

Supplementary information

The charge/discharge mechanism and electrochemical performance of CuV_2O_6 as a new anode material for Li-ion batteries

Jianjun Ma,^a Shibing Ni,^{a,b*} Jicheng Zhang,^a Xuelin Yang,^{a,b*} Lulu Zhang^{a,b}

^aCollege of Materials and Chemical Engineering, Three Gorges University, 8 Daxue Road, Yichang, Hubei 443002, China.

^bHubei Provincial Collaborative Innovation Center for New Energy Microgrid, China Three Gorges University.

E-mail: shibingni07@126.com.

Experiments

Sample preparation

The chemicals were analytical grade and purchased from Shanghai Chemical Reagents. Natural graphite was obtained from Yichang Hengda graphite company (99.9%). In a typical procedure, 2 mmol $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$, 2~3 mmol V_2O_5 and 2 mmol glucose were dissolved in 30 ml distilled water. After stirring for 20 minutes, the homogeneous yellowy suspension was transferred into a 50 ml teflonlined autoclave, distilled water was subsequently added to 80% of its capacity. The autoclave was at last sealed and placed in an oven, heated at 160 °C for 24 h. The final products were washed by distilled water and ethanol both four times and dried in an oven, then sintered in air atmosphere at 600 °C for 5h (the products obtained with 2 and 3 mmol V_2O_5 were defined as sample a and b, respectively). For preparing CuV_2O_6 /natural graphite (defined as $\text{CuV}_2\text{O}_6/\text{NG}$), natural graphite and CuV_2O_6 with weight ratio of

1:1 were manually rubbed for 30 min.

Structure and morphology characterization

The structure and morphology of the resulting products were characterized by X-Ray powder diffraction (Rigaku Ultima IV Cu K α radiation $\lambda=1.5406$ Å), field-emission scanning electron microscopy (FE-SEM JSM 7500F, JEOL) and transmission electron microscopy (JEOL, JEM-2100F) equipped with selected area electron diffraction (SAED). For the morphology and structure characterization of the electrode after charge and discharge tests, the cell was disassembled and the electrode was washed with ethanol.

Electrochemical characterization

Before the assembly of Li-ion battery, a mixture of CuV₂O₆/natural graphite (80 wt%), acetylene black (10 wt%), and sodium alginate (SA, dissolved in deionized water, 0.02 g mL⁻¹, 10 wt%) were coated on copper foil and cut into disc electrodes with a diameter of 14 mm using a punch. Coin-type cells (2025) of Li/1 M LiPF₆ in ethylene carbonate, dimethyl carbonate and diethyl carbonate (EC/DMC/DEC, 1:1:1 v/v/v)/CuV₂O₆/natural graphite disc electrode were assembled in an argon-filled dry box (MIKROUNA, Super 1220/750, H₂O<1.0 ppm, O₂<1.0 ppm). A Celgard 2400 microporous polypropylene was used as the separator membrane. The cells were tested in the voltage region between 0.02 and 3 V with a multichannel battery test system (LAND CT2001A). When calculating the specific capacity of the electrode, the weight of both CuV₂O₆ and natural graphite was considered as the total weight of active materials. The cyclic voltammetry (CV) measurement of the electrodes was carried out on a CHI660C electrochemical workstation at a scan rate of 0.2 mV s⁻¹ between 0 and 3 V. Electrochemical impedance spectroscopy (EIS) measurements were performed on CHI660C electrochemical workstation under open circuit

conditions over a frequency range from 0.01 Hz to 100 kHz by applying an AC signal of 5 mV in amplitude throughout the tests.