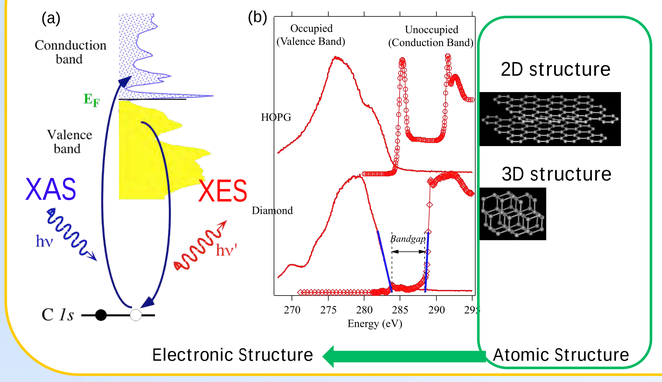
In-situ soft x-ray spectroscopy in battery and catalysis related researches at Beamline 8.0.1.3 and 6.3.1.2.

Yi-Sheng Liu[1*], Timothy Arthur[2], Per-Anders Glens Suzuki[1] and Jinghua Guo[1]

[1] Advanced Light Source, Lawrence Berkeley National Lab, Berkeley, United State, CA 94720
[2] Toyota Research Institute of North America, Ann Arbor, United State, MI 48105
*E-mail: ysliu2@lbl.gov

Abstract
Advanced Light Source (ALS) is one of the most active synchrotron Radiation facilities in the world. Increase demands of sustainable energy resources and energy storage applications make that ALS and our scientists are dedicated to help, to support and to provide fundamental aspects by using Synchrotron Radiation based spectroscopies. Especially, aggressively development of various *in-situ* experimental instrument and capability at the ALS is one of the most important goal to build a functional device in the real world such as ion/air batteries, catalysts and fuel cells. Beamline 8.0.1.3 Wet-RIXS and Beamline 6.3.1.2 ISAAC end stations are soft x-ray spectroscopic (X-ray Absorption and X-ray emission spectroscopy) beamlines that are one of most active beamline in the ALS in *in-situ* soft x-ray spectroscopy. The capabilities of *in-situ* setups for both beamline that cover various fields of interests of such as JCAP and JCSER from solid, liquid to gas phase reactions. Also for a long collaboration with TOYOTA, we had used *in-situ* XAS technique combined with UHV compatible electrochemical cells to identify and monitor the composition/decomposition process of Magnesium ions in Mg ion battery. Furthermore, multivalent metal ion battery, air-battery and high temperature exhausting catalyst projects are under development. Aiming to give a comprehensive understanding of the physical/chemical phenomena behind in electronic structure by using *in-situ* x-ray spectroscopies.

Soft X-ray Spectroscopies probe electronic structure



•Experimental techniques:
X-ray absorption spectroscopy (XAS)
X-ray emission spectroscopy (XES)

Advantages:
- elemental selectivity
- site selectivity
- Oxidation states, chemical and structural sensitivity

Multi-Dimensional Soft X-ray Mesoscale Probes:

Key Electronic Structure
- Conduction and valence bands
- Ligand p-band and metal d-orbital levels

