

Developing a platform for rapid multimodal operando analysis of batteries

Project title:	Developing a platform for rapid multimodal operando analysis of batteries
PRISMAS Research Area:	Clean Energy
Supervisor:	William Brant
Hosting University:	Uppsala University
Partners:	Northvolt
Link to position:	Apply here

1. Project summary:

Energy storage devices such as lithium-ion batteries are exquisitely complex chemical systems with multiple components interacting in ways dependent on the operating conditions. The intertwined reactions subsequently create changes that manifest over multiple length and time scales. This project will aim to implement an electrochemical cell for simultaneous rapid X-ray diffraction and X-ray absorption spectroscopy together with realistic electrochemical cycling. The project will specifically focus on rock salt oxide derived cathode materials for lithium and sodium ion batteries. To support the implementation and uptake of the cell by researchers from academia and industry, routines for processing and analysing the large quantity of data produced will be developed. Such developments will subsequently pave the way for high throughput studies providing unprecedented insight to the chemical mechanisms responsible for aging and degradation.

2. Keywords (up to 5)

Operando diffraction, X-ray absorption spectroscopy, Lithium ion batteries, high throughput

3. Project outline

- **State of the art:**

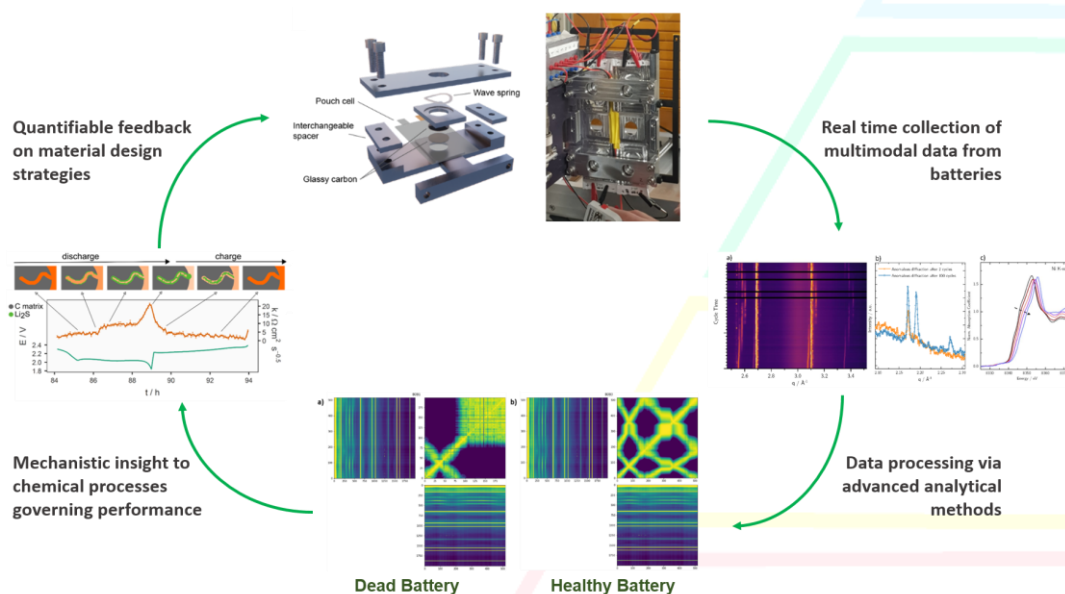
The chemical processes which govern battery performance are notoriously difficult to probe. The critical processes occur while a battery is in operation and involve reactive, short lived intermediate species. Therefore, characterisation must be performed under *operando* conditions [1]. I.e, non-evasively during electrochemical cycling of a realistic device. Two highly popular methods for probing changes inside a battery are X-ray diffraction (XRD) and X-ray absorption spectroscopy (XAS). Together the techniques provide highly complementary data on the atomic and electronic structure of a material, respectively. In a battery, the electrode materials which are often crystalline, undergo reduction and oxidation reactions which change their electronic structure and subsequently the atomic structure. As such, changes observed via XRD and XAS can be used as proxies for evaluating the state of health of a battery [2]. This project will unlock the full potential of these techniques by combining them together with advanced electrochemical characterisation tools such as impedance and intermittent current interruption [3, 4]. As such, in a single multimodal experiment a holistic picture of structure and function can be captured. This will greatly streamline the design and development of materials for lithium and sodium ion batteries by rapidly identifying key markers for

degradation and aging.

- **Project objectives:**

The project will focus on developing a platform for multimodal *operando* experiments using ARD and XAS. Initially commercially available positive electrode materials for lithium-ion batteries will be explored, for example, $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$ (LNMO) and $\text{LiNi}_{0.8}\text{Co}_{0.1}\text{Mn}_{0.1}\text{O}_2$ (NCM811). These are materials which are investigated by a number of researchers within the Ångström Advanced Battery Center and so are a suitable starting point to establish analysis routines. These are also materials which are sourced from commercial partners, such as Northvolt, who have a stake in the research that will be performed.

The PhD student in the project will construct an experimental platform for performing combined *operando* XRD and XAS on multiple lithium-ion batteries during electrochemical cycling. Currently a multicell holder exists for the DanMAX beamline which was designed by our team. This will be modified for compatibility with the Balder beamline and the experiment designed such that measurements can be automated. Data analysis routines will be developed to cross-correlate measurement results from XRD, XAS and electrochemical data. Several analysis methodologies will be explored including sequential Rietveld refinement [5], pearson correlation analysis [6] and other chemometric approaches [7]. Spectroscopic and structural insights will be compared against multiple electrochemical performance metrics such as coulombic efficiency, capacity loss and internal resistance. You will be trained how to interpret the resulting data and use this to explain battery performance from a deep understanding of chemical and structural changes.



To facilitate the development of cell holder and analysis pipelines, a ~6-month secondment at MAX IV Laboratory in Lund is envisioned using the Balder beamline. This secondment could be extended depending on the need. In addition, it is likely that visits to other synchrotron facilities will occur during the PhD such as the DESY synchrotron light source in Germany and the Diamond light source in the UK. In addition, to facilitate uptake of the *operando* cell and data analysis pipelines by industry frequent exchanges will be held with our industrial partners.

- **References:**

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