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Elucidating structural transformations of electrodes while they are being used: The wonderful world of in situ synchrotron X-ray diffraction

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Electrodes account for a significant proportion of battery function, where atomic-scale perturbations or changes in the crystal structure during an electrochemical process permit the reversible insertion/extraction of charge carriers. A method to both understand battery function and improve their performance is to probe the crystal structure evolution in operando or in situ, i.e., while an electrochemical process is occurring inside a battery. In my group we heavily utilize the Powder Diffraction Beamline to track the evolution of the lattice parameters and/or charge carriers, e.g. sodium and potassium, in electrode materials used in rechargeable alkali-ion, primary lithium-metal, Li-S and solar batteries.

In undertaking in situ and in operando experiments there are a number of critical factors that need to be considered, for example optimised cell design to marry electrochemical performance with sufficient diffraction signal. Once the practicalities of such experiments are achieved, the parameter space that can be explored and correlated allows for unprecedented insight into function. Electrochemical parameters such as applied current rates, potential cut-offs and long term cycling can be correlated to chemical parameters such as composition and particle size distribution. Using this information we can design next generation electrode materials, optimising electrochemical performance parameters at a crystallographic level.

In addition to diffraction, my group is expanding our footprint with in situ analytical techniques, including in operando neutron imaging, in operando X-ray absorption spectroscopy and in situ solid-state NMR allowing us to probe non-crystalline components in devices. The combination of these techniques provides more (and multi-scale) insight into the mechanism of device operation and the interactions at play.

This talk will provide a flavor of the work being undertaken in my group, emphasizing the highlights and our future directions.

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