Chemical selective
- Elemental selective; Chemical bonding; oxidation states

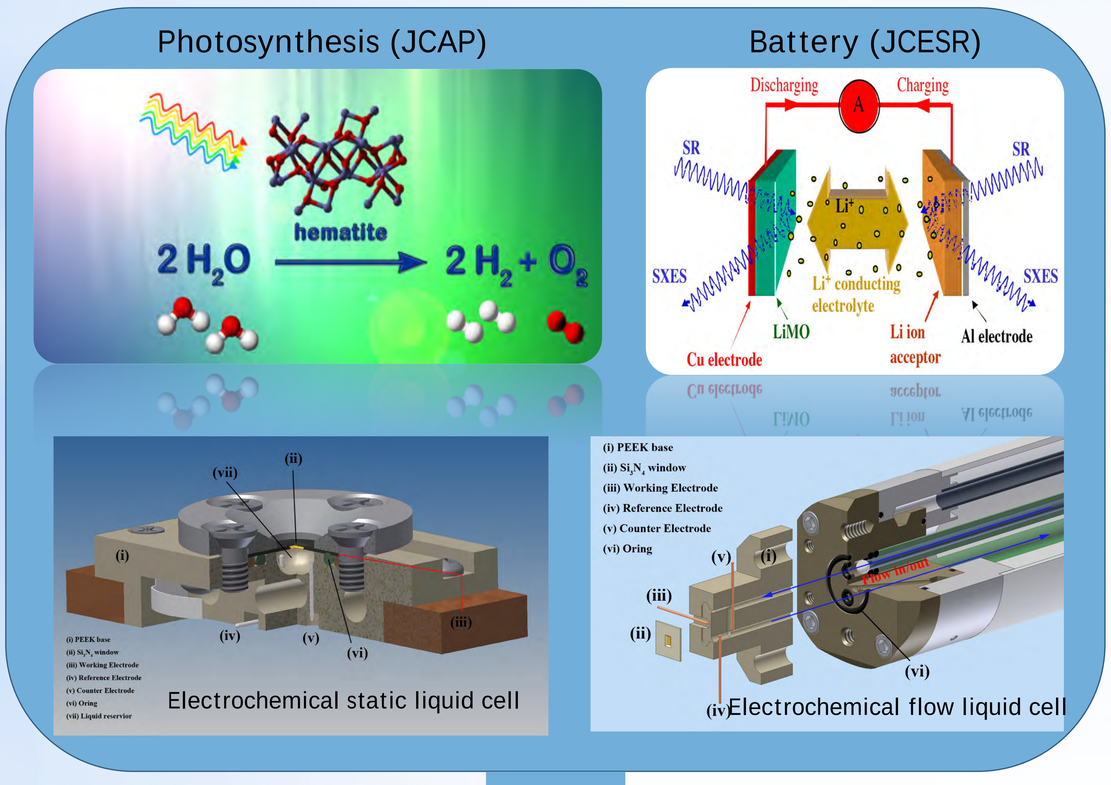
Spatial Resolved (10 – 100 nm)
- XAS: 5 - 100 nm probing depth
- XES and RIXS: 100 nm probing depth

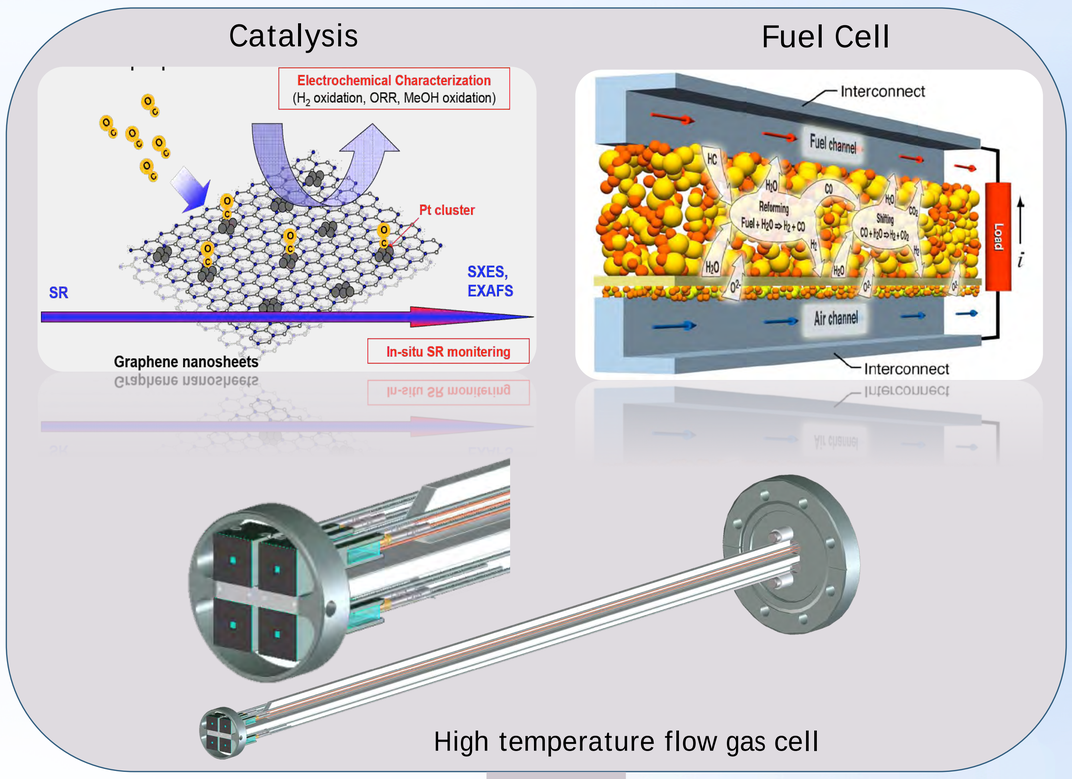
Dynamics while alive:
- Charge transfer, ion transport, electron injection …
- In-situ/in-operando environment (intermediate/transient states)
- Multi time domains (fs, ps, ns, us, and ms, …)

