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NSLS-II Strategic Plan

Photon Sciences Directorate

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Executive Summary

As the National Synchrotron Light Source II (NSLS-II) construction nears completion, Photon Sciences at Brookhaven National Laboratory is entering an exciting new chapter with one of the newest and most advanced synchrotron facilities in the world. NSLS-II will enable the study of material properties and functions with nanoscale resolution and exquisite sensitivity by providing world leading capabilities for X-ray imaging and high-resolution energy analysis. NSLS-II will begin operations at a time when the world is entering a new era with a global economy fueled largely by scientific discoveries and technological innovations. NSLS-II will provide the new research tools needed to foster new discoveries and create breakthroughs in such critical areas as energy security, environment, and human health.

NSLS-II is poised to play a leadership role in enabling and producing high-impact research in key science and technology areas for many years to come. NSLS-II will support the DOE scientific mission by providing the most advanced tools for discovery class science in condensed matter and materials physics, chemistry, and biology – science that ultimately will enhance national and energy security and help drive abundant, safe, and clean energy technologies. NSLS-II will fuel major advances in materials that will enable new energy technologies – such as nanocatalyst-based fuel cells; the widespread, economical use of solar energy; the use of high temperature superconductors in a high capacity and high reliability electric grid; advanced electrical storage systems for transportation and harnessing intermittent renewable energy sources; and the development of the next generation of nuclear power systems.

The vision for the next decade of Photon Sciences at BNL is to develop the world leading capabilities of NSLS-II and to leverage them to enable and conduct a broad range of high-impact, discovery class science and technology programs. BNL has a four-fold strategy for achieving this: (1) creating a vibrant environment that attracts world class scientists pioneering new research areas; (2) developing and operating world class beamlines with breakthrough capabilities; (3) advancing enabling technologies in optics, detectors, instrumentation, methods, and analyses; and (4) catalyzing innovation and facilitating university-industry-government collaborations via focused workshops with topical communities identifying needs and opportunities that support the theme of discovery to deployment.

The NSLS-II Strategic Plan presented here summarizes the strategic science directions, approach, and development plan for the next 5-10 years in order to achieve this vision. The Plan is informed by many years of strategic planning during the conceptualization and construction phases of NSLS-II, including the reports and inputs from a large number of community workshops, advisory committees, review panels, the scientific grand challenges identified by the DOE-BES in *Directing Matter and Energy: Five Challenges for Science and the Imagination*, as well as the Priority Research Directions identified in the DOE-BES Basic Research Needs Workshop series.

Through this approach, Photon Sciences has identified the following five priority research areas that NSLS-II is poised to make pivotal contributions to:

- *Emergent Behavior from Complexity* - This priority area aims to understand and control the emergent macroscopic properties and dynamic behavior in materials with complex quantum, molecular, and nanoparticle interactions. This is one of the grand challenges that impacts technologically important areas such as superconductivity and multifunctional electronic materials.
- *Mastering Materials Discovery and Processing* - This priority area is closely connected to the US materials genome initiative and aims to achieve materials properties and functions by

design through understanding and control of molecular self-assembly, and control of materials environments and failure mechanisms in a diverse range of materials systems.

- *Catalysis and Energy Systems* - This priority area aims to understand and control the chemistry of energy conversion in support of DOE clean energy initiatives through development of efficient catalytic and photovoltaic materials, and better understanding and design of critical materials interfaces in energy storage and other energy systems.
- *Environment and Climate Science* - This priority area aims to understand and ultimately control the complex geochemical and biogeochemical processes in the Earth environment including Earth atmosphere. Focus areas include the transport of nutrients and toxins, element cycling and sequestration, plant ecosystems for biofuels, and impact of aerosol particles on environment and health.
- *Structure and Functions of Life* – This priority area aims to provide fundamental understanding of how life functions at the molecular, cellular, systems, and evolution levels through protein structure discovery, structure to function correlation, and biological imaging.

In support of these priority research areas, Photon Sciences is currently developing a suite of thirty cutting-edge beamlines at NSLS-II, along with associated sample environments and support technologies. These will exploit the unique characteristics of NSLS-II to open up new regimes of scientific discovery and investigation, and enable exploration of many grand scientific challenges. These beamlines will provide world-class scientific capabilities in such areas as nanoscale to mesoscale structural and chemical imaging (HXN, SRX), coherent scattering on complex materials and dynamics (CSX-1, CSX-2, CHX), photoelectron spectroscopy and imaging (ESM, SST-1, SST-2), advanced x-ray scattering for materials self-assembly and membrane science (SMI, LIX), inelastic scattering on complex nanoscale disorder and electronic excitations (IXS, SIX), science-driven high-throughput structural biology (FMX, AMX, NYX, XFP), and in-situ and in-operando diffraction, spectroscopy, and imaging (XPD-1, XPD-2, ISR, ISS, FXI). Additional capabilities will be provided by a suite of best-in-class beamlines in diffraction (IXD, MPP, BMM), scattering (CMS), spectroscopy (QAS, TES, FIS/MET), and imaging (XFM, MID). These 30 beamlines, with phased completions in the 2014-2018 time period, will collectively support a large, highly engaged, and productive user community and enable world-class science addressing the grand challenges in the identified five priority areas, as well as others.

We are also working to develop additional beamlines to complete the beamline portfolio with other key capabilities. Currently nineteen additional beamlines have been proposed by the user community and recommended for development following review by our Science Advisory

NSLS-II: 30 Beamlines under Development

AMX	Automated Macromolecular Crystallography
BMM	Beamline for Materials Measurements
CHX	Coherent Hard X-ray Scattering
CMS	Complex Materials Scattering
CSX-1	Coherent Soft X-ray Scattering
CSX-2	Coherent Soft X-ray Spectroscopy
ESM	Electron Spectro-Microscopy
FIS/MET	Frontier Infrared Spectroscopy
FMX	Frontier Macromolecular Crystallography
FXI	Full-field X-ray Imaging
HXN	Hard X-ray Nanoprobe
ISR	In-situ and Resonant Scattering
ISS	Inner-Shell Spectroscopy
IXD	In-situ X-ray Diffraction
IXS	Inelastic X-ray Scattering
LIX	X-ray Scattering for Life Science
MID	Metrology & Instrumentation Development
MPP	Materials Physics and Processes
NYX	New York State Structural Biology Center
QAS	Quick X-ray Absorption and Scattering
SIX	Inelastic Soft X-ray Scattering
SMI	Soft Matter Interface
SRX	Sub-um Resolution X-ray Spectroscopy
SST-1	Spectroscopy Soft and Tender 1
SST-2	Spectroscopy Soft and Tender 2
TES	Tender Energy Spectroscopy
XFM	X-ray Fluorescence Microscope
XFP	X-ray Foot-Printing
XPD-1	X-ray Powder Diffraction
XPD-2	X-ray Pair Distribution Function Analysis

Committee. Once built out, these additional beamlines will significantly advance the DOE mission and leverage the capital investment made in NSLS-II.

A critical part of our plan is to continue research and development in such areas as advanced nano-focusing x-ray optics, high-quality large-format crystal analyzers, smart and fast pixel array x-ray detectors, coherent x-ray optics and optical metrology techniques, precision engineering and mechanical metrology, and new techniques and tools for *in situ* and *in operando* studies. Advancing these enabling technologies and novel sample environments is essential to maintaining our leadership capabilities and will drive the cutting-edge in synchrotron beamline technologies.

As the experimental activities ramp up at NSLS-II, advanced techniques and detectors will drive higher data rates and volumes and increase the complexity of experimental datasets. In order to achieve the full scientific potential of NSLS-II, BNL is developing a high-performance data management infrastructure with a flexible architecture, as well as dedicated software tools for data analysis, mining, and visualization to enable both real-time analysis during experiments as well as post-experiment analysis. This will be critically important to maximizing the scientific productivity and impact of NSLS-II.

Another key ingredient for achieving our vision is to create a vibrant environment at NSLS-II that attracts world-class scientists pioneering new research areas. Building upon the over thirty-years of success at NSLS, we are developing a world-class scientific and technical workforce, fostering open and cooperative discussions for discovery and innovation, and integrating community interests and participation into lasting partnerships. Following upon the success of the Synchrotron Catalysis Consortium (SCC) at NSLS, we are working to form cross-cutting science centers to integrate science across beamlines, provide specialized instrumentation, and expand the user community through outreach. The beamline development process, the open designs of the Laboratory and Office Buildings, the initiatives for integrated centers and partnerships, and physical colocation of science-oriented beamlines are just a few examples of ways in which we are working to encourage and promote community interactions, communications, and engagement.

Looking further ahead, we are working to develop concepts for future NSLS-II accelerator and insertion device upgrades to ensure that NSLS-II stays world leading in future decades. We will also contribute to the development of future light sources through the development of novel accelerator concepts and by identifying and developing the science drivers that define the performance requirements for future light sources

Finally, this Strategic Plan represents the Photon Sciences vision in 2014, and is a living document.

1. Vision, Strategy, and Approach

This strategic plan describes a comprehensive and ambitious science and technology agenda for Photon Sciences at BNL over the next 5-10 years. It was developed at an exciting time when the NSLS-II construction project is nearing completion and NSLS-II is about to begin operations in the fall of 2014. As such, the content of this report naturally consists of two integral parts. First, it serves as a consolidated report that captures the outcomes from the vast number of strategic planning activities in BNL Photon Sciences over the past decade, dating back to the early conceptualization of NSLS-II and leading up to this update of our strategic plan. Second, this report looks ahead to the first decade of NSLS-II operations, outlining the exciting science directions and programs that NSLS-II will be enabling, the additional scientific facilities that NSLS-II plans to develop, and the strategic programmatic initiatives that NSLS-II plans to pursue.

1.1 Vision and Strategy

NSLS-II will be the newest and highly optimized 3rd generation synchrotron facility in the world when it starts operations in 2014 at Brookhaven National Laboratory. When fully commissioned and built out, NSLS-II promises to provide unprecedented high brightness and photon flux as well as excellent beam stability over a broad range of photon energies from infrared to soft and hard x-rays, and will be able to accommodate at least 58 beamlines for a wide-range of scientific programs from physical sciences to biological and life science research. At the time of this report, thirty beamlines are under various stages of design and construction, and are scheduled to enter the NSLS-II user science program in the 2015-2018 timeframe.

The NSLS-II vision for the next decade is to be an internationally renowned synchrotron facility with world leading capabilities enabling a broad range of high-impact and discovery-class science and technology programs.

In order to achieve this vision, NSLS-II has developed a four-fold strategy: (1) creating a vibrant environment that attracts world class scientists pioneering new and high-impact research areas; (2) developing and operating world class beamlines with breakthrough capabilities; (3) advancing enabling technologies in optics, detectors, instrumentation, methods, and analyses; and (4) catalyzing innovation and facilitating university-industry-government collaborations via focused engagements with topical communities identifying needs and opportunities that support the theme of discovery to deployment.

1.2 Strategic Approach

Our vision and strategy have been developed through many years of strategic planning involving the broad scientific community and the key stakeholders, with many activities dating back to the early conceptualization phase of NSLS-II plus substantial community engagement during the NSLS-II construction. Examples of these activities include large numbers of community workshops, advisory committee meetings, beamline development workshops, beamline advisory teams, and expert panel reviews. Throughout the planning process, our discussions are guided by three key critical questions:

- What are the grand challenge science and technology questions that NSLS-II can help address?

- What are the strategic strengths and the unique positions of NSLS-II and its community in developing potentially world-leading scientific capabilities and programs?
- How should NSLS-II leverage its strengths and its community to achieve our vision?

The following three sections summarize our thoughts and answers to the above questions.

1.2.1 Grand Challenge Science

Our answers to the first question are very much guided by the scientific grand challenges that the broad scientific community have identified through strategic discussions organized by the DOE-BES [1], the Priority Research Directions in the DOE-BES Basic Research Needs Workshop series [2-3], as well as in other scientific disciplines by the National Academies of Sciences [4], the National Science Foundation [5], the National Institutes of Healths, and the DOE-BER [6]. At NSLS-II specific workshops and meetings, the scientific community and the NSLS-II staff have worked together to identify and define specific priority areas of research where NSLS-II should play important roles and make critical contributions. We have grouped these NSLS-II specific research priority areas into five categories:

- ***Emergent Behavior from Complexity*** - understanding and control of the emergent properties and dynamic behavior in materials with complex interactions. Key grand challenge questions include:
    - How do we control materials and processes at the level of electrons?
    - How do remarkable properties of matter emerge from complex correlations of atomic and electronic constituents and how can we control these properties?
    - How do we characterize and control matter away - especially very far away - from equilibrium?
- ***Mastering Materials Discovery and Processing*** - understanding and control of materials synthesis and directed-assembly, materials behavior and degradation in real and extreme conditions. Key grand challenge questions include:
    - How do we design and perfect atom- and energy-efficient synthesis of new forms of matter with tailored properties?
    - Can we master energy and information on the nanoscale to create new technologies with capabilities rivaling those of living systems?
    - Can we imagine the ability to manufacture at the mesoscale – directed assembly of mesoscale structures that possess unique functionality that yields faster, cheaper, higher performing, and longer lasting products, as well as products that have functionality that we have not yet imagined?
- ***Catalysis and Energy Systems*** - understanding and control of the chemistry of energy conversion and storage for clean energy. Key grand challenge questions include:
    - Can we understand and control the fundamental catalytic reaction mechanisms to design and prepare improved catalysts and processes for energy conversion, particularly as they function in the presence of complex feedstocks at high temperatures and pressures?
    - What are the critical physical and chemical phenomena at nanoscale and mesoscale in key constituents that govern the operation and the lifetime of energy storage devices, and how do we design better systems to achieve desired performance?
- ***Environment and Climate Science*** - understanding and ultimately control of the complex geochemical, biogeochemical, and atmospheric processes in the Earth environment. Key grand challenge questions include:

  - What are the roles of Earth system components (atmosphere, land, oceans, see ice, and the biosphere) in determining climate?
  - How is the information stored in a genome translated into microbial, plant, and eco-system processes that influence biofuel production, climate feedbacks, and the natural cycling of carbon?
  - What are the biological, geochemical, and physical forces that govern the behavior Earth's subsurface environment?
- ***Structures and Functions of Life*** - fundamental understanding of how life functions at the molecular, cellular, systems, and evolution levels. Key grand challenge questions include:
  - What is the physics and chemistry of life?
  - How do cells work, how do they interface with the environment, and how do single cells develop into multi-cellular organisms?
  - How do genomes generate organismal robustness and diversity, and what is the molecular basis of evolution?
  - How are biological systems integrated from molecules to ecosystems?

