Energy Storage at NSLS II

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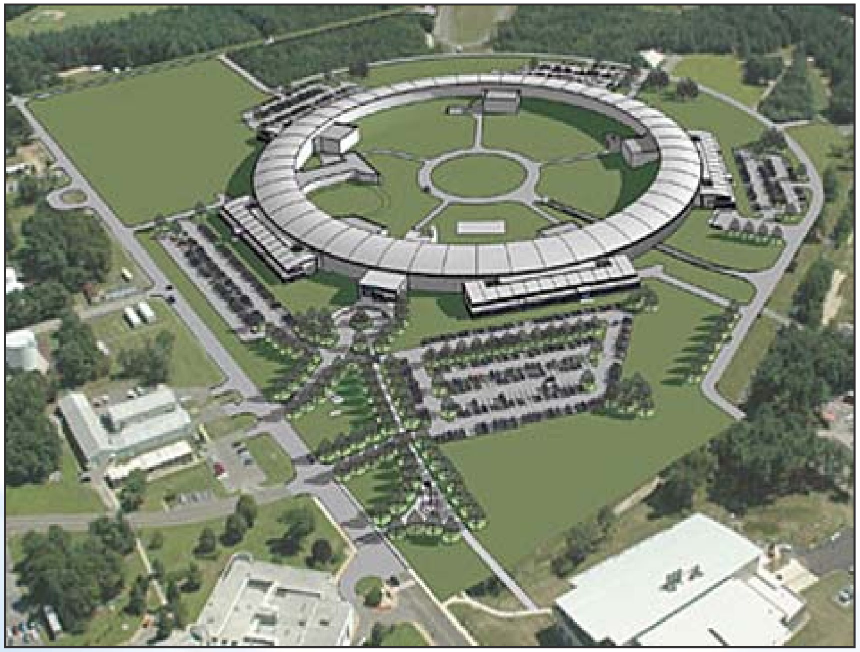
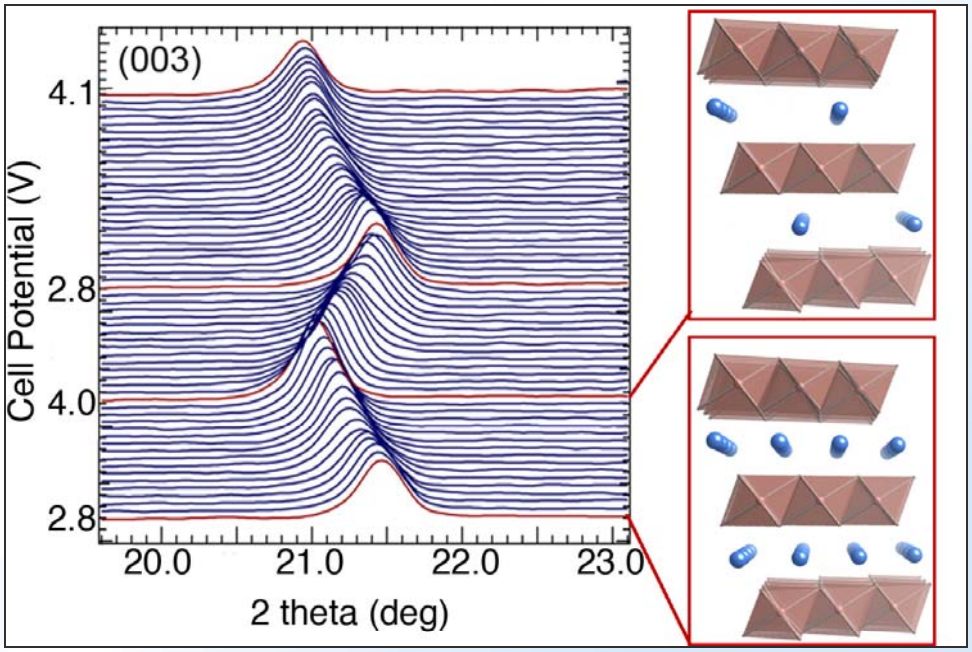
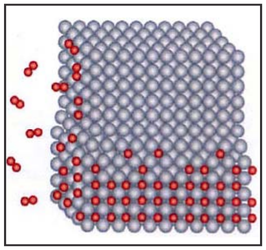




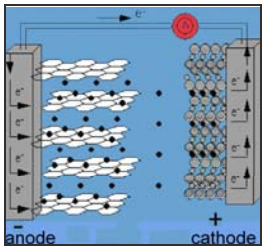
Energy Storage Interests

Materials for hydrogen storage and carbon capture



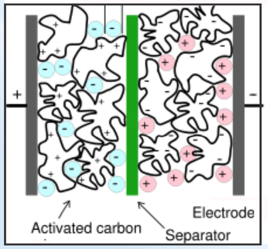
I. H and C-solid interactions; role of transition metal catalysts
II. physical, chemical, mechanical properties of complex materials
III. Materials with tunable thermodynamic and kinetic properties

