

# Combined in situ XRD and XAS studies on materials for Li-ion batteries

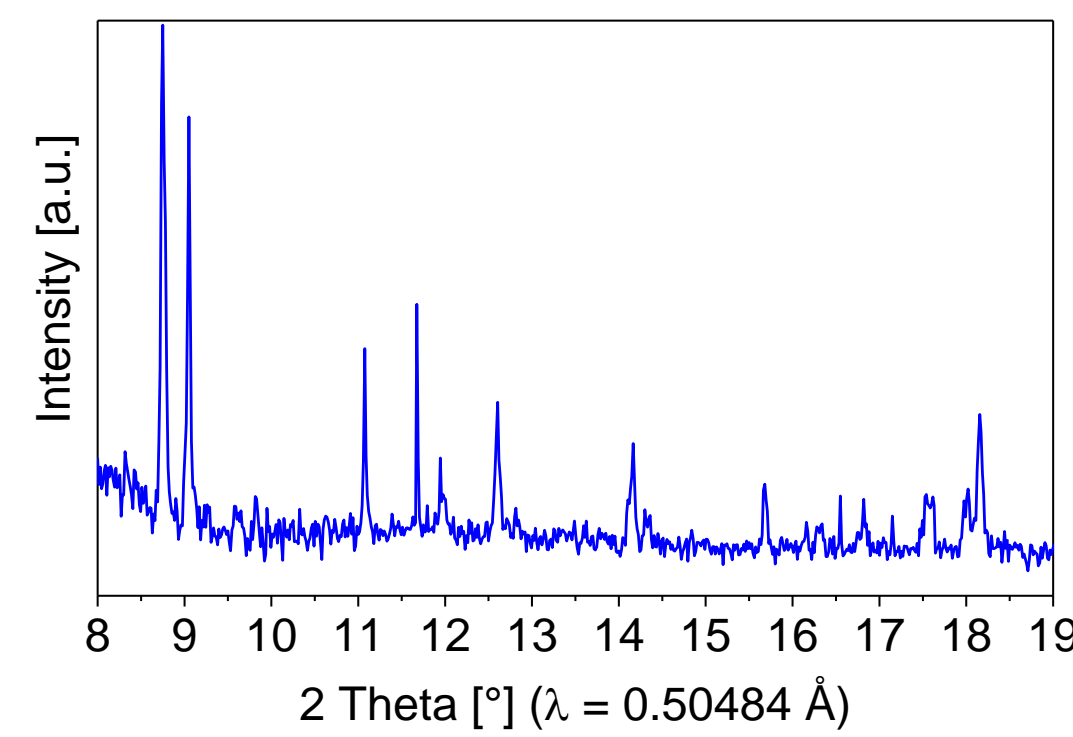
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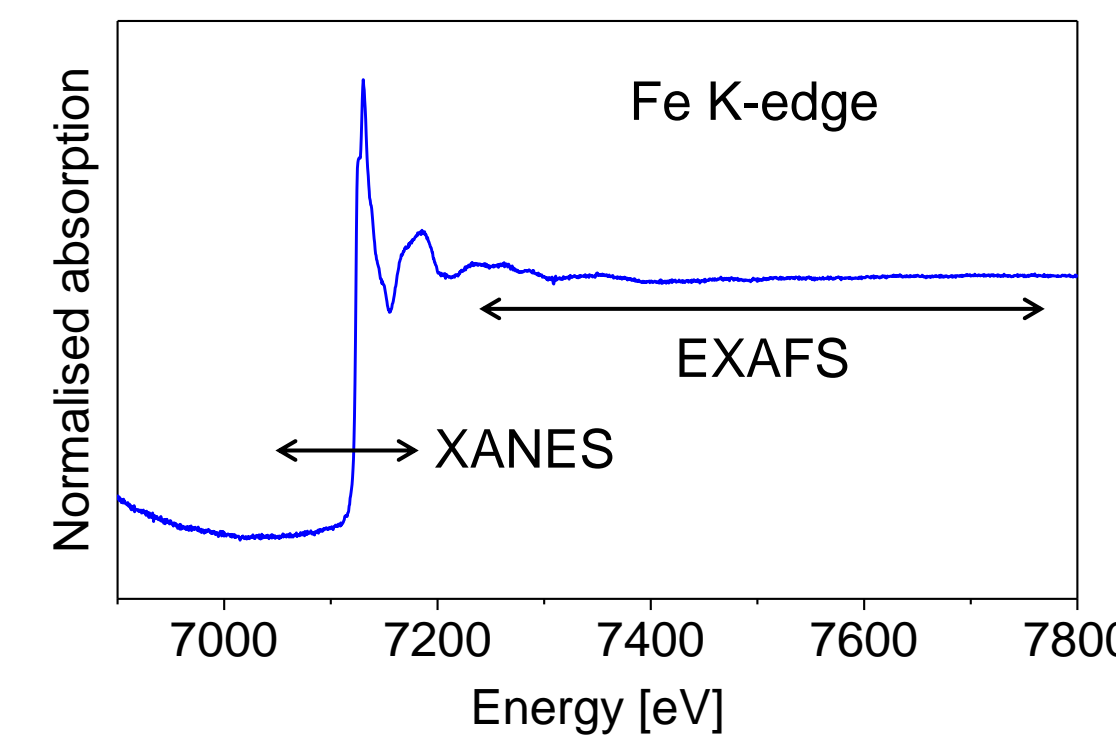
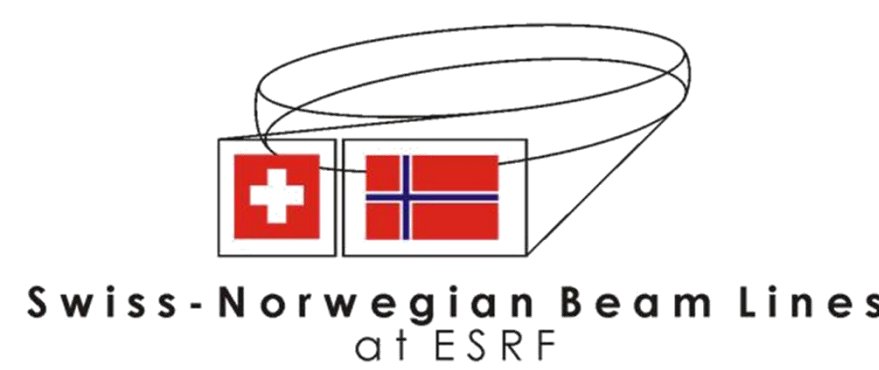
**Goal:**  
Construction and validation of a combined in situ cell for XRD and XAS to study reaction mechanisms of materials for Li-ion batteries

