XAFS using Combined Soft and Hard X-rays under Operando and In/Ex-situ Conditions to Solve Reaction Mechanisms in Batteries and Electrocatalysts

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Core-hole based X-ray spectroscopies used under *ex situ*, *in situ* and *operando* conditions provide information vital to unraveling the mechanisms of charge transfer and structural re-organization of electrochemical materials. In this presentation, we will specifically look at how the core-hole techniques of X-ray absorption can be used in the study of electrochemically active materials such as in batteries and fuel cells, particularly by tuning to resonances in both the soft and hard x-ray regimes.

First we will examine the role of oxygen in the charge compensation of $LiMO_2$ compounds and the consequences of such for battery safety and for unprecedented changes to electrical/magnetic properties. The electronic and atomic structure local to oxygen was first examined indirectly using hard x-rays by *operando* resonant K-level measurements of M atoms in battery cathodes of working batteries. The results were then complemented by direct *operando* measurements at the K-edge of oxygen atoms in the cathode using soft x-rays. It will be demonstrated that the detailed electrochemical roadmap for the reaction mechanisms in LiMO2 cathodes could only be revealed by a combination of soft and hard x-ray based experiments. Next, we will look at the effects of dimension, strain and charge transfer on the electrochemical activity and durability of electrocatalysts for both low and high temperature fuel cells. Again, it will be demonstrated that a thorough employment of XAFS and its complementary core-hole methods at both soft and hard x-ray regimes is necessary to reveal a detailed story of the reaction mechanisms in working electrocatalysts.