

ECXAS: A data aggregation tool for battery study in ROCK beamline

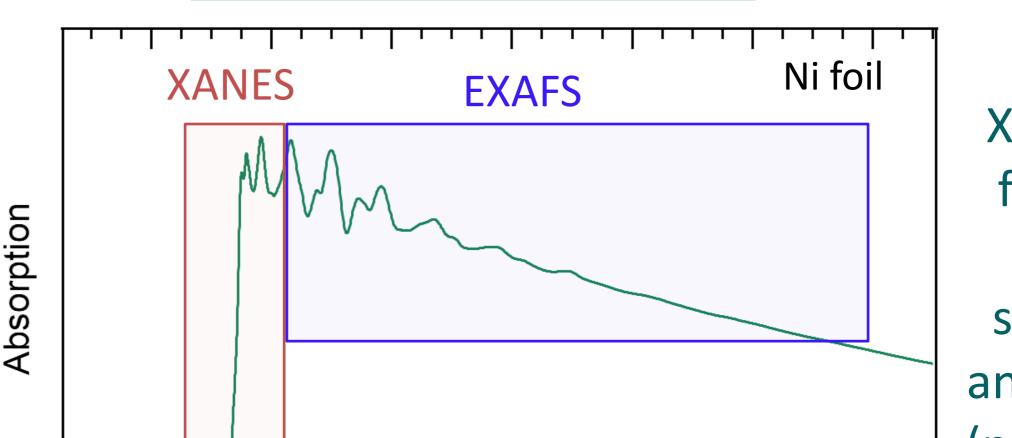
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<u>Why?</u>

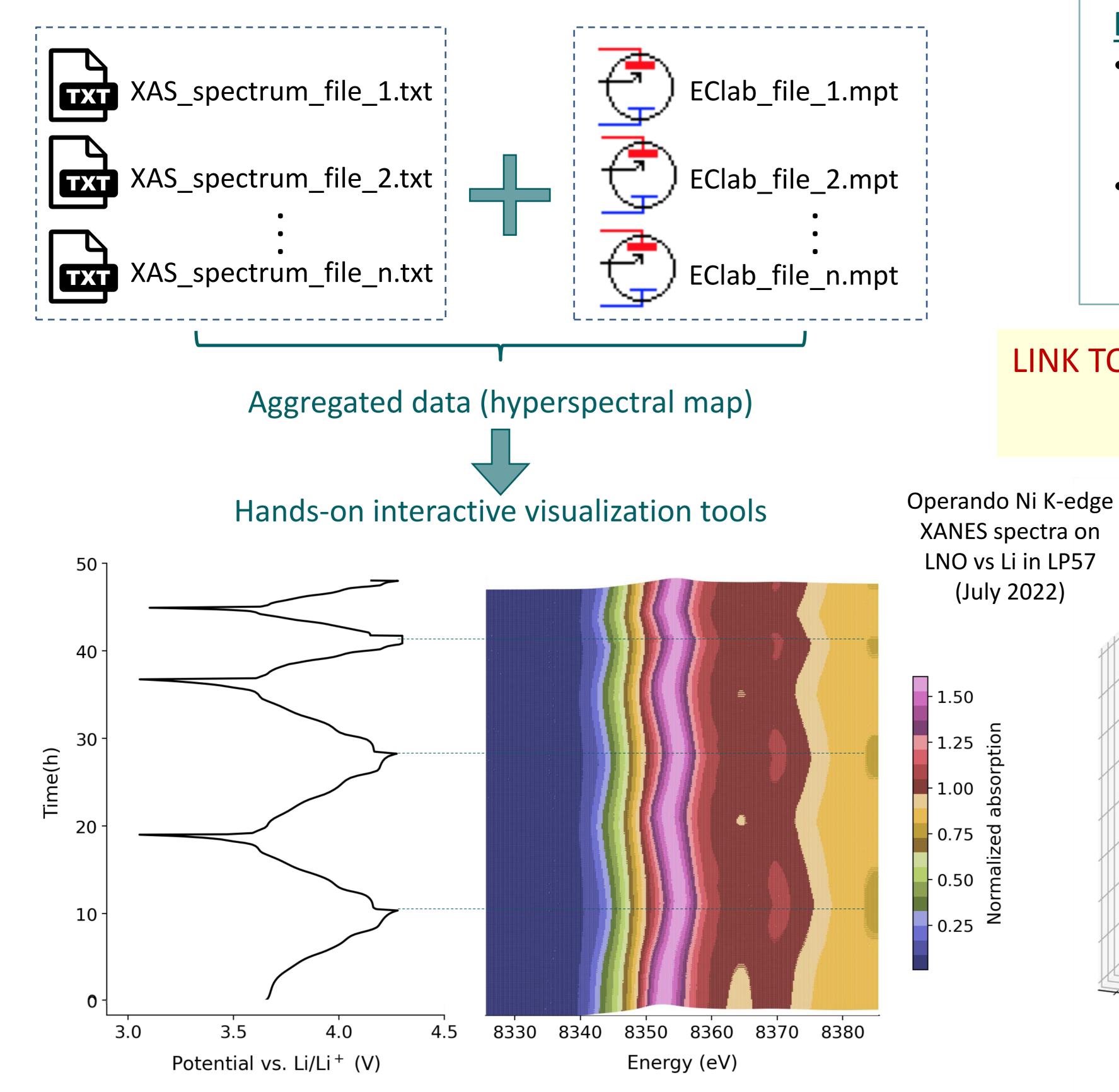
- Battery materials study requires insight from multiple techniques
- **e.g**. operando x-ray absorption experiments coupled with electrochemical characterization
- Additional complexity in synchrotron-based experiments: continuously increasing time/space resolution.
 - → higher data dimension and larger data volume.