**XRD (X-ray diffraction):**

- Phase identification
- Long range order

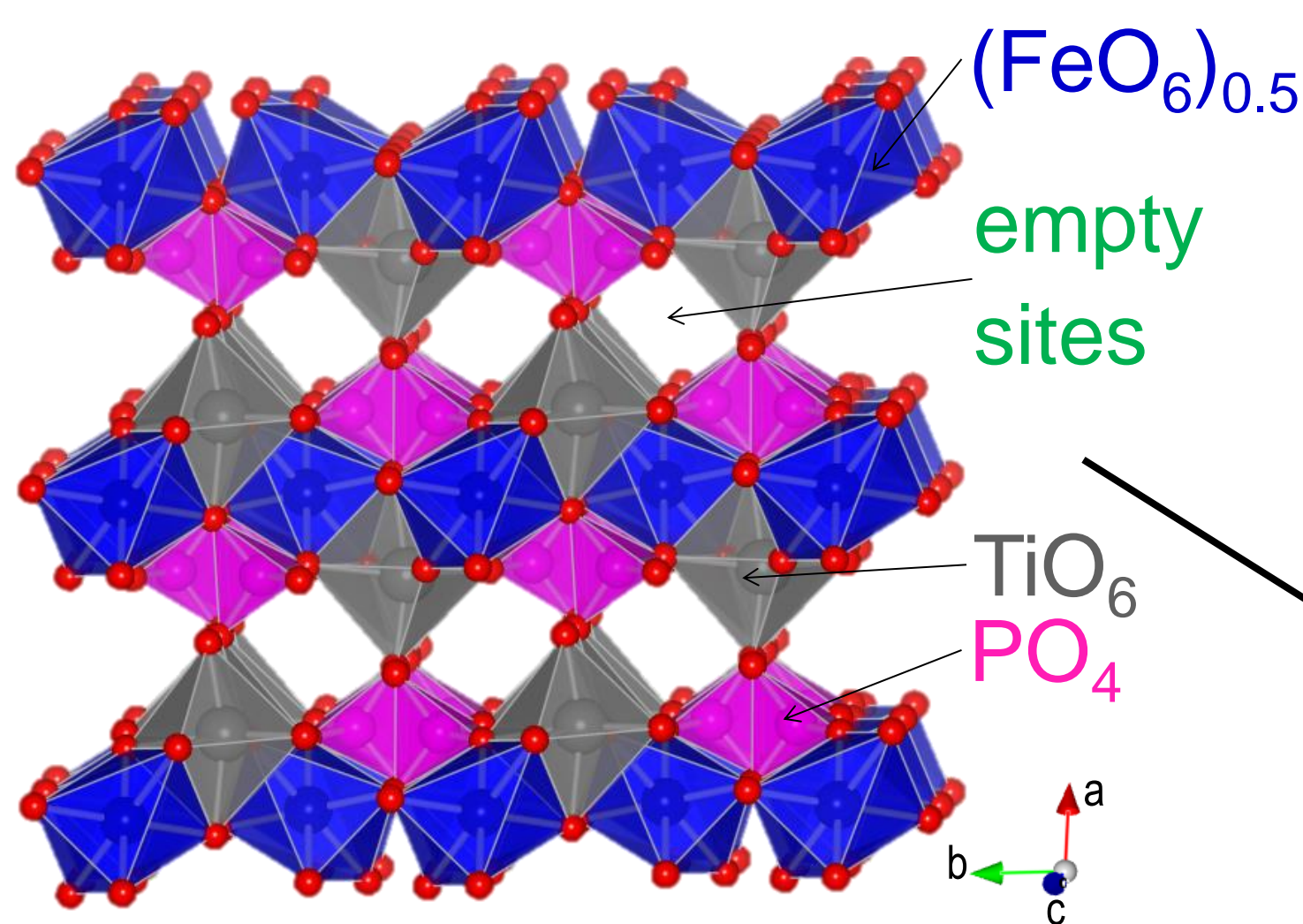


Combination at:



**XAS (X-ray absorption spectroscopy):**

- XANES: Oxidation state & coordination
- EXAFS: Short range order



**Studied material: Fe<sub>0.5</sub>TiOPO<sub>4</sub>**

1.5 empty sites per formula unit  
But reaction with 5-3 Li<sup>+</sup> per formula unit

How are the extra Li<sup>+</sup> accommodated?  
What is the reaction mechanism?

Successful combination of XRD and XAS in one in situ cell



**In situ cell:**

- Easy and quick to assemble
- Exchangeable window material
- Good lithiation behaviour
- Dendrites in delithiation
- Very little overpotential

