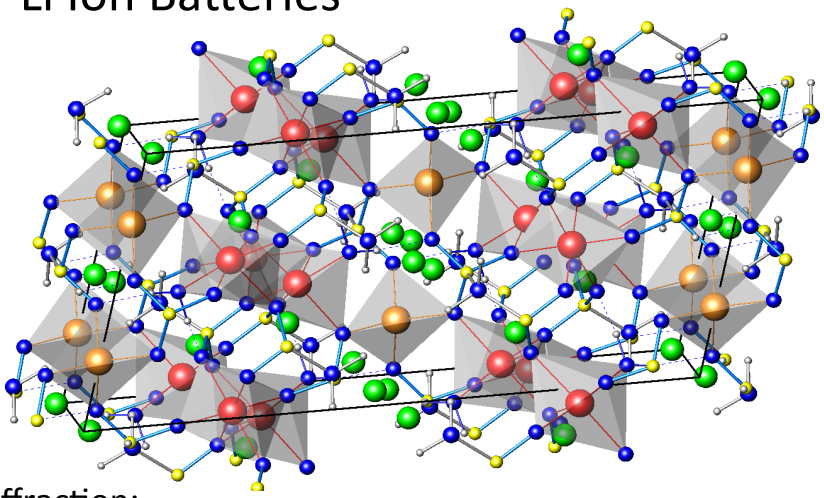
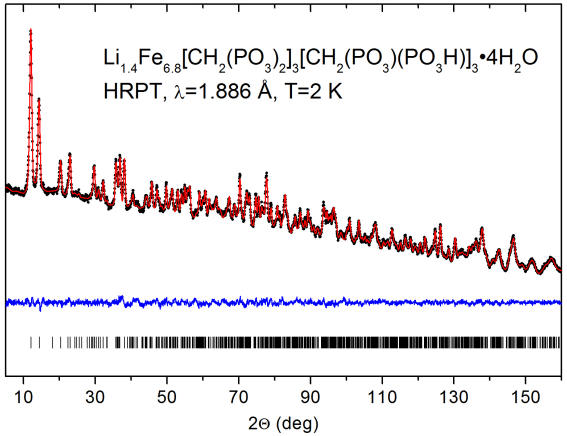
Lithium Iron Methylenediphosphonate: A Model Material for New Organic–Inorganic Hybrid Positive Electrode Materials for Li Ion Batteries



- Search for organic–inorganic hybrid materials as a promising option for the future battery electrode materials: model material ($Li_{1.4}Fe_{6.8}[CH_2(PO_3)_2]_3[CH_2(PO_3)(PO_3H)]\cdot 4H_2O$)
- a specific charge of up to 128 (mA h)/g upon galvanostatic cycling after 200 cycles at a theoretical value of 168 (mA h)/g.
- Operando X-ray absorption near-edge spectroscopy: confirms the reversible cycling of Fe ions between Fe(II) and Fe(III)
- Structure determination based on neutron and X-ray powder diffraction:
  - ✓ SLS data (Material Sciences Beamline) used to index the pattern and find the most probable space group;
  - ✓ HRPT data used to determine the structure
- One of the most complex crystal structures ever determined at HRPT:
  - ✓ Sp. Gr. C 2/c, 18.8 x 8.31 x 8.96 x 107.1 (V=1340 $Å^3$),
  - ✓ 19 independent atoms, ~60 internal structure parameters.
- three different Fe positions, also confirmed by Mössbauer spectroscopy.



- proves the applicability of transition-metal diphosphonates as positive electrode materials for Li ion batteries.

Reference:

S. Schmidt, D. Sheptyakov, J-C. Jumas, M. Medarde, P. Benedek, P. Novák, S. Sallard, and C. Villevieille, Chemistry of Materials 2015, 27, 7889–7895.