Karlsruhe Institute of Technology

Institute for Applied Materials

Novel Sol-gel processing and eletrochemical characterization of monoclinic Li_3FeF_6

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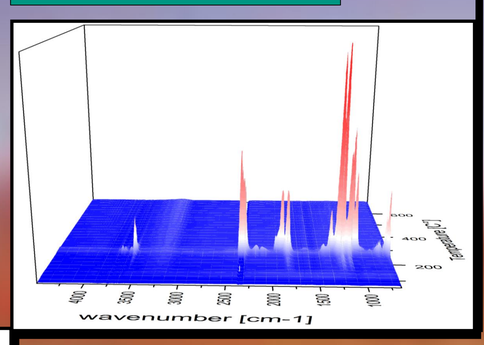
Introduction:

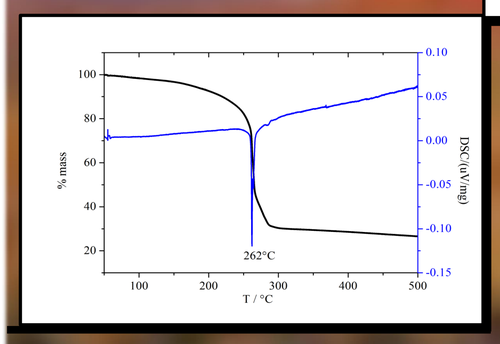
To find new cathode materials for future applications in lithium ion batteries, lithium transition metal fluorides seem to be an interesting class of materials. In principle the Li intercalation voltage can be increased by replacing oxygen in the cathode host structure for the more electronegative fluorine. An easy scalable pyrolytic sol-gel process with trifluoroacetic acid as fluorine source is used to synthesize monoclinic Li_3FeF_6 using non toxic chemicals. For usage as a cathode in lithium ion batteries monoclinic Li_3FeF_6 was ball milled with carbon and binder down to nano-scale. A fully reversible capacity of 129 mAh/g can be obtained for the first cycle. To the best of our knowledge this is the first performance based battery test for lithium transition metal fluorides up to 1C with a capacity up to 71 mAh/g. The redox couple Fe^{3+}/Fe^{2+} of the host structure during Li insertion/deinsertion could be confirmed with ex situ XPS and cyclic voltammetry.

