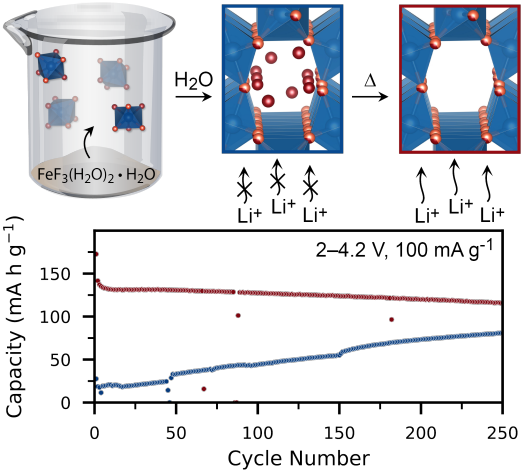
Dissolution-Precipitation Synthesis of Pyrochlore-Type Iron Hydroxy Fluoride for Low-Cost Lithium-Ion Batteries

J. F. Baumgärtner[1,3], M. Wörle[1], C. P. Guntlin[1], F. Krumeich[1], S. Siegrist[1], V. Vogt[1], D. C. Stoian[2], D. Chernyshov[2], W. van Beek[2], K. V. Kravchyk[1,3]*, M. V. Kovalenko[1,3]*

[1]Laboratory of Inorganic Chemistry, Department of Chemistry and Applied Biosciences, ETH Zürich, Vladimir-Prelog-Weg 1, CH-8093 Zürich, Switzerland, [2]Swiss–Norwegian BeamLines at the European Synchrotron Radiation Facility, 38000 Grenoble, France, [3]Laboratory for Thin Films and Photovoltaics, Empa – Swiss Federal Laboratories for Materials Science and Technology, Überlandstrasse 129, CH-8600 Dübendorf, Switzerland

Iron (III) fluorides are appealing low-cost stationary energy storage materials due to the virtually unlimited supply of the constituting elements and high energy densities.[1] The pyrochlore modification is of particular interest because its 3D interconnected channels may potentially enable fast Li-ion diffusion.[2] However, the prohibitevely large cost for synthesis or cathode architecture prevent commercialization. Herein, we present a facile dissolution-precipitation synthesis to access pyrochlore iron (III) hydroxy fluoride (Pyr-IHF) from soluble iron (III) fluoride precursors, enabling to produce Pyr-IHF at a low cost of *ca*. 14 \$ kg^{-1}.[3] Without the need for elaborate cathode designs, we demonstrate superior capacity retention of > 80% after 600 cycles at high current densities of 1 A g^{-1}. Guided by *operando* X-ray diffraction experiments, we selectively synthesize Pyr-IHF of different solvent content inside the channels. Rate capability tests of Pyr-IHF cathodes provide the first experimental evidence for Li-ion diffusion occurring through the 3D channels.



[1] F. Wu, G. Yushin, *Energy Environ. Sci.*, **2017**, 10**,** 435–459
[2] C. Li *et al., J. Am. Chem. Soc.* **2013**, 135, 11425–11428
[3] J. F. Baumgärtner *et al., Manuscript Submitted*, **2023**