In the Chapters that follow, we outline with more details on our plans for scientific facilities at NSLS-II, and how these facilities are poised to make critical contributions to these science areas.

1.2.2 Critical and Relational Analysis

Our answers to the second question come from our extensive critical and relational analyses of the national and international standing of NSLS-II and its scientific communities. As the newest synchrotron facility in the world, NSLS-II is designed and constructed to be world leading from the start, with many advanced characteristics:

- First light source facility constructed to achieve 0.6 nm-rad horizontal e-beam emittance
- Largest medium-energy facility with world-leading circumference and beamline capacity (4th largest circumference closely following Spring-8, APS, and ESRF)
- World-leading high brightness and coherence in the soft to 25 keV hard x-ray range
- Broad range of synchrotron spectrum from IR on soft-bending magnet to very hard x-rays using superconducting wigglers
- Advanced beamlines with cutting-edge x-ray optics, detectors, and instrumentation
- Exceptional storage ring beam and experimental floor stabilities
- Special sunken bypass corridors and the green-field site to accommodate long beamlines
- Advanced integrated control system with time-stamping from the onset
- A dedicated, world-class staff with the skills sets required for the new NSLS-II facility.

Closely matching these world-leading characteristics is a world-class, devoted scientific community that is highly engaged and excited about doing world-class and high-impact science at NSLS-II. While this could be said for any new facility coming online, the NSLS-II community has several unique aspects including:

- There is already a large existing scientific user community at NSLS that has a tradition of being highly engaged and productive for the past three decades
- There are strong genuine interests from both existing and new scientific communities about taking advantage of the unique NSLS-II properties to develop unique scientific capabilities and partnerships
- NSLS-II is ideally located in the greater northeast US, a region that is vibrant and dynamic with a high concentration of world-renowned academia and industrial institutions - home to 45% of

the top fifty US national universities (including seven in the top ten) and to headquarters of over 130 Fortune 500 companies (including Pfizer, Merck, Bristol-Myers, Honeywell, Corning, DuPont, General Electric, and IBM)

- NSLS-II's home institution, Brookhaven National Laboratory, is a DOE multidisciplinary national laboratory that conducts basic and applied research in a broad-range of discovery-to-deployment disciplines. BNL science departments, including Center for Functional Nanomaterials (CFN), have strong interests in developing research programs at NSLS-II in the areas of condensed matter and materials physics, catalysis and energy storage, nanoscience, and environmental and biological sciences
- BNL is managed by Stony Brook University and Brookhaven Science Associates, consisting of six premier research universities - Columbia, Cornell, Harvard, MIT, Princeton, and Yale. Considerable interests exist among these institutions to form cooperative partnerships with NSLS-II to pursue research in energy and health
- BNL is in close partnerships with many science consortia and organizations in the region, with particular emphasis on research and development of tomorrow's energy technologies. This includes partnerships with New York Battery and Energy Storage Technology consortium (NY-BEST), as well as with several newly funded Energy Frontier Research Centers in the region, including the Center for Emergent Superconductivity led by BNL, the NorthEast Center for Chemical Energy Storage led by SUNY – Binghamton, and the Center for Mesoscale Transport Properties led by Stony Brook University.

These unique aspects of the NSLS-II facility, its strongly engaged community, and its social-scientific setting in the region represent enormous opportunities for NSLS-II and lay the foundation for defining the NSLS-II strategic science directions for the next decade. In Chapters 2 and 4, we capture the outcomes of these interactive discussions and outline what science capabilities we are developing and plan to develop in the coming five to ten years to take advantage of the unique strengths of NSLS-II and its community.

1.2.3 Cooperative Partnership with Community

In order to encourage community engagement and to leverage the enthusiasm and intellectual capital in the NSLS-II community, we have been working with the community in cooperative partnership in the development and the operations of NSLS-II beamline facilities and associated science programs. This approach has been and will continue to be used in the following ways.

- *Beamline Development Process*: All beamlines at NSLS-II are developed through open calls for Beamline Development Proposals (BDPs) to solicit ideas and concepts from the scientific community about specific research needs and specific beamline facilities at NSLS-II. The beamline development proposals are peered reviewed and rated by the PS SAC, and PS management makes the decision to approve or disapprove each proposal based on the SAC input. To date, forty-nine beamline development proposals have been approved by PS through this process based on three rounds of BDP calls since 2008.

- *Beamline Advisory Teams*: All NSLS-II beamlines under construction are each overseen by a Beamline Advisory Team (BAT) during their construction period. The role of the BAT is to represent a segment of the scientific community and to advise the beamline development group on the scientific and technical scope of the beamline as well as on the beamline design to ensure that each beamline is developed to meet the community needs.

- *User-Assisted Science Commissioning in Phased-Commissioning of Beamlines*: In order to efficiently commission NSLS-II beamlines and promote the community engagement in the commissioning process, NSLS-II has developed a *phased commissioning* strategy to commission each beamline after its construction is completed. Using this strategy, scientific capabilities will be commissioned sequentially based on scientific priorities determined through interactions with the BAT and user community. Once a specific scientific capability is commissioned, user operation will commence for that capability, interleaved with commissioning activities of other capabilities. This approach will permit thorough technical commissioning of all planned science capabilities while achieving early high-impact scientific productivity at the beamline.

  In addition, commissioning of each science capability will progress naturally in two phases – *technical commissioning*, where the focus is on beam delivery through the main beamline optical system into the experimental endstation, and *science commissioning*, where the focus is to evaluate the endstation instrument and data acquisition system for the planned science experiments. NSLS-II welcomes direct participation of the user community during the science commissioning phase of each beamline. This is done by soliciting first-experiment proposals through special announcements of newly available beamlines during regular calls for General User and Partner User Proposals, which are peer-reviewed and rated by the NSLS-II Proposal Review Panel for allocation of science commissioning beam time at the beamline.

- *Partner Users at NSLS-II Beamlines:* NSLS-II welcomes community participation in beamline construction and beamline operations, through the Partner User approach. Using this approach, a partner user group may make specific contributions to a beamline or beamlines to enhance the scientific capability at the beamline(s) or to co-operate the beamline operations. In recognition of their contributions, the Partner User receives appropriate portion of the available beam time at the beamline(s) upon peer review and approval by PS management.

- *Programmatic Initiatives and Science Consortia*: In order to enhance scientific impact, cultivate innovation, encourage collaboration, and ensure that NSLS-II stay at the scientific frontier in the always-evolving science and technology landscape, NSLS-II plans to work and partner with the community, and develop and implement a number of focused programmatic initiatives in selected target areas. Each initiative will function as a cross-cutting integrated research consortium that will (a) engage the research community to define the scientific challenges in a specific field of science through workshops, seminars, and other outreach activities, (b) drive and coordinate the development of special equipment at NSLS-II beamlines and support laboratories such as sample environment, ancillary instruments, and analysis software, and (c) provide scientific and technical assistance and education to the general users and partner users at NSLS-II beamlines in the corresponding field of research.

In Chapter 5, we outline our plans for several programmatic initiatives that are strategically important to NSLS-II.

1.3 Crosscutting Themes and NSLS-II Strategic Objectives

Crosscutting all research areas discussed in community engagement and strategic planning meetings are three emerging scientific themes and the associated NSLS-II strengths that we have identified as the strategic directions NSLS-II will pursue. In addition, a set of related strategic objectives have been

developed in order to guide and drive the development of NSLS-II scientific facilities to meet the research needs of the community. These themes and NSLS-II strategic objectives are discussed below.

- **Complexity and Dynamics**: From simple material systems with self-organized interacting phases to intrinsically heterogeneous functional systems, complexity and its dynamics is increasingly one of the key characteristics in scientific studies in the 21st century. NSLS-II high brightness will enable world-leading coherence, nano-imaging, and inelastic scattering capabilities that will be ideally suited for fundamental understanding and ultimately control of intrinsic and emergent heterogeneities and associated naturally-occurring, unclocked, and irreversible processes.

    - *Strategic Objective 1*: NSLS-II will develop world-leading high-spatial-resolution nanoprobe and imaging, high-coherent-flux coherent scattering, and high-energy-resolution inelastic scattering capabilities to meet the research needs in complexity and dynamic systems.

- **In-situ Functional Systems**: There is a clear need and demand in the scientific community for advanced characterization tools to allow in-situ and in-operando studies of real or realistic functional materials systems under working conditions that are relevant to natural or industrial processes. NSLS-II high brightness and flux in a broad range of synchrotron spectrum will enable correlated in-situ and in-operando capabilities in scattering and diffraction, spectroscopy, and imaging studies in a variety of functional systems critical to future energy, environment, and human health.

    - *Strategic Objective 2*: NSLS-II will leverage its strengths and the existing expertise in the scientific and industrial community to develop novel and world-class in-situ and in-operando capabilities to meet the research needs on functional systems.

- **Mesoscale Science**: Building upon the enormous atomic-scale scientific knowledge acquired in the past century, it has become clear that the structural and chemical information at the mesoscale – broadly defined as the length and time scales between the atomic and the macroscopic world, may hold the key to how to control the emergent macroscopic properties and processes of materials, environmental, and biological systems. Taking advantages of high brightness and small source size, NSLS-II is in an ideal position to develop a suite of advanced structural and chemical imaging tools that span multiple length and time scales, enabling mesoscale studies in a variety of scientific disciplines with the potential of matching experimental gauge volumes with those directly accessible by theory/modeling.

    - *Strategic Objective 3*: NSLS-II will develop a set of most-advanced, correlative, multi-scale structural and chemical imaging capabilities, including coordinated developments at multiple beamlines, as well as theoretical and modelling tools to meet the research needs in mesoscale and multiscale sciences.

2. Current State of NSLS-II

2.1 NSLS-II Accelerator System

NSLS-II has been designed and constructed to deliver photons with high average spectral brightness in the 2 keV to 10 keV energy range exceeding 10^{21} ph/s/0.1%bw/mm^2/mrad^2, and high spectral flux exceeding 10^{15} ph/s/0.1%bw. This cutting-edge performance will be supported by the NSLS-II accelerator with a very high-current electron beam (I = 500 mA) and a sub-nm-rad horizontal emittance down to 0.6 nm-rad by the use of damping wigglers and a diffraction-limited vertical emittance at a wavelength of 1 Å (vertical emittance of 8 pm-rad). The electron beam will be stable in its position (<10% of its size), angle (<10% of its divergence), dimensions (<10%), and intensity (±0.5% variation). The latter requirement provides for constant thermal load on the beamline front ends and x-ray optics.

The optimized NSLS-II storage ring lattice consists of 30 DBA cells, with straight sections alternating in length between 6.6 m and 9.3 m, with low and high values of horizontal beta functions, respectively. The performance goal of the 0.6 nm-rad horizontal emittance for the NSLS-II storage ring will be achieved when operating with a full complement of insertion devices, including damping wigglers. The initial horizontal emittance of 0.9 nm-rad will be somewhat larger than this, due to the fact that only a limited number of insertion devices, including three 7 m damping wigglers, will be installed at the start of operations. The main design parameters of the NSLS-II storage ring are summarized in the table below.

