

Electronic Supplementary Information

Temperature-driven structural evolution of carbon modified LiFePO₄ in air atmosphere

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Materials synthesis

Carbon coated LiFePO₄ was prepared via a solid-state reaction. Typically, stoichiometric amount of Li₂CO₃ (AR), Fe(II)C₂O₄·2H₂O (AR) and NH₄H₂PO₄ (AR) were dispersed in acetone and ground for 2 h by high energy ball milling at the inert atmosphere of N₂. 2 wt% sucrose was added to the mixture prior to ball-milling. After evaporation of acetone, the resulting powder was loaded into a tube furnace, heated from room temperature to 600 °C at a heating rate of 2 °C min⁻¹, held at this temperature for 12 h, and then cooled slowly to room temperature.

Materials characterization

X-ray diffraction (XRD) patterns were recorded on a Rigaku Dmax-2400 automatic diffractometer (Cu Kα) using a step scan mode, with 0.02° 2θ step size and 10 seconds for data collection for each step. Transmission electron microscopy (TEM) observation was performed on a FEI Tecnai G2 F20 microscope. Fourier transform infrared spectroscopy (FTIR) was measured on a Bruker Tensor 27 spectrometer with a 2 cm⁻¹ resolution and a 32 scans mode. X-ray photoelectron spectroscopy (XPS) was performed on a Kratos Axis Ultra spectrometer with Al Kα monochromatized X-ray source.

Electrochemical evaluation

Electrochemical tests were performed on a 2032-type coin cell. The working electrodes were composed of 80 wt% active material, 10 wt% acetylene black, and 10 wt% polyvinylidene fluoride binder. Li foil was used as the counter electrode and the celgard2400 microporous membrane as separator. The electrolyte is 1 mol l⁻¹ LiPF₆ solution dissolved in ethylene carbonate/dimethyl carbonate (1:1 by volume). Cyclic voltammetry (CV) was conducted on a CHI 660E electrochemical workstation. Galvostatic tests were carried out at 25 °C using a Land battery test system.

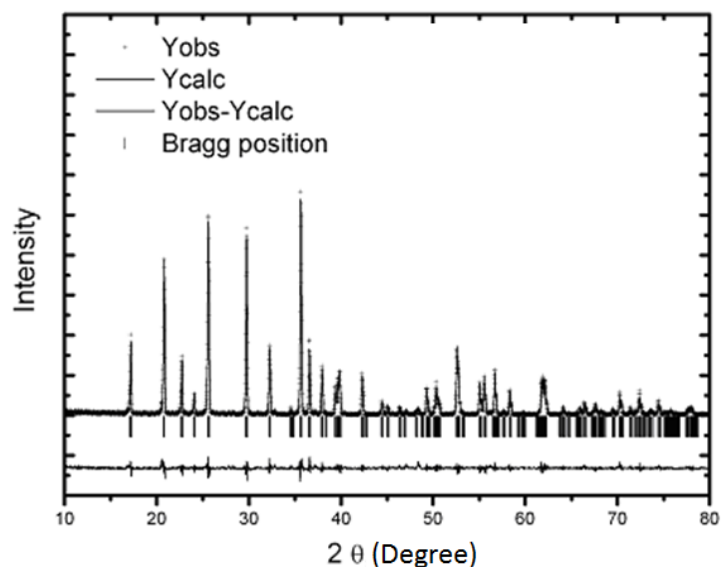


Figure S1. Rietveld refinement results of LiFePO_4 based on the olivine structure (Pnma). The refinement gives good results as seen from the match patterns between the observed and calculated ones. Refinement merits: $R_p = 7.01$, $R_{wp} = 11.2$, $S = 1.71$.

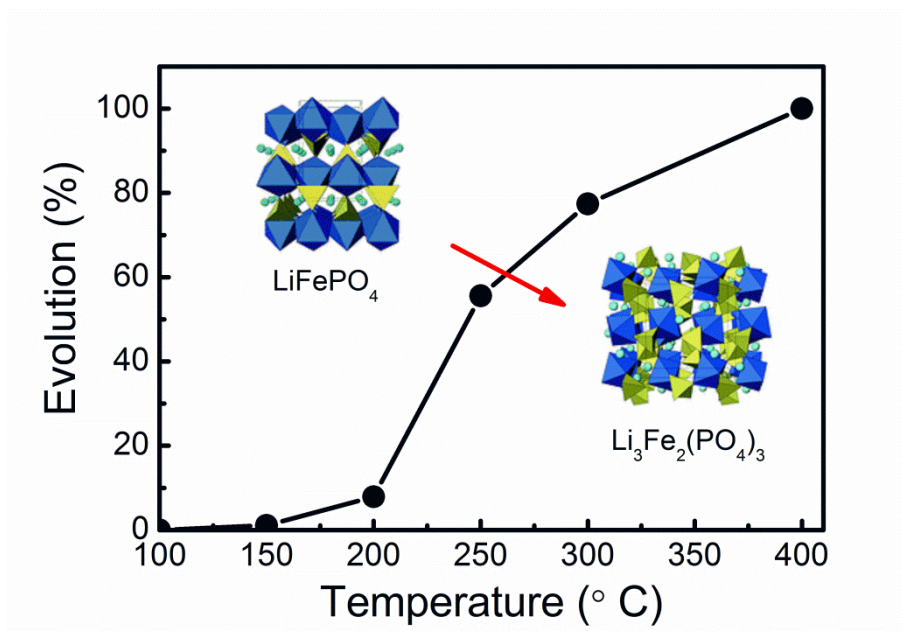


Figure S2. A quantitative evolution map of carbon coated LiFePO_4 upon when exposed to air atmosphere.