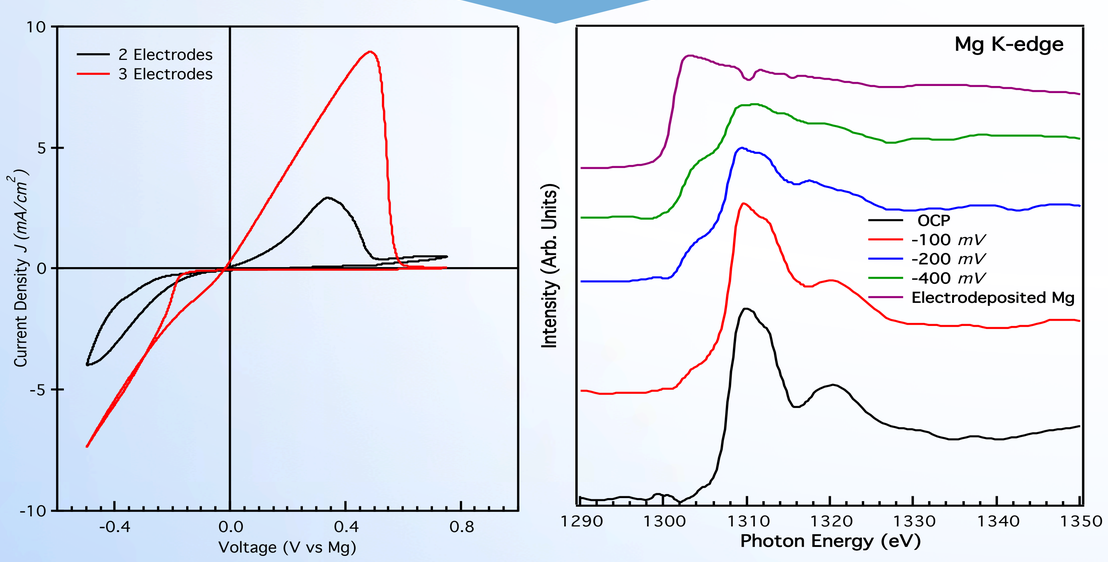
Model Systems (Cells) Characterization:
- Simplify and expose the key interfaces

Our interests @ BL6 and BL8:
Charge Transfer in Energy Conversion and Energy Storage

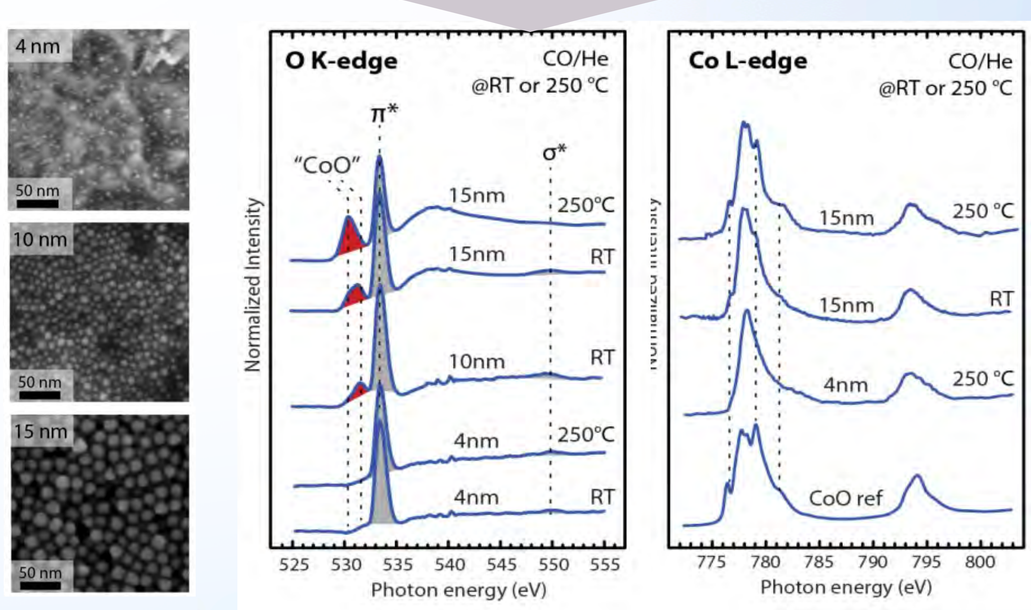
In-situ cells for varying proposed experiments:
Photosynthesis and Battery: Static /flow liquid Electrochemical cell
Catalysis: Flow gas cell.







In-situ XAS studies in Mg metal ions composition/decomposition on cathode in Mg battery:
Left: Electrochemistry CV curves under experimental conditions.
Right: In-situ XAS spectra under reaction.



In-situ XAS in high temperature Co nanoparticle redox in CO/He gases:
Left: SEM images of Co nanoparticles on Au substrate.
Right: In-situ XAS spectra of O K-edge and Co L-edge under redox conditions.