H}_2\text{O} \) were both obtained from Sigma-Aldrich. The VOTP ALD reaction sequence was: i) dose VOTP to 1.0 Torr for 120 seconds; ii) evacuate reaction products and excess VOTP; iii) dose \( \text{N}_2 \) to 20.0 Torr for 60 seconds and then evacuate \( \text{N}_2 \) (repeat 5 times); iv) dose \( \text{H}_2\text{O} \) to 1.0 Torr for 120 seconds; v) evacuate reaction products
and excess \( \text{H}_2\text{O} \); vi) dose \( \text{N}_2 \) to 20.0 Torr for 60 seconds and then evacuate \( \text{N}_2 \) (repeat 5 times). This sequence constitutes one cycle of \( \text{V}_2\text{O}_5 \) ALD. The \( \text{V}_2\text{O}_5 \) ALD was performed at 150 °C.

\textit{Materials Characterization}

The phase, crystallinity and microstructure of the \( \text{V}_2\text{O}_5/\text{G} \) were characterized by XRD using PAN analytical x-ray diffraction system and scanning electron microscopy by a Carl Zeiss Ultra 1540 Dual Beam FIB/SEM System, respectively. The surface area and pore size distribution were measured using a Quantachrome AUTOSORB-1 instrument, and the samples were heated at 150 °C under vacuum for 12 hours before testing. Thermogravimetric analysis (TGA) was performed in air from 20 °C to 800 °C at a heating rate of 10 °C/min in a TA Instrument TGA-Q50.

\textit{Electrochemical measurements}

The electrodes were made by mixing \( \text{V}_2\text{O}_5/\text{G} \) nanocomposites with polyvinylidene fluoride and carbon black at a weight ratio of 75:15:10 in 1-methyl-2-pyrrolidinone solvent. The slurry was coated on copper foil by blade and dried under vacuum at 80 °C overnight. All of the cells were assembled in an argon-filled dry box with Li metal as the negative electrode. A Celgard separator 2340 and 1 M LiPF\(_6\) electrolyte solution in 1:1 w/w ethylene carbonate and diethyl carbonate (Novolyte) were used to fabricate the coin cells. Cyclic voltammetry (CV) measurement was carried out using a potentiostat VersaSTAT 4 (Princeton Applied Research) at a scan rate of 0.5 mV s\(^{-1}\). Galvanostatic charge/discharge cycles were performed at a voltage range of 3-0.01 V using an Arbin BT 2000 testing station.
Fig. S1 Images of graphene and V$_2$O$_5$/G composites, showing the highly enhanced density after ALD
Fig. S2 TGA analysis of \( \text{V}_2\text{O}_5 / \text{G} \) under air atmosphere at a heating rate of 10 \(^{\circ}\text{C} \text{ min}^{-1} \).
Fig. S3 SEM image of pristine graphene
Figure S4 shows the discharge capacity of pristine graphene at various current densities. We take 501 mAh g$^{-1}$ as the capacity for graphene at the same current density as V$_2$O$_5$/G (Figure 2c).

The capacity contribution of V$_2$O$_5$ in the composite can be extracted after considering the contribution from pristine graphene, as following:

$$C_{V_2O_5} = \frac{C_{\text{total}} - C_G \times W_G}{W_{V_2O_5}}$$

Where, $C_{V_2O_5}$, $C_{\text{total}}$, $C_G$ are discharge capacitance of V$_2$O$_5$, V$_2$O$_5$/G composite, and graphene, respectively. $W_G$ and $W_{V_2O_5}$ are the mass percentage of graphene and V$_2$O$_5$ in the composites.

Therefore,

$$C_{V_2O_5} = \frac{C_{\text{total}} - C_G \times W_G}{W_{V_2O_5}} = \frac{892 - 501 \times 0.408}{0.592} = 1161 \text{ mAh g}^{-1}$$
Fig. S5 SEM image of V$_2$O$_5$/G after charge/discharge for 100 cycles at a current density of 200 mA g$^{-1}$

References