Main Parameters of the NSLS-II Storage Ring	
Ring energy (GeV)	3.0
Ring current (mA)	500
Ring circumference (m)	792
Number of DBA cells	30
Number of 9.3 m straights	15
Number of 6.6 m straights	15
β_h in 9.3 m straights (m)	20.1
β_v in 9.3 m straights (m)	3.4
β_h in 6.6 m straights (m)	1.8
β_v in 6.6 m straights (m)	1.1
Vertical emittance (nm-rad)	0.008
Horizontal emittance (nm-rad)	0.6
RMS energy spread (%)	0.1
RMS pulse length (ps)	15-30
Time between bunches (ns)	2
Revolution period (μs)	2.64
RF frequency (MHz)	500
Number of RF buckets	1320
Number of bunches	1056
Average bunch current (mA)	0.47
Average bunch charge (nC)	1.25

2.2 Current Suite of NSLS-II Beamlines

Based on the strategic planning and the beamline development proposal process outlined in the previous Sections, NSLS-II has worked with the community and strategically identified thirty beamlines to be developed as the early suite of scientific facilities. These thirty beamlines (see sidebar on page 2) are currently under various phases of design and construction using several beamline construction projects (described in Section 2.3 below), and will start user science operations in the 2015-2018 timeframe. In addition, we anticipate receiving financial support from DOE-BER to develop three additional beamlines in the near future, and we include these three beamlines in this Section. The key scientific capabilities of all these thirty-three world-class beamlines are summarized below, with the three BER beamlines identified by asterisks.

2.2.1 Nanoscale to Mesoscale Imaging

This suite of advanced imaging beamlines take full advantage of the NSLS-II high brightness and small source size and will provide world-leading capabilities in in-situ nano- to meso- multiscale imaging of heterogeneous structures and chemistry.

- Hard X-ray Nanoprobe (HXN) – A 110m-long beamline for structural and X-ray fluorescence imaging with world-leading 1-10 nm spatial resolution (Figure 1)
- Submicron Resolution X-ray Spectroscopy (SRX) – world-leading high-throughput chemical imaging capability with sub-100 nm and sub-um spatial resolution at ~ms dwell time/pixel with fly-scan capability
- Full-field X-ray Imaging (FXI) – State-of-the-art transmission hard X-ray microscopic imaging at 10-20 ms time-resolution & 30 nm spatial-resolution, and full 3D nano-tomography in <1 minute
- X-ray Fluorescence Nanoprobe (XFN*) – high-resolution X-ray fluorescence scanning probe with 20-30 nm spatial resolution in the 2-15 keV energy range
- X-ray Fluorescence Microscopy (XFM) – High-throughput X-ray fluorescence imaging and tomography with ~um resolution for larger systems
- High-resolution X-ray Topography at Metrology and Instrumentation Development (MID) beamline – High resolution imaging of materials defects in variety of industry relevant energy materials.

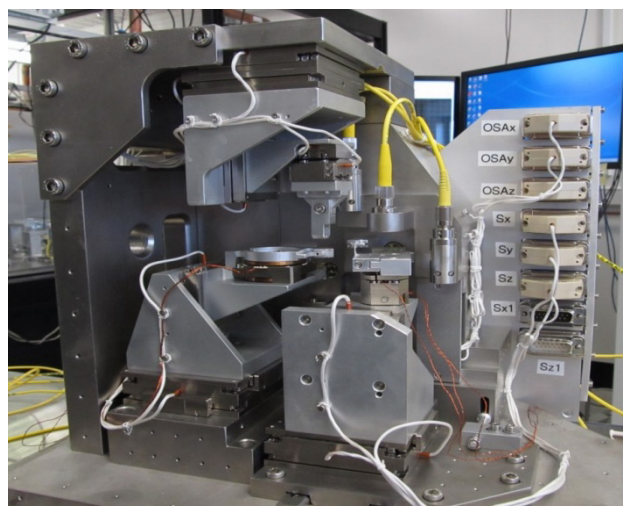


Figure 1: New 10nm X-ray microscope to be installed inside its endstation vacuum chamber at HXN – a 110m long beamline at NSLS-II. The microscope is designed and built with a compact, sub-nm precision laser interferometer position-feedback system based on diode lasers. It is designed to accommodate both Fresnel zone plates and multi-layer Laue lenses (MLLs) as the final focusing optic [7].

Collectively, this suite of dedicated imaging beamlines at NSLS-II will enable a wide-range of *in-situ* structural and chemical studies of heterogeneous materials and biological systems.

2.2.2 Coherent Scattering for Heterogeneous Complexity and Dynamics

Two advanced beamlines are being constructed to take full advantage of the NSLS-II high coherence in the soft and hard x-ray regimes for coherent scattering and imaging of mesoscale complexity and dynamics.

- Coherent Hard X-ray Scattering (CHX) – X-ray photon correlation spectroscopy with world-leading hard x-ray coherent flux and detection system for fast dynamics into the sub-ms regime
- Coherent Soft X-ray Scattering (CSX-1) – Coherent soft x-ray scattering and imaging with world-leading high-coherent flux and detector for probing correlated electronic textures and dynamics
- In addition, X-ray Scattering for Life Sciences (LIX) beamline under development as part of the Structural Biology suite also allows coherent scattering and ptychography imaging capability for multi-modal structural studies of membrane macromolecular assemblies.

Collectively this suite of world-class coherent scattering & imaging beamlines at NSLS-II will enable advances in understanding and control of heterogeneous systems and out-of-equilibrium dynamics.

2.2.3 Inelastic X-ray Scattering

Two world-class beamlines on inelastic X-ray scattering are being developed to provide advanced tools for studying collective dynamics of nanoscale disorder and electronic excitations.

- Inelastic X-ray Scattering (IXS) – Inelastic X-ray scattering with world-leading sub-meV to 0.1 meV energy resolution at 9.1 keV for studying low-energy excitations from nanoscale heterogeneity and disorder.
- Soft Inelastic X-ray Scattering (SIX) – a long beamline for inelastic soft X-ray scattering with a state-of-the-art spectrometer located in a satellite building providing world-leading ~10 meV energy resolution at 1 keV (Figure 2) for probing weak correlated electronic excitations with high sensitivity.

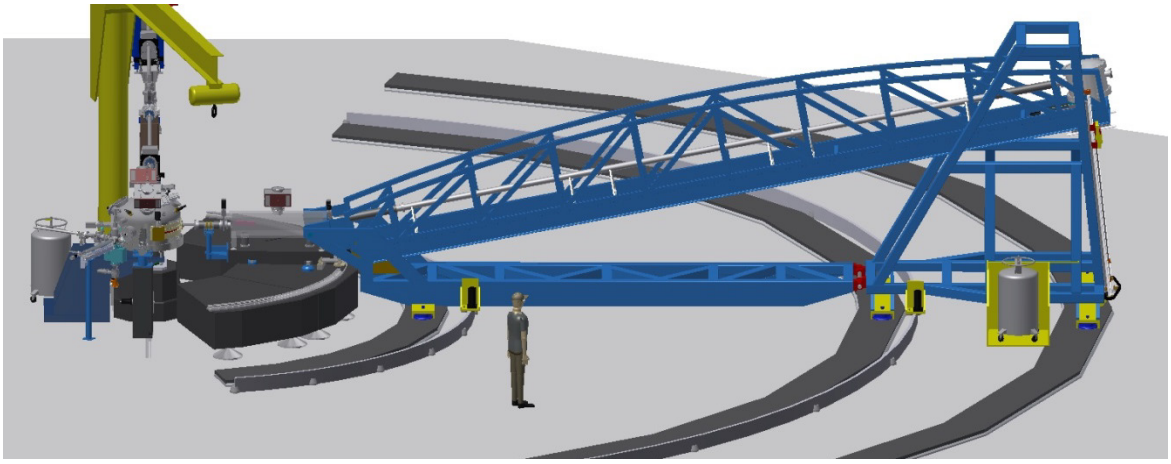


Figure 2: Endstation at the SIX beamline consists of a sophisticated sample chamber, with an in-vacuum spectrometer on a 15m long arm to achieve ~10 meV resolution at 1 keV and a wide-range of momentum transfer, for RIXS applications.

These two world-class inelastic scattering beamlines at NSLS-II will enable novel advances in understanding and control of weak-energy excitations and the corresponding emerging properties in real materials systems.

2.2.4 In-situ Photoelectron Spectroscopy and Imaging

- Electron Spectro-Microscopy (ESM) – Combined LEEM /PEEM as well as u-ARPES (Figure 3) provide world-class spatially resolved photoelectron spectroscopy and imaging capabilities for electronic structures in crystals as well as polycrystals

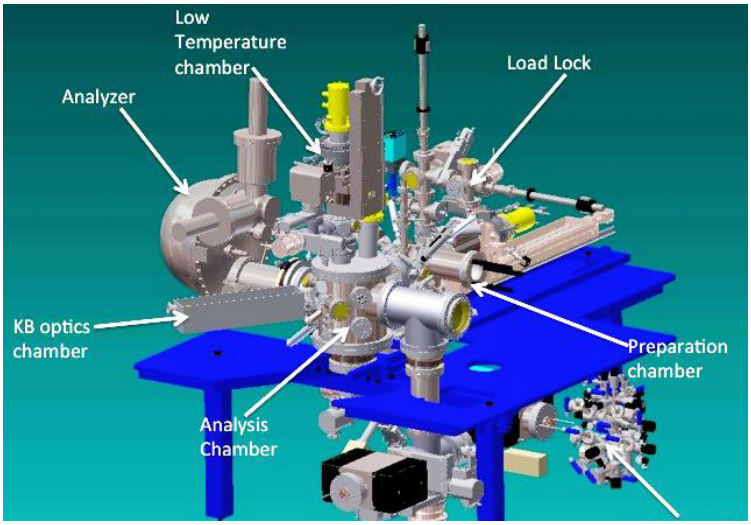


Figure 3: ESM u-ARPES endstation consists of a suite of interconnected UHV systems including an in-situ sample preparation chamber, a sample load lock, a low temperature sample environment chamber, and an analysis chamber.

- Coherent Soft X-ray Scattering and Spectroscopy (CSX-2) – allows studies of element specific magnetization responses using X-ray Magnetic Circular Dichroism (XMCD) technique in real complex magnets and at the interfaces of microelectronic materials, and the ambient pressure photoelectron spectroscopy (AP-PES) with world-leading soft x-ray beam size and flux enables chemical activity studies at up to atmosphere pressure ambient conditions
- NIST Spectroscopy Soft and Tender (SST-1, SST-2) – These two beamlines in partnership with NIST enables X-ray photoelectron spectroscopy and near edge X-ray absorption fine structure (NEXAFS) spectro-microscopy to the materials science of important societal challenges in energy, health, environment, and national security.

This suite of cutting-edge NSLS-II photoemission and soft x-ray spectroscopy beamlines enable research towards materials-by-design by controlling electronic structures and processes.

2.2.5 Advanced Scattering for Materials Self-assembly

- Soft Matter Interface Beamline (SMI) – Simultaneous small-angle / wide-angle x-ray scattering at gracing incidence, and special x-ray reflectometry for liquid interfaces, including wider x-ray energy range of 2-24 keV to access to element edges important to soft matter e.g. P, S, K, Ca.
- Complex Materials Scattering (CMS) – High-throughput small- and wide-angle x-ray scattering in transmission and reflection mode covering broad q-range of $4x10^{-4}$ to 7 A^{-1}, with an auto-sample-changer and versatile sample environment for stimuli-responsive *in-situ* experiments, and micro-beams for heterogeneous sample mapping of complex hierarchical materials
- In-situ and Resonant Scattering (ISR) – enables real-time studies of thin-film synthesis and growths that aim to control the nucleation kinetics during the growth process.

These world-class materials scattering beamlines at NSLS-II will enable advanced studies of wide range of functional architectures based on soft-matter and the control of self-assembly process by rational materials design.

2.2.6 Hypothesis-Driven Structural Biology

- Frontier and Automated Macromolecular Crystallography (FMX/AMX) – A pair of micro biological crystallography beamlines on canted undulators with world-leading micron-sized x-ray flux densities in the 5-30 keV range, and a suite of automated novel crystal mounting and handling systems (Figure 4), including an acoustic-droplet ejected system and a dynamic slit system to adapt beam to crystal size, to enable high-throughput, hypothesis-driven, and challenging projects using multi-crystal serial crystallography at cryo- or room temperatures.

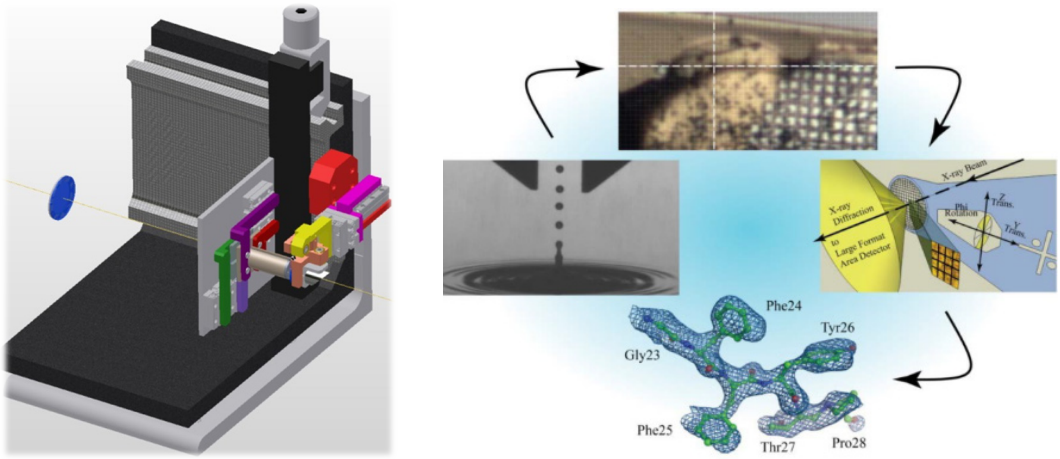


Figure 4: Sophisticated endstations at the FMX and AMX beamlines, with automated crystal mounting and handling such as acoustic droplet ejection (Right, Ref. 8), as well as a dynamic adaptive slit system to match anisotropic crystal shape during data collection (Left) will enable advanced structural biology projects potentially using multi-crystal serial crystallography with room temperature data collection.