Example of XAS spectrum

XANES region is a fingerprint of an atom oxidation state (edge shift) and local geometry

New tool for asynchronous data aggregation and semi-automated data processing becomes thus decisive during and after each experiment.



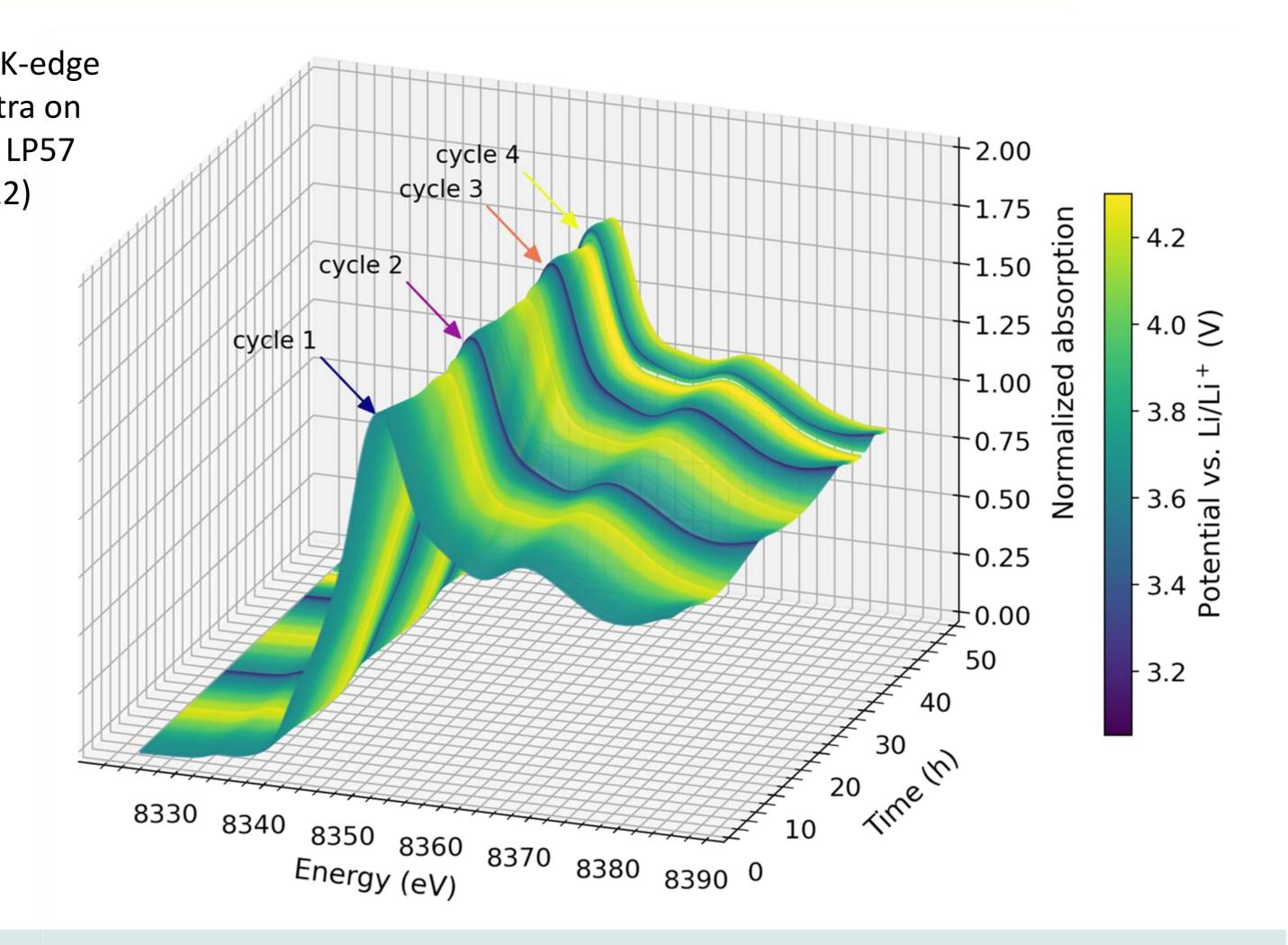
= pre-edge + edge + XANES 8200 8400 8600 8800 9000 9200 9400 Energy (eV)

