Li₂FeP₂O₇ as cathode material for Li-ion batteries Andreas Blidberg, Torbjörn Gustafsson, Fredrik Björefors Uppsala University, Department of Chemistry - Ångström Laboratory

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To meet the growing demand for Li-ion batteries, inexpensive cathode materials made from abundant natural resources are required. Today's cathode materials are to a large extent based on cobalt, which is considered a strategic metal¹. Iron based cathode materials provide possible alternatives to cobalt based ones. Today LiFePO₄² has become the state-of-the-art iron based cathode material due to its high power efficiency with a structure stability resulting in high intrinsic safety. The drawback is the low potential (3.4 V vs. Li⁺/Li).

With the intention to investigate a number of existing and novel iron based materials regarding their electrochemical properties as cathodes, initial studies of $\text{Li}_2\text{FeP}_2\text{O}_7^3$ have been conducted in this work. $\text{Li}_2\text{FeP}_2\text{O}_7$ was synthesized, characterized, and used in pouch cell batteries. Figure 1 shows an XRD-pattern of the synthesized product.



Figure 1. XRD-pattern of the synthesized Li₂FeP₂O₇

 $Li_2FeP_2O_7$ offers a quasi two-dimensional diffusion pathway of Li-ions, which enables high electrochemical capacity even without nanosizing. It has been shown that reduction of the particle size by a combustion synthesis instead of a ceramic synthesis does not affect the electrochemical performance to a large extent. On the contrary, combustion synthesis provides a possible route to industrial up-scaling⁴. Materials with one-dimensional lithium diffusion, such as LiFePO₄, are also more sensitive to defects upon cycling, which could block the Li⁺ diffusion in a large part of the material.

In addition to the advantageous 2D lithium diffusion, Li₂FeP₂O₇ provides a slightly higher potential than LiFePO₄. It is also possible to increase the potential further by manganese doping. In Li₂FeP₂O₇ iron is either present in FeO₆ octahedral sites or FeO₅ bipyramidal sites, with some mixing of FeO₅ sites with LiO₅ sites. However, the FeO₅ sites can be stabilized by doping the material with manganese, resulting in some redox activity approaching 4 V^5 , compared to 3.5 V vs Li⁺/Li for the pure Li₂FeP₂O₇. If the Fe⁴⁺/Fe³⁺ redox couple can be accessed, there is also the possibility of extracting two Liions per Li₂FeP₂O₇ formula unit, resulting in a theoretical capacity of 220 mAh/g. There has been some indications that the $Fe^{4+/}Fe^{3+}$ redox couple could be active at potentials higher than 5 V vs. Li+/Li⁶, but more stable electrolytes than the standard organic liquid electrolytes are required to investigate this further.

These aspects of Li₂FeP₂O₇ together with cycling data for

half cells will be presented in this contribution.

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