- NYSBC Biological Microcrystallography (NYX) – Being developed in partnership with New York State Structural Biology Consortium (NYSBC), the NYX beamline provides cutting-edge optimized single- and multiple-wavelength anomalous scattering (SAD and MAD) capabilities in the 6-17.5 keV range. It is expected that the specialized features of NSLS-II beamline NYX will further promote the development and optimal use of SAD and MAD in biological crystallography
- X-ray Scattering for Life Science (LIX) – Time-resolved solution scattering for studying macromolecule conformational changes in solution and advanced grazing-incident scattering for structural studies of membrane complexes
- Correlated Spectroscopy and Macromolecular Crystallography (SM3*) – provide unique simultaneous optical spectroscopic and X-ray macromolecular crystallography capability for the structural biology community
- X-ray Foot-printing (XFP) – Being developed in partnership with Case Center for Synchrotron Biosciences, the XFP beamline provide a unique X-ray coupled mass spectroscopy capability for structural studies from non-crystalline macromolecule specimens, enabling investigations of more complex biological systems and allowing access to timescales in the microseconds range.

This suite of world-class structural biology beamlines at NSLS-II will bring structural biology at SR to a new level, enabling discovery-class as well as hypothesis-driven projects in life sciences.

2.2.7 In-situ and In-operando X-ray Diffraction and Spectroscopy

- X-ray Powder Diffraction (XPD-1) and In-situ X-ray Diffraction (IXD) – X-ray powder diffraction beamlines at NSLS-II offer cutting-edge capabilities with a wide suite of in-situ sample cells under extreme conditions and real-world in-operando sample environments
- X-ray Pair Distribution Function Scattering (XPD-2) – provides dedicated PDF capability for in-situ studies of nanoscale deformations in advanced energy materials
- In-situ Resonant Scattering (ISR) – In-situ capabilities include real-time diffraction and scattering in thin-film growth chamber, a 6-350K sample environment, and a gas handling / exhaust system
- Materials Physics and Processes (MPP) – X-ray reflectivity and diffraction under in-situ conditions for micro-electronic materials, including a rapid-annealing specimen handling system
- Inner Shell Spectroscopy (ISS), Quick Absorption & Scattering (QAS), Tender Energy Spectroscopy (TES), and Beamline for Materials Measurements (BMM) – offer an advanced suite of *in-situ* X-ray spectroscopy capabilities, including a state-of-the-art confocal X-ray spectrometer at ISS (Figure 5), with a set of specimen environments and a hazardous gas handling system for characterization of catalytic reactions and processes under industrial relevant conditions.

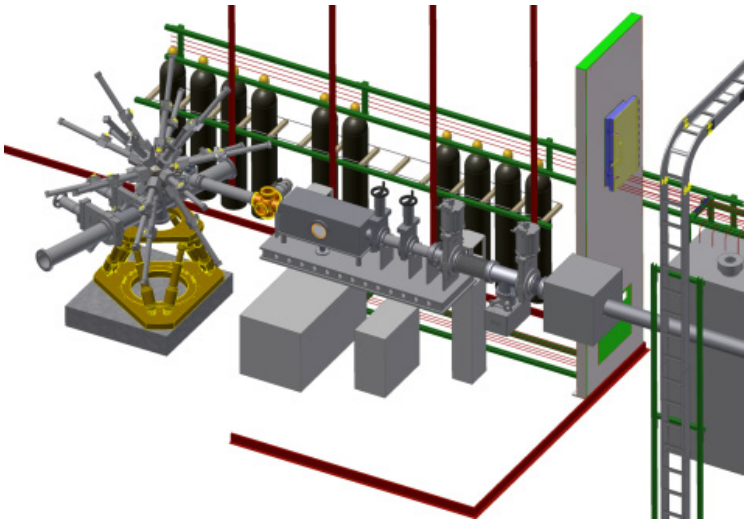


Figure 5: State-of-the-art in-situ and in-operando X-ray spectroscopy endstation planned for in-situ catalysis at the ISS beamline, with a suite of confocal X-ray emission spectrometers, in-situ specimen environments, and a hazardous gas handling system.

2.2.8 Infrared Spectroscopy and Imaging

- Frontier Synchrotron Infrared Spectroscopy under Extreme Conditions and Magneto, Ellipsometric and Time-Resolved Optical Spectroscopy Beamline (FIS/MET) – In-situ optical studies of hydrogen metallization at multi-megabar pressure and low temperature and condensed matter and materials studies using infrared spectroscopy
- Full-field Infrared Spectroscopic Imaging (IRI*) – enables in-situ studies of organic composition of materials by vibrational spectroscopy, with micromolar detection sensitivity and sub-micron spatial resolution

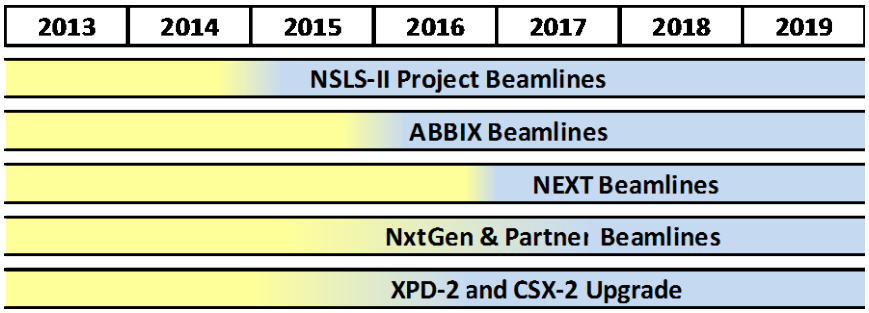
This suite of world-class IR beamlines at NSLS-II will benefit from the high brightness of the NSLS-II source and the exceptional stability of the NSLS-II facility.

2.3 NSLS-II Beamlines Acquisition Strategy

As discussed previously, all NSLS-II beamlines are being developed with the engagement and participation of the scientific community through beamline development proposals and beamline advisory teams. Funding for NSLS-II beamlines are obtained through one of the following acquisition strategies:

- NSLS-II leads the discussions with potential federal funding agencies to secure funding through beamline construction projects
- An external group leads the discussion with potential funding sources in their fields of research interests to secure funding for the construction of an NSLS-II beamline
- A combination of the above approaches, but with clear understandings of individual parties' responsibilities
- NSLS-II allocates a portion of its operating funds as capital equipment funds to develop beamline upgrades, or to develop new beamlines based on reusing existing equipment.

Using these strategies, NSLS-II has established and is currently pursuing the following beamline construction projects, with planned timelines shown in the figure below (yellow – design/construction, and blue – operations):



- NSLS-II Project Beamlines: Seven insertion device (ID) beamlines are being completed within the NSLS-II construction project on six ID ports, funded by DOE-BES, consisting of IXS, HXN, CSX-1, CSX-2, CHX, SRX, and XPD-1 beamlines. These beamlines will start operations in 2015.

- NSLS-II Experimental Tools (NEXT) Project: Six ID beamlines are being developed as a Major Items of Equipment (MIE) project, funded by DOE-BES, consisting of ESM, FXI, ISR, ISS, SIX, and SMI beamlines. These beamlines plan to start operations in 2017.

- Advanced Beamlines for Biological Investigations with X-rays (ABBIX): Three ID beamlines on two beam ports are being developed, funded by NIH based on an inter-agency agreement between DOE and NIH. This includes FMX, AMX, and LIX beamlines. These beamlines plan to start operations in 2016.

- Partner Beamlines: Five beamlines are being developed through funding secured by external groups. Specifically, National Institute of Standards and Technology (NIST) is constructing two ID beamlines (SST-1, SST-2) and one 3PW beamline (BMM), New York Structural Biology Consortium (NYSBC) is constructing the NYX undulator beamline, and Case Western Reserve University received an NSF grant to construct the XFP beamline on a 3PW port. These beamlines plan to start operations in the 2016-17 timeframe.

- NSLS-II NxtGen Beamlines: Eight beamlines based on 3PW, BM, and IR sources, consisting of CMS, QAS, TES, XFM, IXD, MPP, FIS/MET, and MID beamlines, are being constructed with planned funding allocated through the NSLS-II operations. Making extensive use of the existing beamline equipment transferred from NSLS, these beamlines plan to start operations in the 2016-18 timeframe.

- XPD-2 Beamline and CSX-2 Upgrade: NSLS-II plans to use a portion of its operating funds to support the full build-out of the XPD-2 branchline at XPD. With its hutch and utilities already provided through the NSLS-II construction project, it is a cost-effective way to deliver a fully independent ID beamline at a minimal cost. In addition, NSLS-II is adding an additional set of KB mirrors to the CSX-2 beamline to accommodate a cutting-edge ambient-pressure photo-electron spectroscopy (AP-PES) program at the CSX-2 in partnership with the CFN. Both the XPD-2 and the AP-PES capabilities are scheduled to operate in the 2015-16 timeframe.

3. Science Priority Areas

The primary mission of NSLS-II is to develop a portfolio of cutting-edge scientific capabilities that enable high-impact research addressing the scientific grand challenges that our society faces today and tomorrow. Guided by the grand challenge discussions in the scientific community and through the NSLS-II strategic planning process outlined above, we have identified a comprehensive list of research areas that NSLS-II will make significant contributions to, and that have potential high-impact in a wide range of scientific and technological disciplines. In this Chapter, we summarize these research areas in five science priority categories: emergent behavior from complexity, mastering materials discovery and processing, catalysis and energy systems, environment and climate sciences, and structures and functions of life. The following sections describe in more detail how the scientific challenge questions in each area lead to the needs for a specific set of scientific capabilities and research tools that should be developed at NSLS-II, and how collectively these capabilities will advance the research fields in each of the priority areas.

3.1 Emergent Behavior from Complexity

Global needs for renewable energy sources and effective ways to store and transmit energy or information motivate physical science researchers to explore increasingly more complex materials or materials architectures with enhanced or emergent properties to drive transformative technologies. The overarching controlling complexity challenge is to understand the organizing principles and correlated interactions of the constituents or local associations when integrated into the complex material architectures so the emergent macroscopic properties can be predicted and ultimately controlled.

In this Section, we describe three science priority areas that have been identified in our strategic planning process and where NSLS-II will play a significant role: *strongly correlated electron systems*, in which complexity results from competing quantum interactions between atoms, *soft complex materials and programmable assembly*, in which the complexity results from competing entropic forces and interactions between the constituent molecules, macromolecules, polymers, nanoparticles, or biological complexes, and *disorder and complex dynamics* in these materials, where the intrinsic dynamic processes often play a critical role in determining the emergent properties.

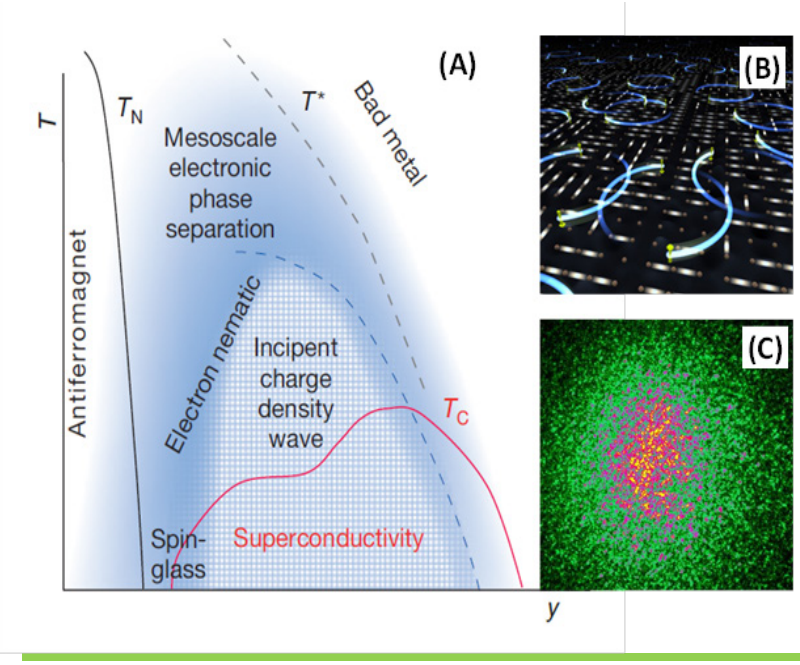


Figure 6: (A) Cuprate phase diagram showing the complexity of charge, spin, and superconducting orders, including a large region of charge correlations, "incipient charge density wave", intimately connected with superconductivity [9]. (B) Schematic illustration of Cooper pairs in a background of charge order in a cuprate. At NSLS-II the high brightness in the soft x-ray regime will allow the study of these correlations using coherent x-ray scattering for the first time, to probe the dynamics of these correlations, their real space arrangement and temperature and doping dependence. (C) Coherent scattering from antiferromagnetic order in a manganite [10] obtained at ALS.