Chemical Energy Storage - Li-ion, flow batteries, Li air, fuel cells



I. Role of (nano)structure on capacity, kinetics and cycle life
II. High capacity electrodes: cathodes with redox centers that accept > 1 electron and alternative anodes (alloy, conversion)
III. Electrolytes stable at higher potentials (4V+)
IV. In situ (nano)electrochemistry (coin, pouch, 18650 cells)

Capacitive storage - hybrid and supercapacitors



I. Electrolytes & electrode-electrolyte interface
II. Materials that exploit multiple charge storage mechanisms
III. Understand charge transfer and develop new hybrid materials

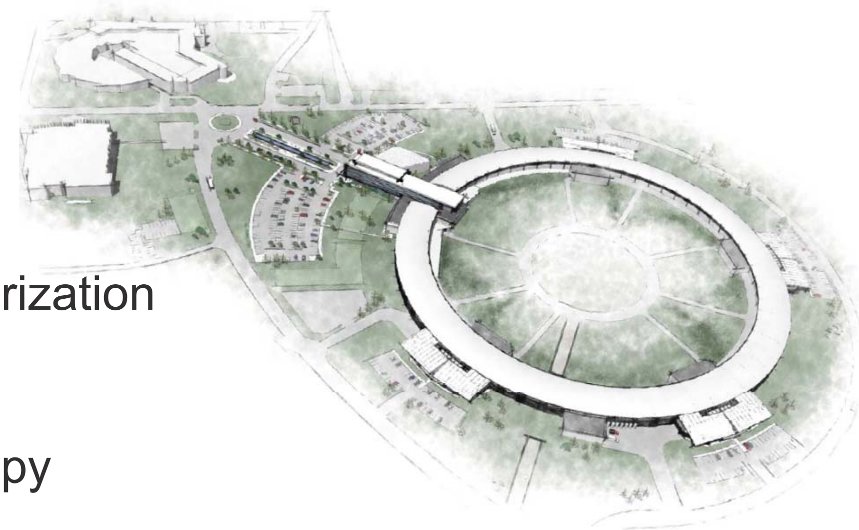
Required Capabilities

• Critical energy storage properties: **performance** (power/energy density), **durability** (calendar and cycle life), **abuse tolerance** (safety characteristics) and **cost**.

• Synchrotron tools can help understand (i) redox processes & charge compensation; (ii) structural transformations & size effects; and (iii) surface and interface phenomena.

Techniques		Charge compensation	Structural transformations and size effects	Surface and interface phenomena	Full battery diagnostics
Scattering / diffraction	XRD		X		X
	μ-XRD		X	X	□
	PDF		X		X
Spectroscopy	XAS (XANES)	X		□	X
	XAS (EXAFS)		X	□	X
	PES	□		X	
Imaging	Tomography		X	X	X
	TXM STXM	X		X	
Dynamics	*In-situ* studies	X	X	□	X

Future Beamlines



Project Beamlines

- **CHX**: Coherent Hard X-ray Scattering
- **CSX**: Coherent Soft X-ray Scattering and polarization
- **HXN**: Hard X-ray Nanoprobe
- **IXS**: Inelastic X-ray Scattering
- **SRX**: Submicron Resolution X-ray Spectroscopy
- **XPD**: X-ray Powder Diffraction

Approved Beamlines (see complete list at www.bnl.gov/nsls2/)

- **QAS**: Quick X-ray Absorption and Scattering - 10ms time resolution
- **BMM**: Hard X-ray Absorption Spectroscopy and Diffraction - Beamline for Materials Measurements - XAFS and XRD (high throughput)
- **ESM**: Electron Spectro-microscopy for Fundamental Studies of the Physics and Chemistry of Materials - chemical mapping 200x300nm
- **IXD**: Powder Diffraction Beamline for In-situ Studies of Structural and Chemical Transformations - rapid XRD measurements with good Q resolution
- **FXI**: Time-resolved Full Field X-ray Microscopy at Nano & Micro Scale - 30nm res.
- **XFM**: X-Ray Fluorescence Microscopy - μEXAFS w/ 1-10μm beam; microtomography