How?

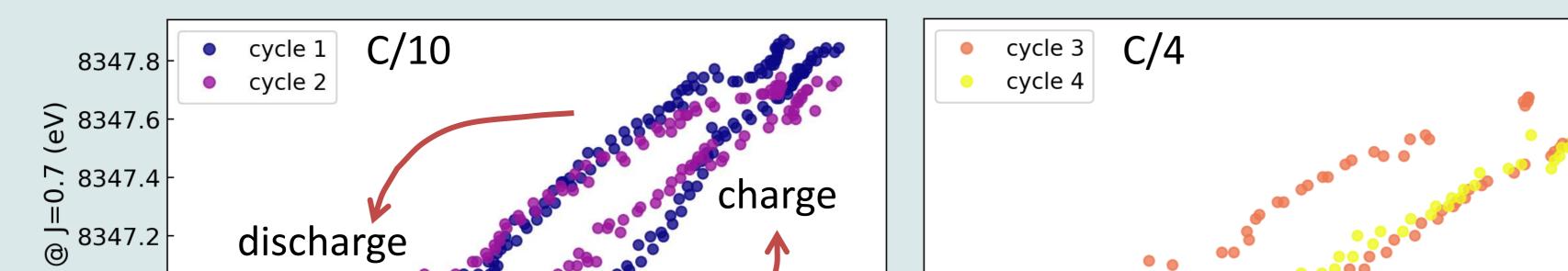
- Python Jupyter notebook with a developed library for data aggregation and interactive visualization tools, focused on the XANES region.
- Easy comparison:
 - Over time (for one cell)
 - Among different types of cells

LINK TO PACKAGE (Jupyter Notebook with example)

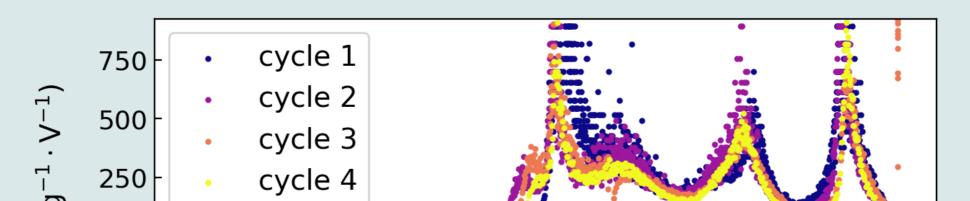
https://github.com/GhostDeini/perex



Evolution of the edge position at different C-rates



Basic visualization of the electrochemical data Differential capacity vs. potential