Complex Correlations and Collective Dynamics: Amongst the defining features of strongly correlated electron systems is the development of complex correlations in charge, orbital, spin degrees of freedoms in electron systems. These may take the form of exotic ground states – charge, orbital or spin order, stripe textures, or short range correlations. In addition, nanoscale heterogeneities typically emerge in these materials, which, while of fundamental importance to the emergent properties, are intrinsically difficult to study because they are spatially heterogeneous and, in general, also fluctuating in time. NSLS-II cutting-edge capabilities in coherent scattering and nanodiffraction imaging at CSX-1 with world-leading coherent flux will play a critical role in investigating these correlations, addressing many of the challenging questions in the community, such as whether the charge and orbital ordered 'stripe' domains are static or dynamic and how such correlations relates to superconductivity in high-Tc cuprates and Fe-based high-Tc materials (Figure 6).

An important part of understanding strongly correlated electron systems is the information on low-energy excitations close to the Fermi surface due precisely to the many competing degrees of freedom that co-exist and often perturb the ground states. This information can be obtained by angle-resolved photoelectron spectroscopy (ARPES) and soft x-ray resonant inelastic scattering (RIXS). At NSLS-II, its high brightness will help the cutting-edge μ-ARPES capability at the ESM beamline to extend the powerful ARPES technique to spatially-resolved studies of valence electron correlations and excitations in heterogeneous specimens. NSLS-II state-of-the-art soft x-ray RIXS capability at the SIX beamline with world-leading energy resolution of ~10 meV and full momentum scan range will enable a wide range of weak excitations be studied for the first time in strongly correlated condensed matter systems, ranging from multi-magnon spectra and dispersing orbiton excitations in cuprates, to weakly

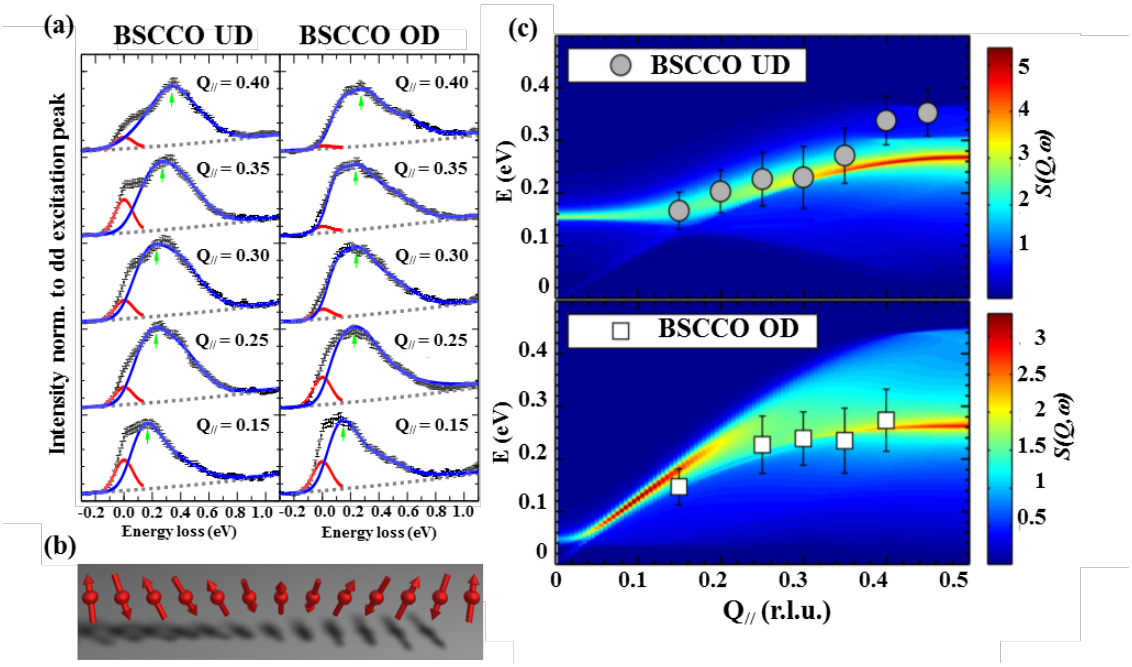


Figure 7: Magnetic excitations in a superconducting cuprate can be predicted using a parametrization of the measured electronic structure. High-resolution RIXS spectra on $Bi_2Sr_2CaCu_2O_{8+d}$ (BSCCO) reveal a dispersive spin-flip excitation in both underdoped (UD, T_c=0 K) and optimally doped (OD, T_c=92 K) samples (a). These collective spin flips propagate in the cuprate as spin waves, as illustrated in (b). The dispersion of these magnetic excitations derived from the RIXS data (solid points) is well described by theoretical calculations of $S(Q,w)$ based on ARPES-derived parameters of the electronic structure (c). This indicates that there may be a unified framework to reconcile the magnetic and electronic properties of the cuprates. Such a framework is key to explaining why high-T_c superconductivity occurs in these materials [11].

exchanged spin waves (Figure 7) in transition metal compounds, and electronic and magnetic structure of oxide heterostructures.

Soft Complex Materials and Programmable Self-Assembly: Soft matter systems exhibit unique properties, rarely observed in hard materials: a complex degree of organization, structural plasticity and reconfigurability, and an ability to integrate both organic and inorganic functional components. These rich materials promise to revolutionize a host of applications, including energy harvesting and storage, smart mechanical responses, tunable optical activities, and interfacing with biological systems [12].

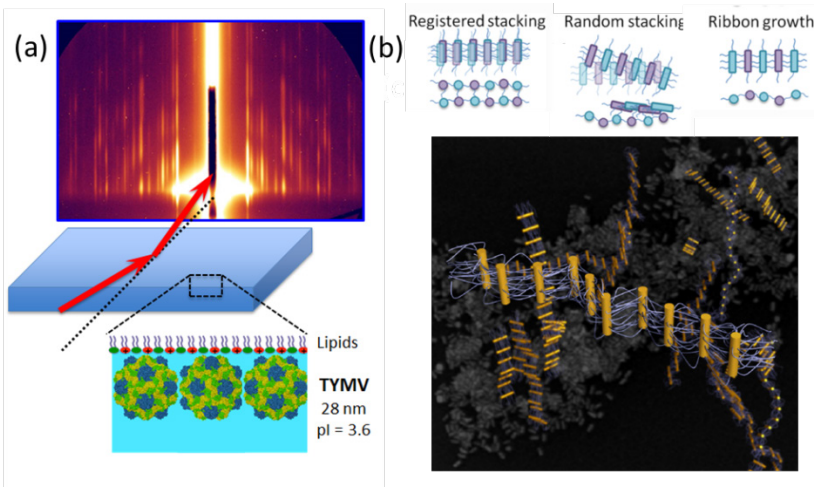


Figure 8: Hierarchical organization of soft matter mesostructures can be initiated, for example, by tuning nanoparticle interactions using (a) a virus with regularly positioned chemical groups [13] or (b) DNA functionalized nanorods [14]. The mesostructures depend on assembly conditions and assembly time. X-ray scattering at SMI elucidates static structures while coherent scattering at CHX measures assembly kinetics.

As shown in Figure 8, several promising concepts have been demonstrated for by-design assembly, including: programming interparticle interactions via bio-recognition (DNA, peptides), particles or molecules exhibiting shape complementarity, the use of anisotropic interactions, and the directed assembly involving use of interfaces of underlying patterns. The complex energy landscapes with a great variety of meta-stable states with comparable energies, relatively weak order and large entropy, high sensitivity to temperature and external pressure, as well as coupling between phenomena lead to multiple relaxation processes on local and global length scales, and over many decades in time. Moreover, the structural plasticity of many soft matter components and their low-excitation energy landscape enable the design of new classes of "smart" materials, for example shape memory polymers [15] or liquid crystal/nanoparticle composites [16], which can not only be assembled into static architectures, but are able to respond, to reconfigure, and to react to external stimuli such as applied fields or changes in chemical environment. At NSLS-II, the suite of advanced X-ray scattering beamlines, SMI, CMS, and CHX, will provide a set of cutting-edge x-ray techniques including coherent scattering and imaging for bulk and for interfaces to help researchers to reveal local and multiscale organizations in systems with complex order, and to track and ultimately control different kinetic assembly pathways and response behaviors in these systems.

Disorder and Mesoscale Dynamics: The study of disordered materials spans the range from defects in otherwise uniform media such as crystals at one end to amorphous and glassy materials at the other. Disordered materials, including disorder in crystals, have profound technological impact. It is often the deviation from perfect periodicity that makes the materials function. Yet it is the imperfections that also make the materials difficult to study. NSLS-II will provide a number of breakthrough capabilities to address this issue. At HXN beamline, the state-of-the-art nano-fluorescence, nanodiffraction, and ptychography capabilities will enable imaging nanoscale defects, local strain-fields around defects or around purposely designed nanostructures at better than 10 nm resolution. The pair distribution function (PDF) capability at the XPD-2 will allow spatially resolved PDF studies for mapping local short-range orders in many nanostructured materials [17]. And, the ultra-high resolution IXS beamline

with sub-meV energy resolution will allow inelastic scattering studies of weak energetic excitations arising from these nanoscale heterogeneities, including soft phonon-like excitations in bio-membranes comprised of active proteins and enzymes.

Understanding the dynamical behavior of these inherently out-of-equilibrium systems is important to guide the design of 'intelligent' soft architectures with responsive viscoelastic and self-healing properties. In high-density complex fluids even before the glass transition temperature is reached, the long-range motion of the units comprising the complex fluid (atoms, molecules, polymer segments, or particles) can be arrested and jam. Both the glassy and jammed states represent kinetically trapped structures that are very far removed from equilibrium so their dynamical behavior span multiple time scales. At NSLS-II, the CHX beamline is design and built to help address these challenges in non-equilibrium dynamics. Taking full advantage of the world-leading coherent flux and the VIPIC detector under development, the x-ray photon correlation spectroscopy (XPCS) capability at CHX will open new research opportunities in studies of dynamic behaviors of heterogeneous, disordered, and glassy materials, with an unprecedented wide-range of time-scales.

Complex Dynamics via Time-Resolved / Pump-Probe Experiments: In many condensed matter systems, ultrafast dynamics excited by femtosecond stimuli are characterized by a rapid decay of an order parameter (*e.g.* spin, charge, and orbital order, crystalline symmetries, ionic valence, *etc.*) followed by a much slower (ps-scale) return to equilibrium as the system thermalizes and the order parameter is re-established. The trajectory back to equilibrium need not be smooth, as metastable states may present bottlenecks in the de-excitation process. The time-scales for pump-probe experiments at NSLS-II are thus well suited to investigate in detail processes such as renormalization of a superconducting ground state after rapid disruption and breaking of Cooper pairs; studies of nuclear motion (*e.g.* phonons) in crystalline and soft-matter systems; mass transport in chemical systems; and spin wave phenomena and other spin dynamics in technologically relevant systems. And, of course, these systems can be interrogated with the high coherence and exceptional beam focusing capabilities afforded by the ultra-low emittance NSLS-II storage ring.

3.2 Mastering Materials Discovery and Processing

Discovery of new materials and mastering materials processing and behavior is at the core of materials science and engineering and at the heart of the modern-day materials manufacturing sector which is essential to economic security and human well-being. Accelerating the pace of advanced materials discovery and deployment is therefore crucial to achieving global competitiveness in the 21st century [18]. NSLS-II will play an important role in this process by providing the most advanced materials characterization tools to enable rational materials synthesis, self-assembly, and processing, to understand and control heterogeneities, disorders, and failure mechanisms in materials, and to study functional materials under operando, extreme, and industrial relevant conditions.

Rational Materials Synthesis and Processing: Synthesis of a new compound or a new hierarchical material and their processing towards desired functional properties [19] typically require many trials-and-errors in a vast and complex thermodynamic and chemical composition landscape. Hence the structure-function relationships are complex, presenting significant challenges and requires efficient and high-throughput tools to navigation through a huge phase space of compositional and processing variables. At NSLS-II, the high-throughput x-ray diffraction and scattering capabilities at the XPD and CMS beamlines will allow automated workflows that integrates robotic sample handling, real-time data reduction and analysis, multi-dimensional parameter-space visualization, and decision making algorithms to enable intelligent high-throughput methods to survey, visualize, and pinpoint structural signatures of interest, such as anisotropy in scattering pattern, in a multi-dimensional parameter space.