Proposed Beamlines

- **STX (2011)**: Scanning Transmission X-Ray Microscopy

Needs and Capabilities

Synchrotron Tool		Technology Issue: Electrochemical performance	Degradation mechanism during cycling and storage	New material for electrodes	Polymer/liquid electrolytes	Electrode-electrolyte Interface (SEI)	Defects	Safety	3D internal structure
spectroscopy	EXAFS	Catalyst at interface	local environment around specific element	coordination and band length change		element specific		Decrepitation of materials when hydrogenated	
	XANES	In-situ oxidation state	range reduction of valance changes	redox in-situ	element selective ion complexing	charge transfer process		thermal decomposition during heating	
	PES		Electronic energy-band structures			Bulk/surface electronic structure			
	IR microspectroscopy	2D element mapping			Identify species present	Identify species present			
Scattering/ Diffraction	Single-crystal /Powder XRD	Dynamic studies	Irreversible structural damages	Temperature dependent in-situ structure determination		interface structure		In-situ phase transformation during cycling	
	High energy XRD		Location specific structural changes in real battery					Commercial battery in situ	
	u-XRD			phase transformations in micron region			Grain structure, orientation, stress, strain	in-situ cracking and stress	
	PDF					In-situ time-resolved formation of nanoparticles	Atomic structure		
	SAXS/WAXS		Particle shape and size change	Particles evolution during cycling	Evolution of structures in real time at nano to micro scales	formation of nanoparticles/ breakage of larger particles			
	GISAXS /GIXD				In-situ PEM structural changes				
	RXS/RXD			Element, charge and orbital ordering phenomena					
Imaging	Micro-XCT	in-situ particles formation	Breakage 3D imaging during cycling	Morphological changes during cycling		non-equilibrium Li battery			Micro 3-D internal structure
	TXM			3D elemental distribution in nano resolution		3D imaging in nano spatial resolution	internal 3D structural imaging	Nanostructural and morphological changes during cycling	3-D internal structure at submicron scale
	SXM	Chemical states and local structure in micron scale	Oxidation state in micron region	2D composition and oxidation mapping		Local oxidation state change			2D elemental imaging
	Topography			Strain distribution			Strain induced by cycling		
	PEEM/LEEM	surface element mapping		Surface 2D mapping					

Discussion Session

Goal: Identify strategies to develop and enhance research programs at BNL and SBU that will benefit from NSLS-II's capabilities

Identify high impact, field changing experiments that can be preformed early at NSLS II and will brand the facility

- In operando imaging of nano particles and nanostructures (tens of nms) during electrochemical cycling
- High resolution valence mapping of cathodes at different states of charge
- Combined XRD/XAS of single particles

What is the expected usage of the currently planned beamlines by the existing research programs and personnel at SBU and BNL?

- XAS and XRD beamlines are currently well utilized for in situ and ex situ studies - future beamlines that incorporate these techniques will likely be well utilized
- Activity on SAXS/WAXS beamlines will likely increase
- PDF and imaging techniques (STXM/TXM) will likely be well utilized

Are there opportunities to enhance BNL/SBU representation in the areas of interest among the existing six NSLS-II beam-line advisory teams?

- PIs on beamline proposals should be encouraged to reach out to energy storage community at BNL/SBU to get input and get researchers involved in the beamline development early.

Is there a need to propose additional beam-lines (beyond those already approved) to provide additional capabilities needed to meet the current and emerging challenges identified by the BNL and SBU community?

FCC - Frontier Chemical Crystallography
• Microcrystallography – single crystal diffraction from μm and sub-μm thick grains
• Multicrystallography – simultaneous single crystal diffraction analysis on hundreds of crystallites
• Tomographic mapping – 3D diffraction tomographic mapping with 100 nm – 10 micron resolution Light element mapping – 2D chemical mapping using x-ray Raman spectroscopy
• Heavy element mapping – 2D chemical mapping and valence state analysis from XRF

ICT - In-situ studies of chemical transformations with high energy diffraction and IR and Raman spec.
• designed to provide time resolved *in-situ* scattering data which can be used to determine structural changes of catalysts under operating conditions and, in general, transformations of advanced materials accompanying variations of temperature and pressure
• partial diffraction measurements (small number of peaks) suitable for monitoring lattice changes in seconds and total diffraction patterns suitable for PDF and HQPR in 10 - 30s.

TRS - Time Resolved Spectroscopy Beamline for *in situ* studies of fast physicochemical processes
• XAS with high temporal resolution (10ms)
• *In situ* and *in operando*, and measure fast kinetics (with sub-second characteristic times) of working catalysts.

What other infrastructure is needed at either BNL or SBU (besides NSLS-II) to attract and support the S&T communities that will utilize NSLS-II.

- A variety of sample cells for in-operando studies
- Specialized reactors for studying synthesis reactions in situ

What are the areas of strength for personnel in the existing research communities at BNL/SBU and what are the most pressing needs for additional expertise or personnel in order to mount leading research initiatives utilizing NSLS-II?

- Expertise on flow batteries, lithium air, super/hybrid capacitors

What are the most effective strategies for strengthening the BNL/SBU research community (e.g., strategic hires, partnerships, etc.), including leveraging industrial collaborations, especially in NYS?

- GE collaboration on Na-$NiCl_2$ cells was very successful - how can we improve and develop more of these partnerships?

What are the funding opportunities to foster and support innovative, high-risk-high-reward R&D that benefits from utilization of NSLS-II at BNL/SBU?

- DOE-BES Battery Hub
- ARPA-E

How do we nurture new communities and/or new investments by these communities in research at NSLS-II?

- Dedicated lab space for energy storage community equipped with glove boxes, cyclers, crimping/decrimping equipment, etc.

- Specialized sample holders and reactors for in situ and in operando studies

Comments on new aspects of the User Access Policy

- More avenues for long-term access - 1 proposal could cover multiple experiments over 2 or 3 cycles

- Opportunities for spreading beamtime over weeks or months

  For example, lifetime (shelf and cycle life) experiments may want to break up beamtime to run 1 day every month for 4 or 5 months