

Exploring Li-Fe-F phases as cathode materials for Li-ion batteries

Tanghong Yi, Chunjoong Kim, Jordi Cabana
University of California, Lawrence Berkeley National
Laboratory
One Cyclotron Rd, Berkeley, CA 94720

Given the worldwide increasing demand of energy, new energy resources and conversion systems are under extensive research, with energy storage playing a very prominent role. Lithium ion batteries, the premier technology for portable power, need further development to meet the needs of different applications and to seize the automotive market. Cost, energy and power density, safety and cyclability are the main issues in lithium ion batteries. Chemical or physical modifications, such as coating, doping, adding additives and nanoengineering, to improve the performance of existing materials is one way to resolve the issues. Exploring new materials with superior electrochemical performance is the other way to solve the challenges that battery technology is facing.

Intercalation electrode materials are still the main object of research on cathode materials. Compounds containing $\text{Fe}^{2+}/\text{Fe}^{3+}$ with strong ionic character have attracted attention due to the merits of cost, safety and environmental friendliness. A lot of research has been done on Li-Fe- PO_4 and Li-Fe- SiO_4 systems,(1-6) but only a few on Li-Fe-F system.(7, 8) Quite a few stable Li-Fe-F ternary phases have been predicted by first principle calculations.(9) However, very few of them have been experimentally synthesized, especially, if the phases contain Fe^{2+} . In this report, we report attempts to make LiFeF_3 and Li_2FeF_4 ternary phases through other alkali metal iron fluorides AFeF_3 and A_2FeF_4 ($\text{A} = \text{Na}, \text{K}$). For instance, cubic KFeF_3 and tetragonal K_2FeF_4 (Fig. 1) are synthesized by solid state method. $\text{K}_{1-x}\text{Li}_x\text{FeF}_3$ ($0 \leq x \leq 1$) and $\text{K}_{2-x}\text{Li}_x\text{FeF}_4$ ($0 \leq x \leq 2$) phases can be achieved by ion exchange method and electrochemical cycling versus lithium. The synthetic methodologies, phase characterization by X-ray and synchrotron diffraction, and electrochemical performance will be presented.

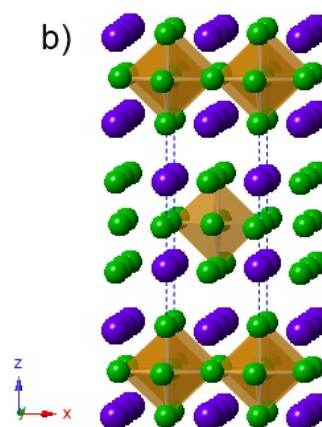


Fig.1: crystal structure of a) KFeF_3 and b) K_2FeF_4 , the mauve, dark orange and green color represent K, Fe, and Fe, respectively.

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