Nearly all current electronic and optoelectronic devices rely on heteroepitaxial interfaces, including compound semiconductor heterostructures and complex oxides. As many novel properties – e.g. interface superconductivity, colossal ionic conductivity, and colossal magnetoresistance - are strongly dependent on stoichiometry and finite size effects, strict control over film composition, quality, and thickness is essential. While deposition methods such as molecular beam epitaxy and pulsed laser deposition can achieve reasonable stoichiometric and excellent thickness control, the details of the dynamic physical processes occurring during growth remain poorly understood, partly because of the many relevant time scales of competing processes and the complexity due to heterogeneous adatom step and islanding kinetics. Key issues include fundamental mechanisms of fast interlayer transport, and the roles of strain in modifying properties such as ferroelectric polarization. At NSLS-II, the ISR beamline will provide the in-situ x-ray reflectivity and scattering capabilities during thin-film growth, and coupled with high-coherence the beamline will allow X-ray photon correlation spectroscopy studies on crystal truncation rods, providing critical insights into the intrinsic nucleation, diffusion, and self-assembly dynamics of the materials during thin-film deposition. These novel and efficient scattering methods and intelligent searches through phase space at NSLS-II beamlines will provide the much needed information critical to the understanding and control of processing and composition parameters and to correlate structures with the desired functions, and ultimately to shorten the materials discovery to deployment cycle.

Mesoscopic Materials under Operando and Processing Conditions: All materials, whether naturally existing or man-made, function under certain operating conditions in a given heterogeneous, non-

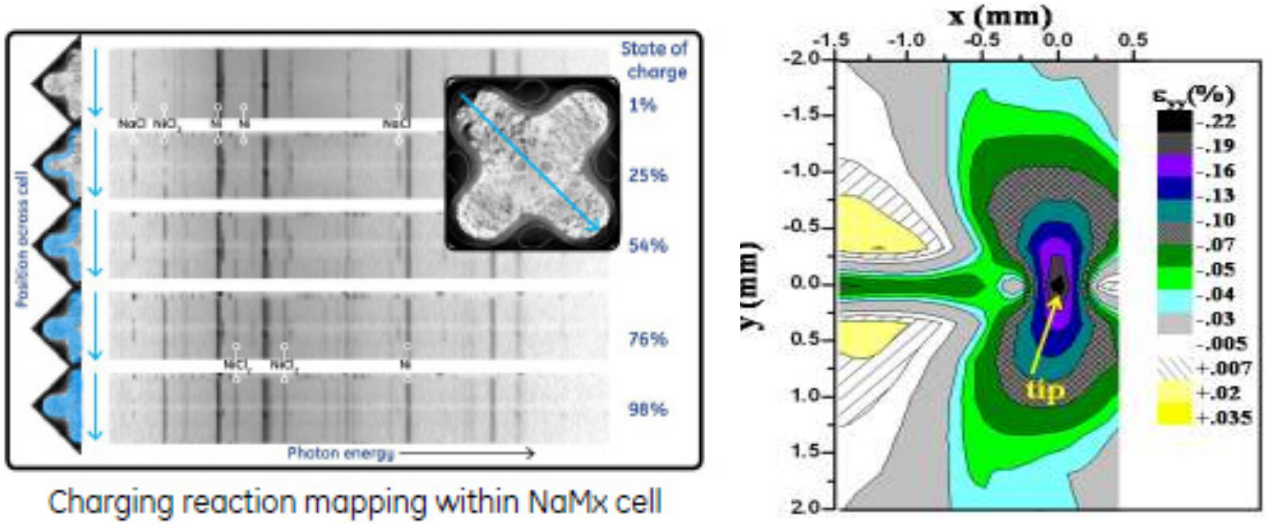


Figure 9: (Left) In-operando XRD imaging studies of structural phases in a General Electric commercial NaMx battery cell as a function of time at different percentages of full charge [20]. (Right) Spatial contour map of the ε_{yy} strain component near the crack tip of a fatigued steel specimen under in-situ loading [21]. Both datasets taken at NSLS using spatially resolved energy dispersive x-ray diffraction. At NSLS-II, advanced diffraction capabilities at XPD and future HEX beamlines will extend these strain-stress studies in-situ studies to much higher spatial resolutions and under in-operando conditions. In addition, nanodiffraction capabilities at HXN will enable unprecedented nanoscale resolution, allowing strain-field studies well into the single grain and grain boundary levels.

equilibrium environment that carries its desired thermodynamic energy flow. For materials produced via industrial processes, their behaviors under thermomechanical and chemical extremes of high pressure and stress, high chemical reactivity, and high and low temperatures are at the heart of many energy problems of crucial importance to the nation. New structural materials that can withstand

higher temperatures and stresses without failure are required for the next generation of efficient turbines and heat exchangers for more efficient jet engines, for steam and nuclear electrical power plants, and for future fusion power applications. Similarly, strong, lightweight materials are needed to reduce energy consumption in future transportation systems. Despite of its importance, our current understandings of the chemical and physical processes related to materials failure mechanisms are still largely based on empirical trials and errors.

At NSLS-II, several beamlines – XPD, HXN, FXI, and SRX, will establish a powerful suite of cutting-edge nano-imaging and nano-diffraction capabilities to address this issue and enable a variety of studies on materials under realistic operando conditions. In addition, the HEX future beamline will allow 3-D orientation and lattice strain reconstructions on the single-grain scale, and determination of the elastic strain tensor components (Figure 9) along with the active plastic deformation defect types and densities. Closely coupled to modelling these methods will allow grain scale micro-mechanics to bridge to mesoscopic mechanical response, leading to critical insights into the materials failure mechanisms in structural alloys materials. This would allow better materials-by-design using variety of materials engineering and manufacturing processes, such as the elasto-plastic deformation processing of the near surface designed to inhibit fatigue crack formation and growth by imposing compressive residual stresses in a near/sub-surface region, and the coating and composite processing where metal part modification by ceramic nano-material coating or carbon composite integration have also become critical to aviation-related manufacturing.

In-situ microelectronics properties and processes: As microelectronics devices shrink and new materials and processes are incorporated to improve performance, the behaviors of interfaces and reduced dimensions have an increasingly major effect in the 3D integrated circuits. Better understanding and control of these nanoscale 3D interfaces requires in-situ structural characterization tools that provide critical information on the chemistry, structure, and atomic-scale strain at these interfaces. The brightness of the NSLS-II will enable nano-imaging of strain-field in these nanoscale heterostructures using coherent diffraction ptychography, as well as the investigation of ultra-thin films and features with high resolution in reciprocal space at the necessary time scales associated with the evolution of key material properties. Real-time diffraction during rapid thermal annealing process enables identifications of structural phase transformations, which, in conjunction with complementary measurements such as optical light scattering, yields vital information about the behavior of thin films and small features during processing. Crystallographic phase formation, grain orientation and size, interfacial and surface roughness, strain, and transition temperatures – all measured during the rapid thermal or laser annealing processes, provide crucial information for development to deployment of tested heterostructures.

In-operando observation of defect motion on power electronic devices during electrical stressing: Based on wide-band-gap SiC and GaN technology, new low cost high efficient semiconductor power electronics devices are developed which will change significantly the way how electric power is distributed in the grid; this work is an essential development to modernize the power infrastructure and to adjust the grid to decentralized power generation as a consequence of the increased utilization of alternative energy resources. They are poised to supersede Si in applications involving, for example, high power switching for more efficient power distribution and inverters for electric vehicles. Currently, excessive defect densities, in both the substrates and epilayers, are inhibiting these applications and extensive research into understanding of defect dynamics during growth with a view to defect reduction is being carried out not only in the US but also in Europe as well as in China and Japan with significant industry and government investment in this key area. NSLS-II MID beamline will enable much improved spatial and angular resolution topographic imaging to be carried out. In particular, in-operando studies of these devices during electrical stressing will allow observation of

defect motion, which will enable strategies to be developed to remove the most dangerous defects from the active areas of the devices, leading to drastically improved performance.

Materials in Extreme Environment: The majority of the condensed matter making up the Earth, and other bodies in the universe, exist at high pressures and high temperatures. Therefore understanding the fundamental properties that dictate large-scale process, e.g. plate tectonics, depends critically on observations of materials structures and properties under high *pT* extreme conditions. Most melt in Earth's interior is present at the 1 – 2% level. Understanding the mechanical properties of this mixture provides insight into the process of plate motion and the mechanism for accumulating the magma chamber. At NSLS-II, large volume high-pressure systems located at XPD-1 with the high-flux, high-energy x-ray beam will provide the ideal platform to define the mechanical properties of such media. A significant property of this system is relaxation time related to the solid – melt interaction. Acoustic velocity measurements with a time constant of a fraction of a microsecond can be coupled with forces oscillation measurements with time constants from 1 to 10,000 seconds indicating the effects of the partial molten region on seismic wave velocities (time constant of 10 to 1000 seconds). This information will provide new insights into identifying partially molten regions in the Earth. In addition, the world-leading IXS capability with sub-meV energy resolution at NSLS-II will be an exciting tool for high-pressure science. It will enable liquid dynamics studies in low-Z materials under extreme pressures in a diamond anvil cell, such as hydrogen, lithium, and sodium, as these simple elements have very complicated phase diagrams, which are not fully understood.

Nuclear materials are another class of materials used in extreme radiation environments. Radiation damage in materials, especially engineering alloys, is a very complicated phenomenon with many competing, path-dependent effects such as defect formation versus recombination, transmutation of elements, development of new phases and amorphization of existing precipitates, acceleration and interaction of thermal and irradiation creep processes and corrosion. The fundamental mechanism of irradiation and thermal creep, embrittlement and fracture properties under extreme radiation flux are needed to ensure safe operation of reactors for long periods at high temperatures. Being able to monitor chemistry and diffraction on the same specimen as a function of time and environment is critical for studying corrosion and irradiation assisted stress corrosion cracking. In situ experiments at far-from-nominal conditions rarely are performed, but are needed by computational modelers to supply valuable data so that estimates of materials performance are not based solely upon extrapolation during reactivity and temperature transients. Such experiments and the enhanced modeling capability that could be validated by the results will create materials with better performance and will provide crucial information for developing the next-generation nuclear power reactors.

3.3 Catalysis and Energy Systems

Devices for energy conversion and storage are integral part of our daily life. Independent if it is the Li-battery of the smart phone, the catalyst in our car enabling our daily mobility, or the availability of electrical power at home, we are dependent on devices with complex structures, combining a wide range of organic and inorganic functional materials. The functionality depends strongly on the working conditions and history of the device, as well as on the interplay of a set of functional materials on different length and time scales. To elucidate these complex correlations of device functionality and structural changes on the various time and length scales is a great challenge and can only be performed in the concert of various experiments conducted under in-situ and in-operando conditions, providing the most relevant information on materials chemistry, structure, interfaces, and functionality. Below we outline three main areas of research that NSLS-II is poised to contribute on.

Multi-scale structure and functionality correlation on electrical energy storage devices: Several constaints limit the needed function of currently available energy storage devices, *i.e.* batteries, including energy content, power delivery and lifetime. In electric cars, the issues are particularly acute

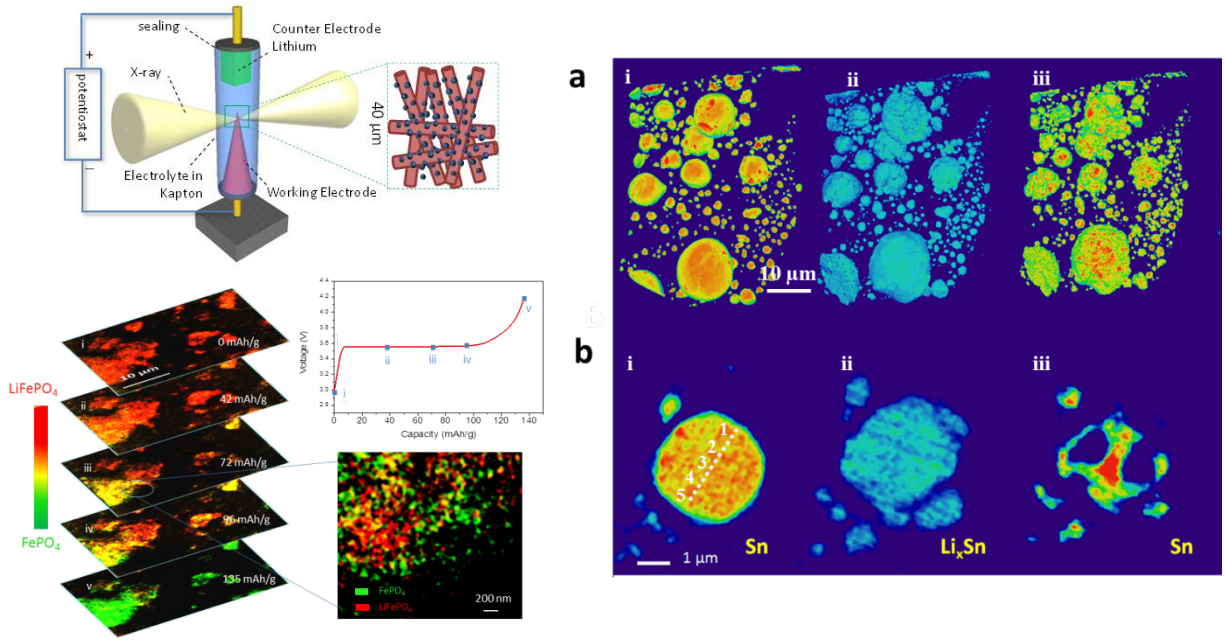


Figure 10: In-operando nano-imaging observations of 3D microstructural and chemical evolution in Sn anode in a Li-ion battery (Right, Ref. 22) during lithiation-delithiation cycles using a specially designed in-situ microcell (Top Left), and of 2D chemical mapping of multi-particle lithium iron phosphate cathode during fast charging (Bottom Left, Ref. 23). Data collected at NSLS. With NSLS-II, the state-of-the-art TXM instrument at FXI will enable in-operando chemical and structural studies of nanostructured electrodes at time-scales

where charge time, driving distance, battery size and cost are not yet at needed levels. Storage solutions for the electric grid hold particular importance as they play a key role in the broader implementation of renewable energy generation which by its very nature is often intermittent. To break through the current barriers it will be necessary to close the critical gaps in our knowledge of the battery materials and their functional interfaces *at the nanoscale,* particularly under in-situ and in-operando conditions. Work pioneered at NSLS using high energy energy-dispersive x-ray diffraction yielded the first in-situ x-ray diffraction profiling/mapping of electrochemical changes in space and time for a large commercial battery (Figure 9) used for diesel-electric hybrid locomotive and grid applications. Extending these investigations at NSLS-II to high spatial and time resolutions as well as higher sensitivities and correlations to functionalities is critical to enable the identifications of parasitic phase/morphology formations (see examples illustrated in Figure 10), which will help development of next-generation energy storage devices with enhanced performance.