3.6

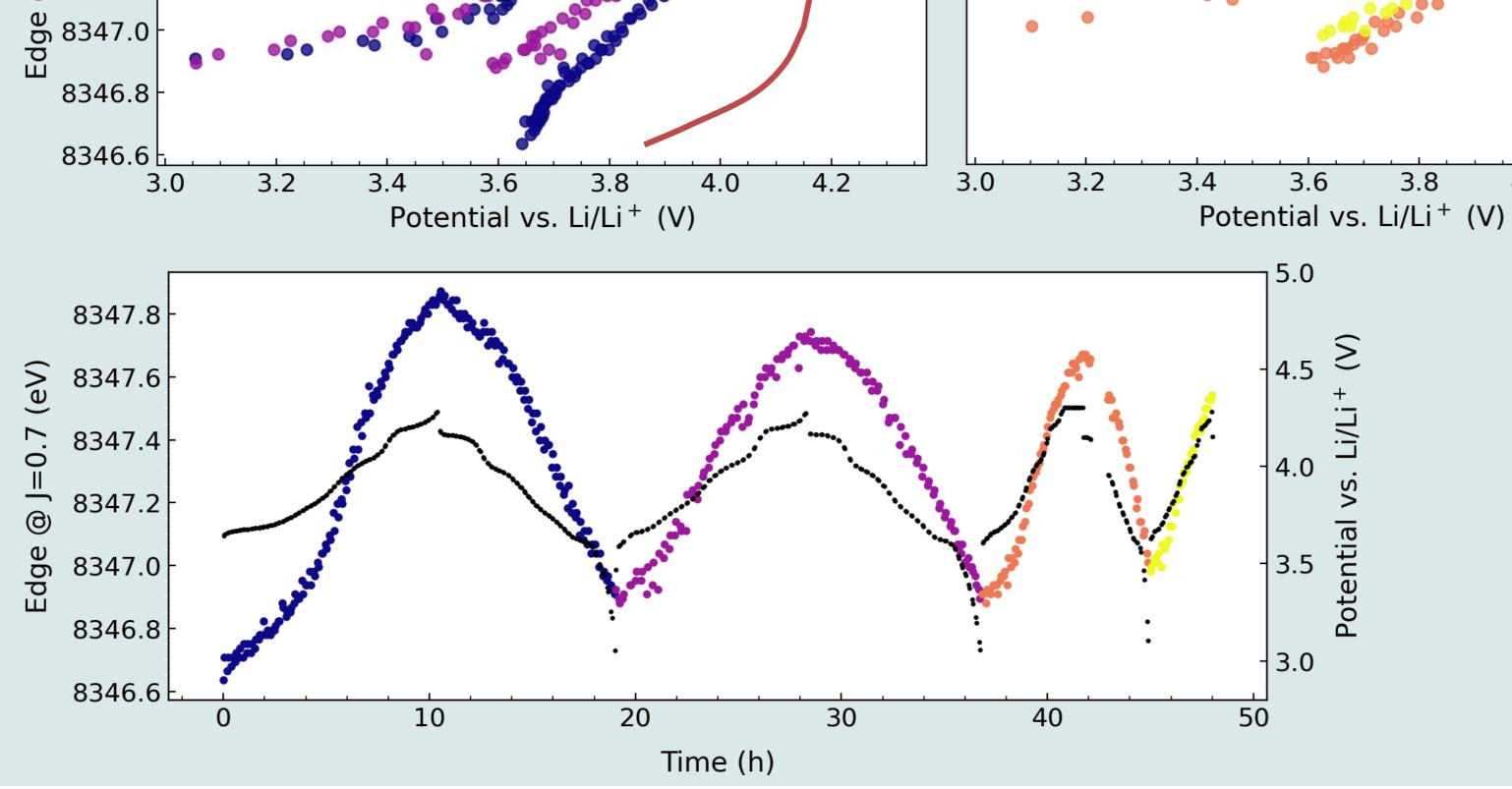
Potential vs. Li/Li⁺ (V)

3.4

3.8

4.0

4.2



Future work:

4.2

4.0

• Try linear combination fitting of spectra using modeled reference samples (e.g. using FEFF, MXAN)

3.2

- Scripts for semi-automatic data processing in Larch python.
 → pre-edge fitting
 - \rightarrow EXAFS region.

(mAh

Vb/Qb

-250

-500

-750

3.0

NOBUGS 2022 – 19-22 September, Paul Scherrer Institut, Villigen, Switzerland