

Supporting information for

Morphology evolution and impurity analysis of LiFePO₄ nanoparticles via solvothermal synthesis process

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Part 1

Three samples with LiOH/H₃PO₄=1.8, 3.0 and 3.15 individually were produced via Fe→(P→Li)feeding sequence. H₃PO₄ was added to LiOH's solution first to form a white suspension, and then FeSO₄'s EG solution was dripped inside. Then a green black slurry was formed. We transferred this slurry into a Teflon vessel, heated it at 180°C for 10 hours, and then cooled down. The obtained precipitates were washed and dried. SEM images of the 3 samples are shown in Fig. S1. The morphology changes from nano rectangular plates to spindle plates with LiOH/H₃PO₄ increases. The orientation of crystal faces are checked through high resolution TEM and select area FFT shown in Fig. S2. The results indicate that the rectangular face is b-c plane(100), while the spindle face is a-c plane(010). The feeding sequence has no influences on the LiFePO₄ crystal morphology evolution.

Part 2

In literatures Scherrer equation (also refers to Debye-Scherrer equation, shown in equation S1) has been applied to determine crystal thickness in a particular orientation(hkl) even mean crystal sizes for spherical crystals. It also used to determine the LiFePO₄ crystal sizes by many researchers.

$$D_{hkl} = \frac{K\lambda}{\beta \cos \theta} \quad (\text{S1})$$

Where D_{hkl} is the average thickness of the crystal in a direction normal to the the diffracting plane (hkl), K is a constant depending on the average crystal size and the X-ray diffraction parameters, here we set it as 0.9, λ is the wavelength of the X-rays, β_{hkl} is the width (full-width at half-maximum) of the X-ray diffraction peak in radians and θ is the Bragg angle.

The data of LiFePO_4 samples were collected in steps of $0.01^\circ(2\theta)$ over the range $28.6\sim 31^\circ(2\theta)$ with a constant counting time of 1s per step.

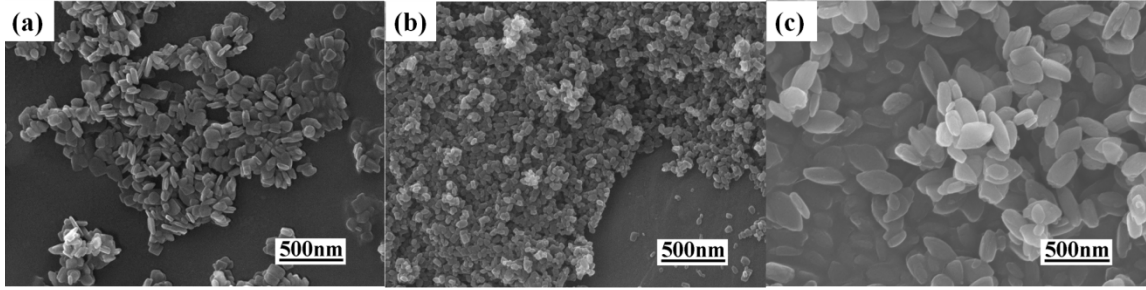


Fig. S1 SEM images of samples made by feeding sequence Fe → (P → Li) with various LiOH/H₃PO₄ mole ratios: (a)1.8, (b)3.0, (c)3.15.