Catalysis for efficient and directed energy conversion: Commercially viable production of clean hydrocarbon-based fuels and bulk chemicals from alternative feedstocks, including those as natural gas and coal, and renewable sources, such as lignocellulosic biomass, requires development of multiple conversion strategies. Heterogeneous catalysts greatly increase efficiency and specificity of the chemical transformations leading to value-added chemicals; however, complex cascade reactions involved in biomass conversion cannot be efficiently controlled without detailed knowledge of catalyst action. Understanding exact chemical nature of the catalytically active site and the interaction of the active phase of the catalyst with the support phase are essential in optimizing multi-step processes. In

addition, efficiency of a conversion process involves sequential chemical transformations depends on the ability to accurately control access of reactant to catalytic sites.

Developing new generations of catalysts for challenging processes required expertise in synthetic techniques, catalytic testing and characterization. The catalyst should be characterized under realistic reaction conditions (*in situ*) and, whenever possible, structural and chemical transformation in the catalytic material during the reaction should be correlated with its chemical activity and selectivity (*operando*). In particular, the following approaches are needed: (a) *operando* investigation under industrial processing conditions using multi-technique approach – applying multiple characterization methods to the catalyst, simultaneously or sequentially allows detection of relevant changes on various length scale from individual atoms to catalyst particles, (b) spatially resolved 2D and 3D characterization approach – enabling analysis on a single-particle/single-site level (Figure 11) using multiple techniques, allowing unprecedented insight into catalyst structure under reaction conditions,

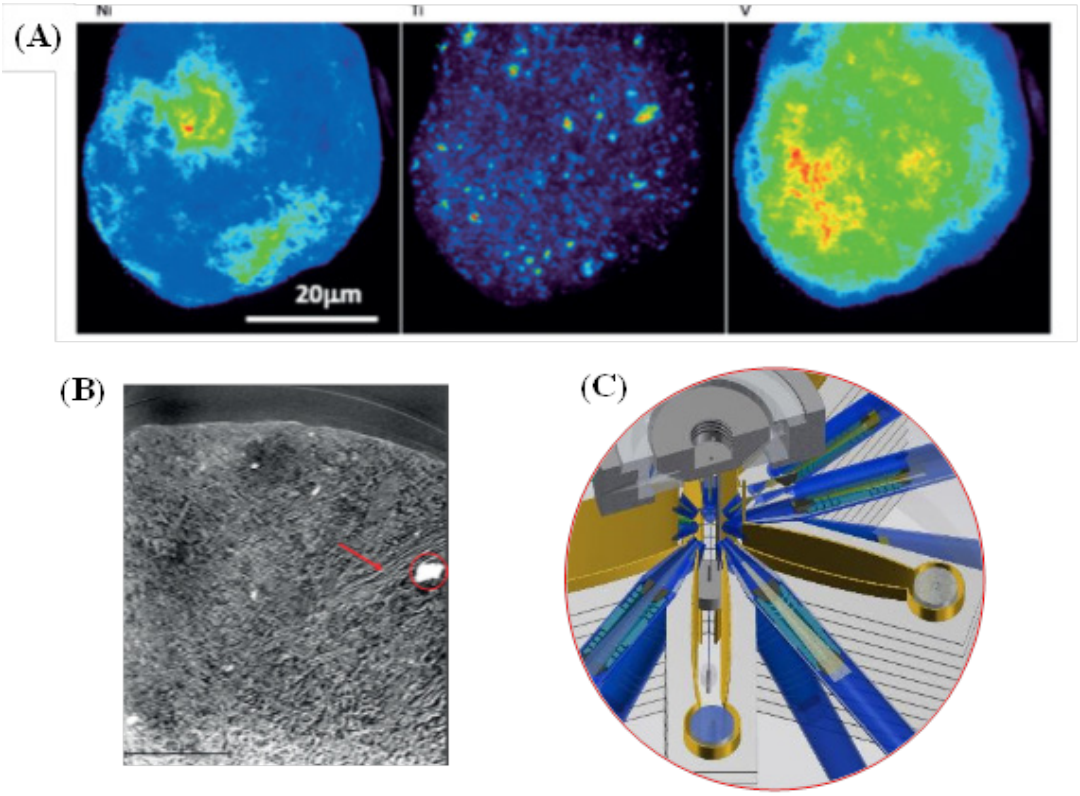


Figure 11: The fluid catalytic cracking (FCC) process is the principle gasoline upgrading technology used in refineries worldwide, involving the circulation of the catalyst continuously between a reactor and a regenerator. In-situ characterizations of FCC catalysts of structural and chemical composition and morphology at the nanoscale for individual microparticles can provide critical understanding of these catalysts function and lead to designer catalysts that are more efficient and effective. Examples shown include (A) an X-ray fluorescence image of elemental distributions in a FCC catalyst microparticle taken at APS with 150-200 nm spatial resolution, and (B) a cross-section of a transmission x-ray micrograph taken at NSLS of the internal microstructures of a FCC particle indicating complex morphologies of constituents and possible defects [Ref. 24]. At NSLS-II a powerful suite of spectroscopy and imaging beamlines *e.g.* ISS, with an in-situ/in-operando mini reactor as the center of the confocal spectrometer as shown in (C), as well as QAS, TES, FXI and SRX beamlines will enable substantial advances in *operando* investigations of catalysts in action, including x-ray emission spectroscopy studies under industrial relevant conditions, high-speed time-resolved 3D nano-tomography and XRF tomographic studies of single catalyst microparticles at 30-50 nm resolutions.

and (c) improved and extended time-resolved capabilities of analysis methods, covering various time scales that are relevant, from femtoseconds (excited state lifetime in a photocatalyst) to minutes and hours (catalyst deactivation). Finally, strengthening the link between experimental and computational channels leads to an efficient flow of information, facilitating catalyst development and optimization.

Nanoscale chemical and electrical metrology of next-generation photovoltaic materials: While crystalline silicon (c-Si) solar cells dominate the commercial market today, thin-film solar cells made from the direct bandgap semiconductor known as copper indium gallium selenide ($CuIn_{1-x}Ga_xSe_2$ − CIGS) ultimately have the potential for lower-cost solar electricity generation than silicon, as a potential alternative to meet the U.S. DOE SunShot goal of a levelized cost of electricity of six cents per kilowatt hour. The cost advantages of CIGS is primarily due to the potential for low-cost, high-rate manufacturing of CIGS resulting from its thin absorber layers (2 microns in CIGS compared to 200 microns in c-Si), which reduces material usage and enables roll-to-roll manufacturing on flexible substrates. These thin absorber layers are enabled by a strongly absorbing and tunable direct bandgap which in principle allows a fine-tuning of material properties as an added benefit.

The photovoltaic performance of CIGS films is currently limited due to its fairly complicated phase diagram along with the existence of ordered defects compounds. Solving this challenge requires powerful new nanoscale probes, such as those at NSLS-II and the CFN, and correlation of these measurements with laboratory-based device characterization. The ultimate performance of photovoltaic devices depends on structural properties that span multiple length scales, from stoichiometry variations over mm, to grain sizes on the order of microns, down to phase segregation at the nanoscale. The strong infrared and x-ray imaging and spectroscopic capabilities of NSLS-II, and the BNL partnership with the U.S. DOE Photovoltaic Manufacturing Consortium (PVMC) in Albany, NY, provide a nation-wide unique opportunity to address these challenges.

3.4 Environment and Climate Science

The world in which we live encompasses complex interactions between humans and the surrounding environment. Dissecting this complexity requires a molecular level understanding of the associations between the interacting partners. Moreover, science today is moving beyond a piecemeal approach to studying individual components in the environment towards an integrated approach to understanding these processes and being able to model and predict their behavior. The natural complexity of these interactions between living systems and the environment dictates the need for a wide range of characterization tools, especially those that can spatially and chemically probe this “interactome.”

The unique capabilities of NSLS-II will allow the scientific community to perform studies on naturally heterogeneous materials down to the nanoscale using a suite of interdisciplinary techniques including x-ray absorption spectroscopy, x-ray diffraction and scattering, x-ray fluorescence micro/nanoprobe, soft x-ray spectromicroscopy, microtomography, and infrared microspectroscopy.

Some key focus areas in environmental biogeochemistry that will be addressed by NSLS-II capabilities will include:

- *Biological systems science:* understanding the interactions between plant and microbial systems for applications such as sustainable biofuel production, improved carbon storage, and environmental contaminant remediation.
- *Environmental biogeochemistry:* investigations of the interfacial processes at Earth’s surface and subsurface in order to maintain sustainability of soil fertility, rare earth elements, fossil fuel production, mineral deposits, and fresh water reservoirs.

- *Climate and atmospheric science:* determination of the fundamental physics of interactions between clouds and aerosols including their impact on terrestrial ecosystems.
- *Planetary science:* characterization of natural and model-system extraterrestrial particulates in order to understand the evolution of our solar system, the origin of life, and the impacts on human space travel.

Biological Systems Science: One particular grand challenge in biological systems science is the complexity associated with the inter-actions between plant and microbial systems which are important to processes such as sustain-able bioenergy production, bio-geochemical cycling of metals and nutrients, carbon biosequestration, and greenhouse gas emissions. For example, cellulosic biofuels are not yet widely available because their biomass is a complex, heterogeneous material that is difficult to degrade into its component sugars and we have a limited understanding of the nanoscale chemical and structural properties of plant cell walls that impart strength and resistance to degradation. Another challenge in optimizing biofuel production is the need to increase biomass yield, which has been shown to be possible by the addition of endophytic bacteria in the environment of the plant root. However, very little is known about the mechanism of plant growth promotion or about the symbiotic relationship between the plant root and the bacteria. Another challenge is to understand how marine and terrestrial microorganisms fixate and cycle carbon in order to recycle the Earth's biomass.

With NSLS-II, X-ray probes with nanoscale resolution can address these grand challenges. As illustrated in Figure 12, for example, diffraction-based X-ray imaging at SRX can be used to determine the structure of crystalline cellulose and soft X-ray spectromicroscopy can assess the chemical effects of enzymatic degradation of the lignocellulosic network in the plant root. Additionally, synchrotron infrared imaging can provide images of the real-time degradation of cellulose at submicron-scale resolution. The NSLS-II nanoprobes can also be used to investigate nutrient cycling and flux at the plant-microbe-soil interface.

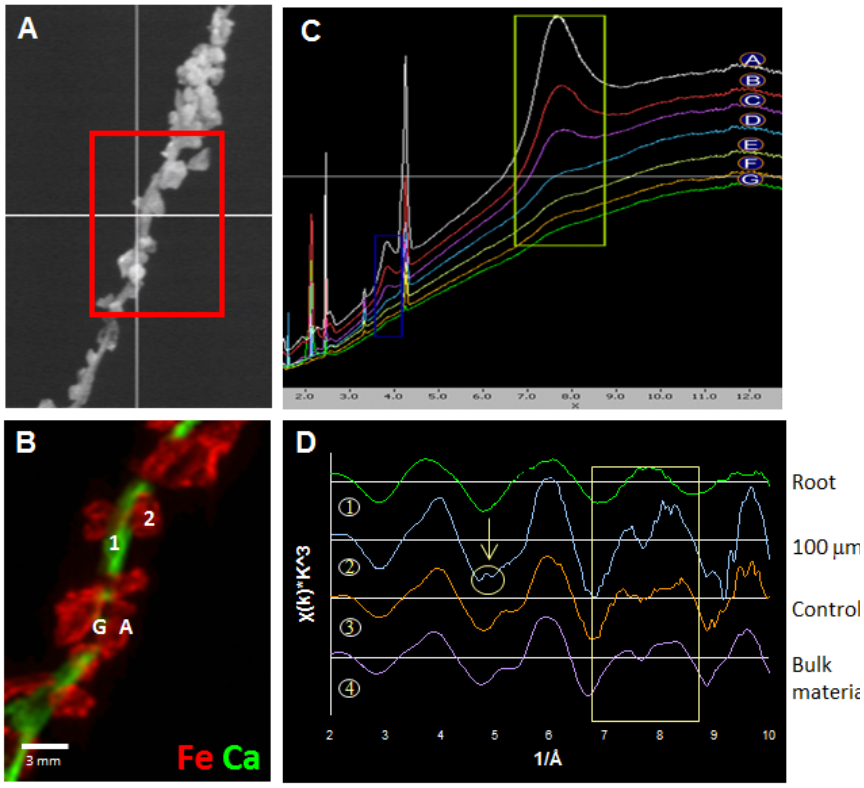


Figure 12: Mechanism of Fe transport across the plant-mineral interface [Ref. 25]. One of the most limiting nutrients in the soil is Fe because of its extreme insolubility. However, the micorrhiza at the plant-mineral interface interact with soil minerals enabling solubilization and transport. Understanding these mechanistic details at the interface requires nanoscale probes with chemical sensitivity such as X-ray fluorescence microscopy, spectroscopy, and diffraction at NSLS-II. (A) Visible and (B) X-ray fluorescence microscopy (XFM) image of a plant root and associated soil particles. X-ray Fluorescence Microscopy distinguishes between the root and rhizosheath through elemental imaging. (C) X-ray microdiffraction shows that soil minerals are solubilized near the plant root. (D) Microbeam X-ray Absorption Spectroscopy identifies the Fe speciation at the root-mineral interface, which shows that Fe solubilizes and chelates to organic acids near root surface.

