XES Nanoprobe for Hard X-Ray Region

Research Team: Nancy Hess, Kyle Alvine, Mark Bowden, John Fulton, Tamas Varga (PNNL)
Key Collaborators: Jerry Seidler (University of Washington), Steve Heald (APS), John Lemmon (PNNL)

Purpose

Build a high spatial resolution x-ray emission spectroscopy (XES) capability for *in situ* analysis of x-ray emission lines in the 5- to 10-keV range. The development of a low-cost, modular XES system with combined nanometer spatial resolution and *in situ* capability will be unique and widely applicable to fundamental materials chemistry challenges.

Expected Outcomes

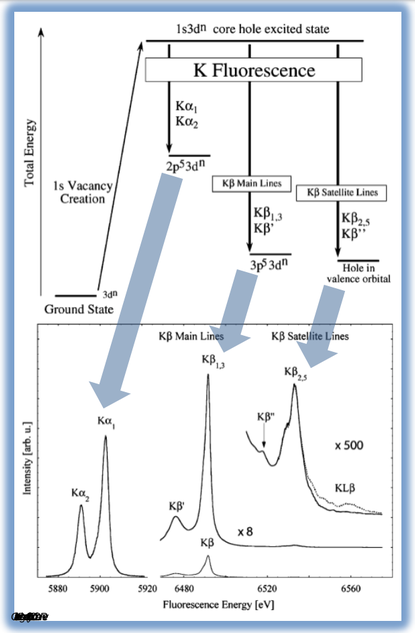
This project will result in the construction of an XES Nanoprobe, first at the APS and ultimately at NSLS2.

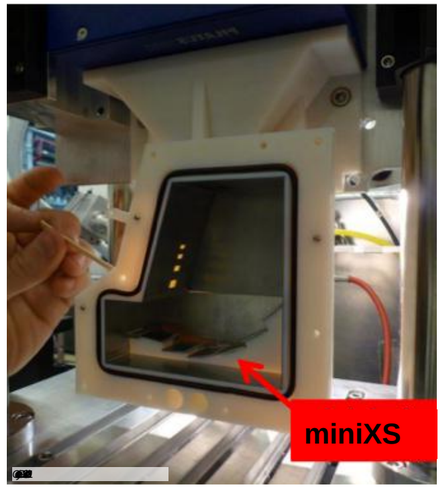
The XES Nanoprobe capability will be demonstrated on two battery systems of current scientific interest: Na/$NiCl_2$ and Ni-doped lithium ion, Li_3Ni.

The fundamental knowledge generated from this project will be published in high-quality journals and lead to programmatic development.

What is Hard XES?

- XES is the measurement of the fluorescent x-rays emitted following the creation of a core hole in the ground state.
- XES gives element-specific, electronic structure information including oxidation state, spin and magnetic state, bond character, and ligand identity.
- Hard XES will probe transition metals, lanthanides, and light actinide elements.
- XES is complementary to XANES and EXAFS measurements.

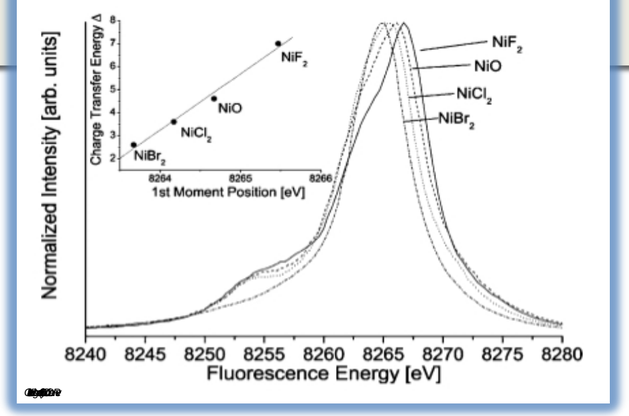




What makes XES Nanoprobe unique?

- Hard, 5-10 keV x-rays allow creation of ***in situ* sample environments**
- miniXS spectrometer is element-specific, modular, low cost, **high resolution and high efficiency**
- Ultimate spatial resolution limited by brightness of synchrotrons
- **Nanometer resolution** attainable at next-generation light sources

Kβ lines in Ni(II) compounds



What are possible applications for the XES Nanoprobe?

- Degradation of Ni-cathode from Na/$NiCl_2$ and lithium-ion battery systems
- 2D domain mapping in magnetic materials
- Other applications: catalysis and energy materials, transition metal centers in biological molecules, and geological materials
- Fundamental studies of lanthanide and actinide electronic structure