

## Approaching Theoretical Capacity of LiFePO<sub>4</sub> at Room Temperature

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Transition metal polyanion compounds, in particular phosphates (e.g. LiFePO<sub>4</sub>[1], α-VOPO<sub>4</sub>[2], and α-LiVOPO<sub>4</sub>[3]) represent a new class of cathode materials in lithium rechargeable batteries. Some of these materials have large theoretical capacities and have shown good stability. In addition, they are normally inexpensive and environmentally favorable. However, owing to their very poor conductivity, Li<sup>+</sup> can only be partially extracted/inserted at room temperature[1-3]. Elevating the temperature was reported to significantly improve the capacity.[4] For example, the capacity of LiFePO<sub>4</sub> was almost doubled from 23°C to 60°C. By coating an electronically conducting layer on LiFePO<sub>4</sub>, almost full theoretical capacity was achieved at 80°C in a polymer electrolyte cell[5]. In the present work, we prepared a LiFePO<sub>4</sub>/C composite which exhibits ~95% Li capacity at room temperature.

The LiFePO<sub>4</sub>/C composite was prepared by mixing CH<sub>3</sub>COOLi, (CH<sub>3</sub>COO)<sub>2</sub>Fe, and NH<sub>4</sub>H<sub>2</sub>PO<sub>4</sub> with a carbon gel, and then heating the mixture at 700°C for 10 hours under an inert atmosphere.

Electrochemical cells were constructed in a Swagelok design, utilizing 1M LiPF<sub>6</sub>/EC-DMC as the electrolyte, and a cathode composite with 10% carbon black, and 5% PVDF binder. Charging/discharging profiles of the LiFePO<sub>4</sub>/C composite at C/10 at 25°C are shown in **Fig.1**. In the first cycle, nearly all of the Li (0.98 Li/LiFePO<sub>4</sub>) was extracted during charge, and 0.95 Li/LiFePO<sub>4</sub> (162 mAh/g) was recovered in the following discharge. The irreversible loss is as low as ~3%. Following cycles displayed excellent reversibility with a discharge/charge efficiency close to 100%.

The rate behavior is illustrated in **Fig.2**. At a low rate, e.g. C/10 or C/5, over 90% of the Li was accessible; at an intermediate rate, e.g. C/2, close to 90%; and at high rates, e.g. 5C, ~70% of the reversible capacity was still accessible.

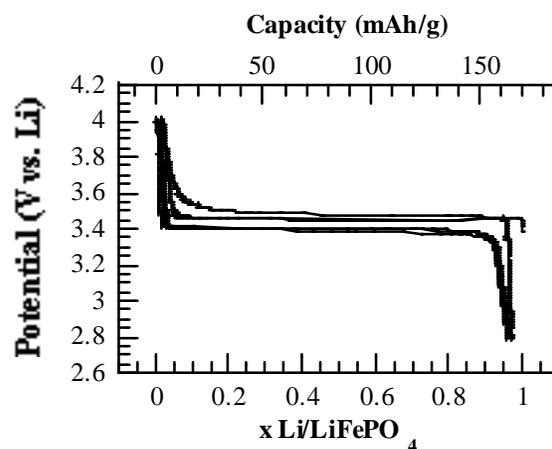
The cycling stability tests were performed at a C/5 for 100 cycles (**Fig. 3a**) and at 5C for 800 cycles (**Fig. 3b**). At both rates, the composite material showed excellent cycling stability. At C/5, after 100 cycles only a subtle loss of capacity was observed. At 5C, the capacity increased on initial cycling to reach a maximum at ~120 mAh/g, and then lost ~8% over 800 cycles.

In conclusion, the LiFePO<sub>4</sub>/C composite successfully achieved almost full capacity with good rate capability and excellent stability, making this material an almost ideal cathode at room temperature. The results of doping this material, and extending the method to vanadium phosphates will also be discussed in the presentation.

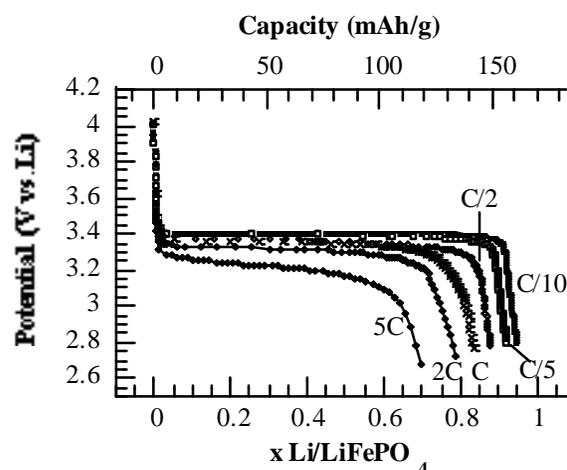
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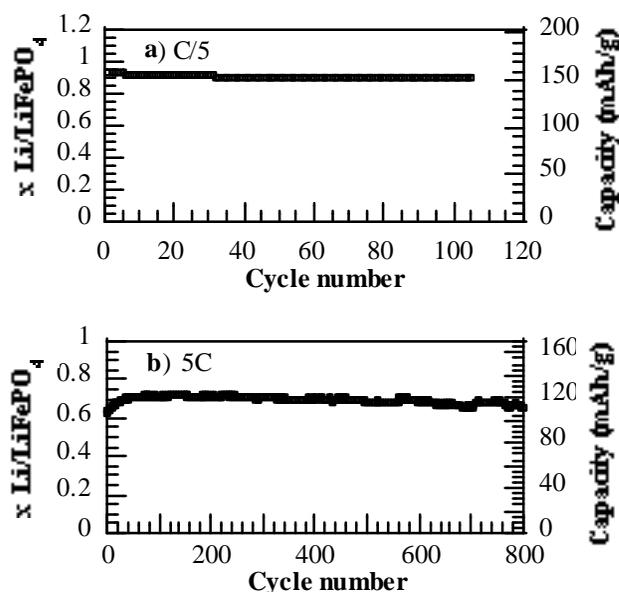
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**Fig.1** The charging/discharging profiles of the first three cycles of LiFePO<sub>4</sub> at C/10 in the potential range from 2.8 V to 4.0 V



**Fig. 2** Discharge curves of LiFePO<sub>4</sub> at various rates.



**Fig. 3** Electrochemical cycling tests of LiFePO<sub>4</sub> at a) C/5; and b) 5C