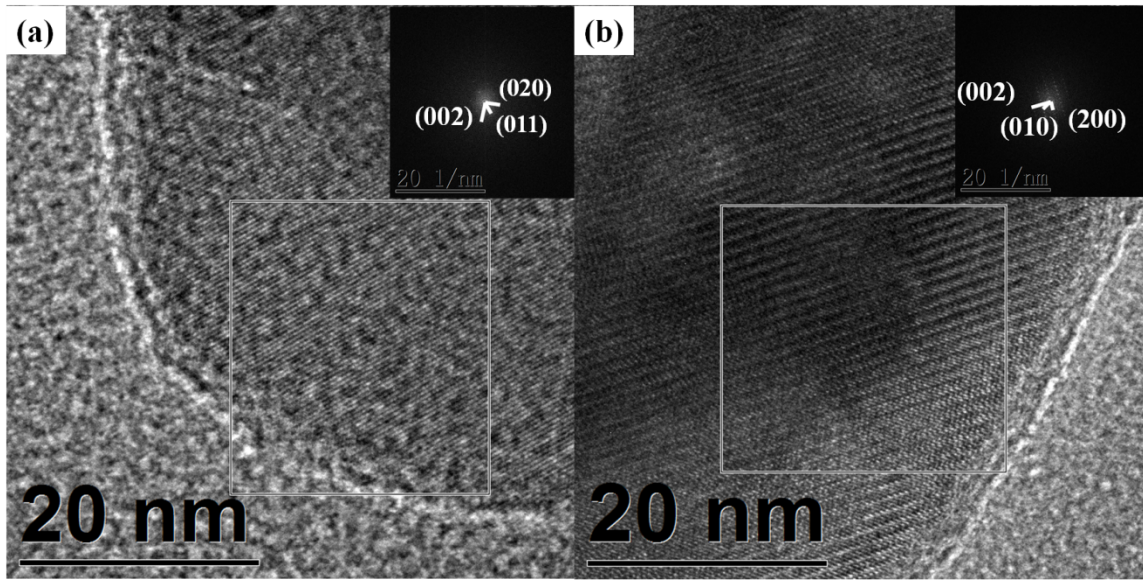


Fig. S2 HRTEM and select area FFT (fast Fourier transform) images of samples made by feeding sequence Fe → (P → Li) with various LiOH/H₃PO₄ mole ratios: (a)1.8, (b)3.15.

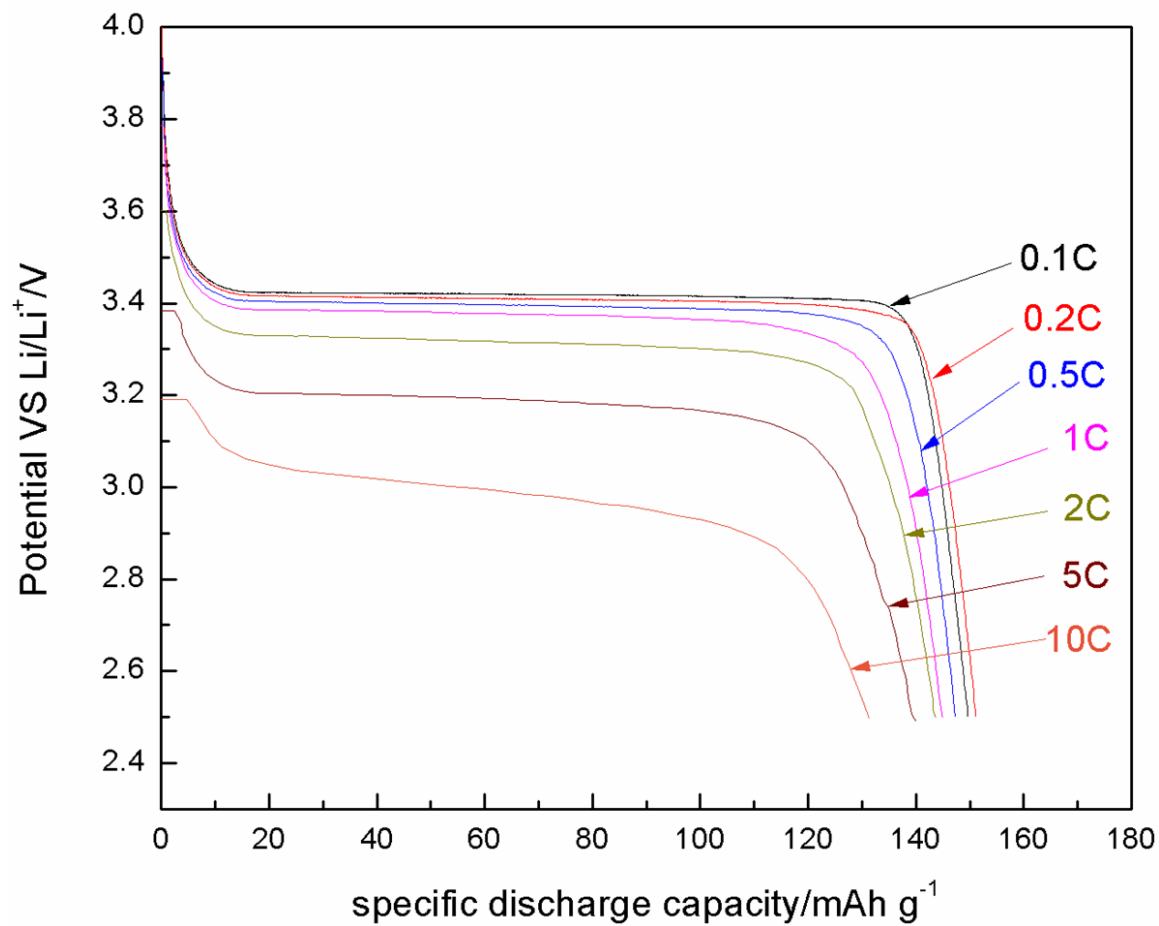


Fig .S3 The first cycle discharge curves of carbon coated LiFePO₄ synthesized at LiOH/H₃PO₄=2.7 at different C rates: 149.6, 151.2, 147.3, 144.9, 143.6, 140.1 and 131.3 mAh g⁻¹ at 0.1C, 0.2C, 0.5C, 1C, 2C, 5C and 10C individually.