Sol-Gel Route
No toxic chemicals
like LiF, F_2, HF

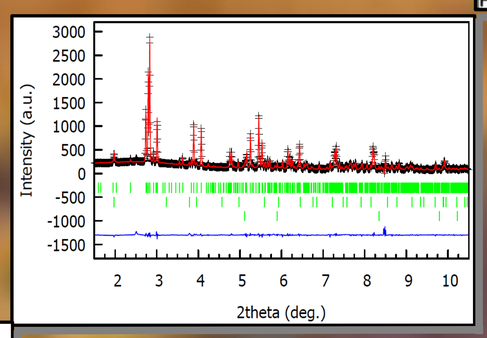
TG-FTIR



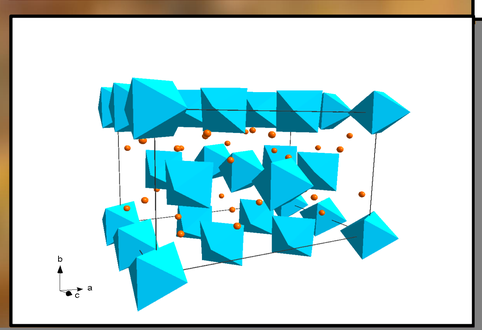
TG-DSC



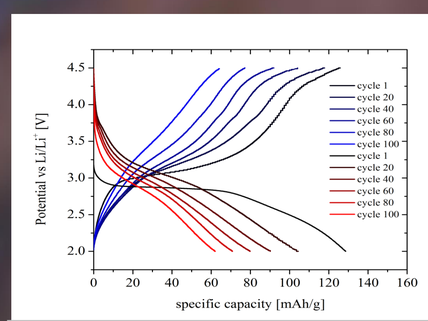
Characterization



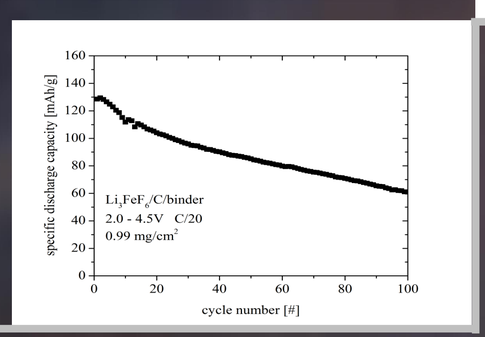
Structure S.G. C/2c



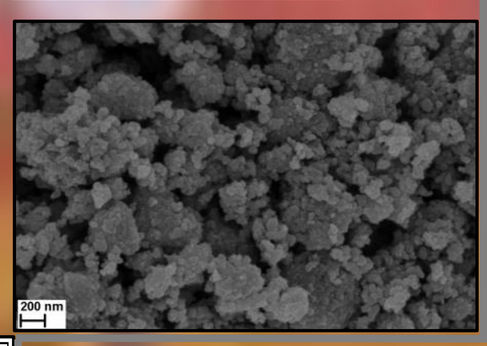
Electrochemistry



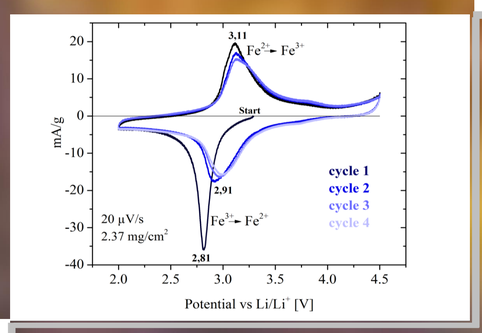
Cycle stability



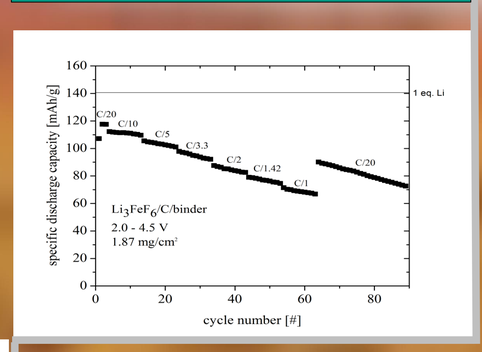
Morphology



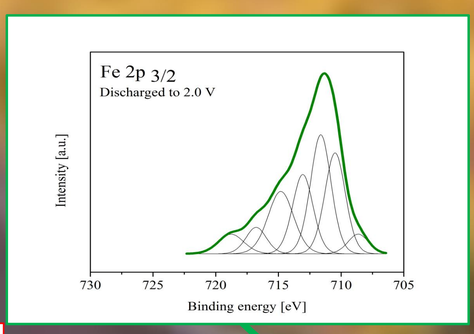
Cyclo voltammetry



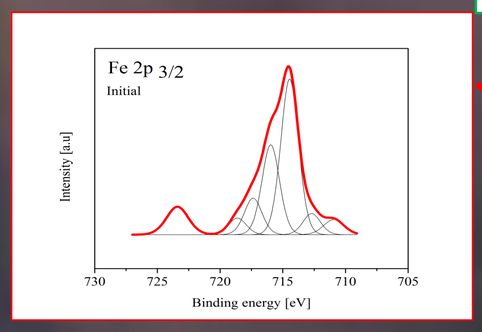
Performance rate test



XPS-analysis



Ex-situ investigation



$Li_3FeF_6 \overset{\pm Li}{\longleftrightarrow} "Li_4FeF_6"$

Conclusions

- A novel synthesis was established for Li_3FeF_6
- 91 % of the theoretic capacity can be obtained
- Even at high discharge rates 50 % of the capacity
- Redox couple Fe^{3+}/Fe^{2+} can be confirmed

Outlook

- In-situ XANES and EXAFS investigations
- Ex-situ NMR and Mössbauer investigations
- Synthesis of new compounds and their electrochemical investigation.