X-ray fluorescence imaging and nanotomography are used to study the 2D and 3D distributions and elemental associations on the submicron scale, and X-ray absorption spectroscopy (XAS) is used to determine the molecular speciation of target elements. Hence, researchers will be able to observe these biogeochemical processes for the first time at the sub-cellular level, providing new information on the mechanism of plant growth promotion and bioenergy sustainability.

Environmental Biogeochemistry: The interfacial processes at Earth's surface and subsurface are critical for maintaining the sustainability of soil fertility, rare earth elements, fossil fuel production, mineral deposits, and fresh water reservoirs. For example, the DOE is committed to remediating the large volumes of soil, sediments, and groundwater contaminated with metals, radionuclides, and a variety of organics at diverse defense facilities and sites across the nation. In modeling contaminant transport, there is a vital need to evaluate how grain boundary geometries in natural systems influence the transport of chemical species in the subsurface.

With NSLS-II, advances in chemical imaging will offer excellent opportunities for imaging mineral-solution reactions in confined spaces in situ within dense geologic media. Direct observations of pore-scale transport may be possible, particularly in 3-dimensions using spatially resolved tomographic techniques. Since the average porosity of many subsurface lithologies has a natural size distribution at about 1 micron, the improvements in spatial resolution of SRX and HXN as well as FXI for tomographic instruments will allow us to image and quantify the distribution of pore spaces, evaluate microbial distribution on pore walls, and micro-spectroscopically evaluate colloidal chemistry at mineral interfaces. Together these tools can help generate a mechanistic understanding of these processes with a goal of developing long-term models for predicting the transport and fate of contaminants in order to produce viable remediation strategies.

Climate and Atmospheric Science: Today we face an increasing challenge to balance the worldwide demand for energy and its impact on climate and the atmosphere. Activities such as mining, construction, and fossil fuel burning are affecting climate processes in the atmosphere and on earth in a negative an unpredictable way. Many of these interactions involve chemical reactions at the surfaces of microscopic aerosol particles, which make them challenging to study, especially in situ. Comprehensive observation and modeling of Earth's system components are underway and include the need for new tools to probe these molecular interactions in model and real-world systems. The chemical sensitivity of the NSLS-II SRX and XFM probes will be instrumental in understanding many of these interactions. For example, anthropogenic atmospheric emissions as a result of mining, smelting, construction, fossil fuel burning, and other activities have significantly altered the natural global cycles for these and other metals. Increased atmospheric emissions has the potential to deliver significantly more bioaccessible iron and other metal micronutrients to the surface waters of the ocean, where it can stimulate primary production and CO_2 fixation. The effects of enhanced delivery of metals on the global CO_2 balance and, therefore, climate remain unresolved. To understand the effects of metal-rich aerosols on ecosystems, climate and human health it is not only important to measure total fluxes and concentrations of metals in air masses but also the oxidation state, chemical bonding, and structure of the metals. With NSLS-II, the spatial distribution and speciation of metals in microscopic aerosol particles can be investigated. The sensitivity of the x-ray fluorescence microprobes at NSLS-II will enable examination of submicron size particles with attogram detection sensitivity.

Planetary science: Synchrotron probes have been instrumental in understanding the origin of minute primitive extraterrestrial materials, analyses that provide unique insights into the conditions at the earliest stages of solar system evolution. Samples of cosmic dust rarely exceed a few micrometers in diameter and are typically aggregates dominated by nanoscale mineral grains and organic matter. For example, both interplanetary dust particles (IDPs) collected by stratospheric-flying NASA aircraft and

cometary dust samples returned to Earth from NASA's Stardust mission, the sizes of most of the individual mineral grains range from only a few nanometers up to a micrometer. It is critical to determine elemental composition and speciation down to trace concentrations in these grains to infer the chemical and physical conditions (composition, oxygen fugacity, and temperature) present in the solar nebula during condensation of the first solids. Since each component in these unequilibrated aggregates can have a different evolutionary path, there is a critical need for x-ray probes with adequate spatial resolution to analyze these subunits individually, especially in light of recent results suggesting that chondritic porous IDPs are the most primitive materials in our collections.

With NSLS-II, the HXN and SRX beamlines will provide some of the highest spatial resolutions available for elemental analysis coupled with highly-focused XAFS, XRD, and microtomography that will be world leading for the non-destructive analysis of these precious resources curated by NASA. A better understanding of the evolution of our solar system will also lead to insights into conditions required for stellar systems to produce planets conducive to the support of life.

3.5 Structures and Functions of Life

The study of Biological systems is fundamental to our understanding of our place in the world, our capacity to exploit this knowledge is fundamental to our health, our ability to produce food and fuels crops and our understanding of environmental change. Exploration of biological structure and function has benefited substantially from access to synchrotron radiation bringing significant, high impact, scientific results over the last decade. However, revealing the atomic structure of a bio-molecule is only part of the issue. In the biological context the environment, dynamics and large-scale organization are also key elements, thus there is a need to combine length scales - the atomic with the meso-scale, the meso-scale with the macroscopic.

NSLS-II brings new opportunities for life science research. Our suite of facilities will allow the combination of the atomic details revealed through X-ray diffraction, with longer scale organization in scattering experiments combined with imaging. To achieve the full potential will require innovation in sample preparation, instrument design and data analysis.

Structures and Dynamics of bio-molecules:

The enzymology of molecular machines: Many biological processes progress through the chemistry of the proteins involved. In many cases it is the coordinated action of tens of thousands of atoms in the form of bio-molecular machines that provides the essential functionality (Figure 13). The significance of these processes is apparent in the awarding of Nobel prizes in the last decade for the unraveling of the function of the ribosome (Yonath, Steitz and Ramakrishnan 2009) and mechanisms of transcription (Kornberg, 2006) both awards supported through the contribution available through synchrotron structural biology including NSLS. NSLS-II structural biology beamlines will provide the world-leading beam characteristics and specimen handling to enable structural studies of tiny biological crystals approaching ~um to sub-um scales. These capabilities, coupled with sophisticated data reduction and merging algorithms for a large number of datasets from multiple crystals, with expand the current studies to higher resolutions with high throughput, allowing hypothesis driven structural biology research on larger biological complexes of interest.

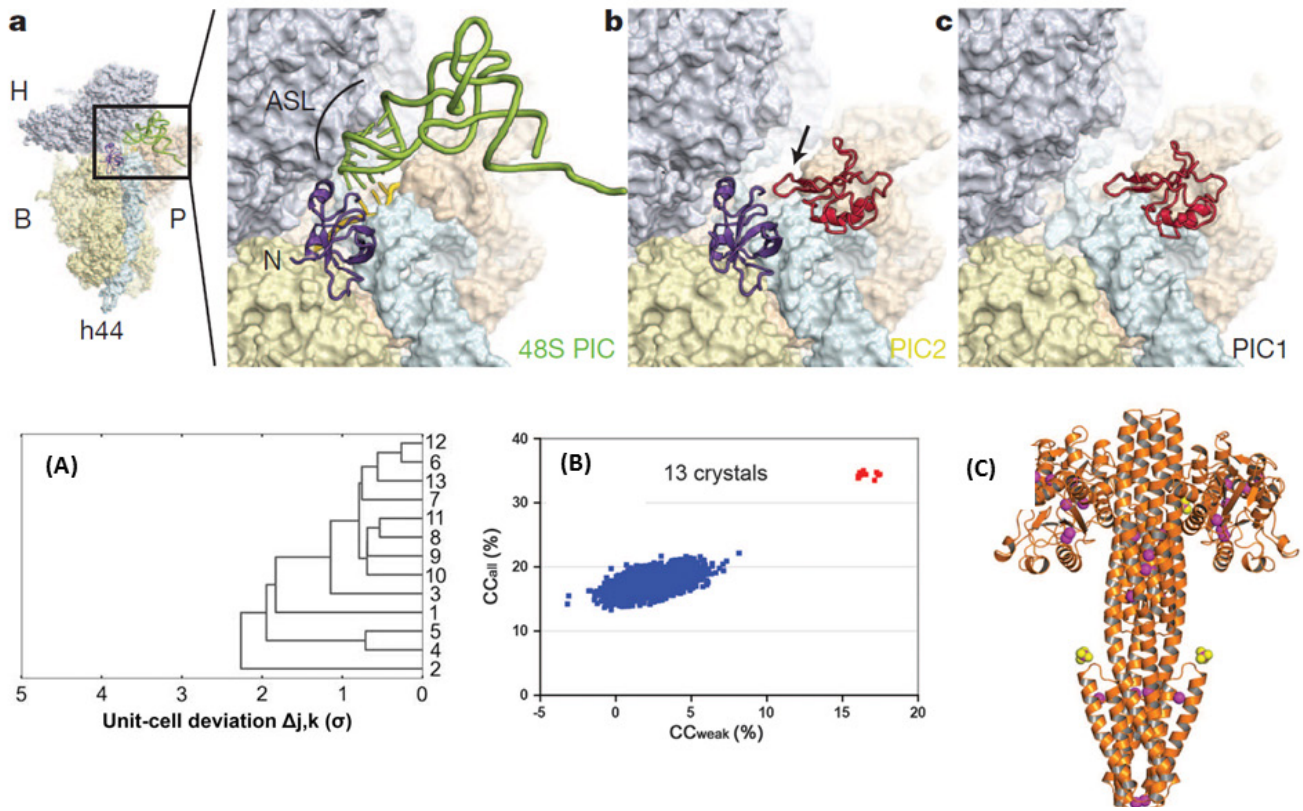


Figure 13: (Top) Revealing the genetic scanning mechanism that begins the protein synthesis process of the cell machinery – Crystal structures of three complexes of ribosome. These pre-initiation complex (PIC) structures provide insights into the steps in mammalian protein synthesis – position of eukaryotic initiation factors eIF1 (violet) and eIF1A (red), recruitment and scanning of mRNA (yellow), selection of initiator tRNA (green), and joining of large and small ribosomal subunits [26]. NSLS-II FMX and AMX beamlines will potentially enable such work at resolutions much higher than the current 7.9-9 A to reveal atomic-scale details of this crucial biological process.
(Bottom) Native structure of biomolecule TorT/TorS$_S$ in (C) from single-wavelength anomalous diffraction (SAD) of 28 sulfur atoms based on datasets on 13 different crystals [27]. The weak sulfur anomalous signals at 7.1 keV required the use of a novel data reduction method based on cluster analysis when merging multicrystal datasets, taking into account systematic differences such as the unit-cell dimensions (A). The structural solutions were obtained on the properly merged dataset as shown in (B). Extensions of such advanced data reduction algorithms to highly-merged partial datasets from a large number of crystals will be essential for structural biology investigations of large bio-molecule complexes at NSLS-II FMX and AMX beamlines.

Membrane transport and regulation: Membrane transport and the regulation of these processes underlies *inter* and *intra* cellular processes. The Noble prize for the GPCR systems (Lefkozitz and Kobilka 2012) and that for the structure and function of ion channels (McKinnon 2003) demonstrates the direct relevance of the NSLS-II in furthering our understanding, in that the biology was built upon many decades of basic research and was only possible due to access to high intensity X-ray beams for micro-crystallography. The potential economic impact of these discoveries is enormous – for example start-up companies are benefiting from this work in the search for new drugs to treat the panoply of Human diseases associated with GPCR proteins. Membrane transport function underlies many process of value to health, and food security, plant-microbe interactions and carbon-exchange.

Mesoscale Structures in Biological Cells

Understanding to plant-microbe interface at the molecular level: The relationship between plants and microbes is a complex, multi-organism system dependent on the environmental forces and the species involved. The complex interaction extends from the molecular scale (e.g. synthesis of nutrients)

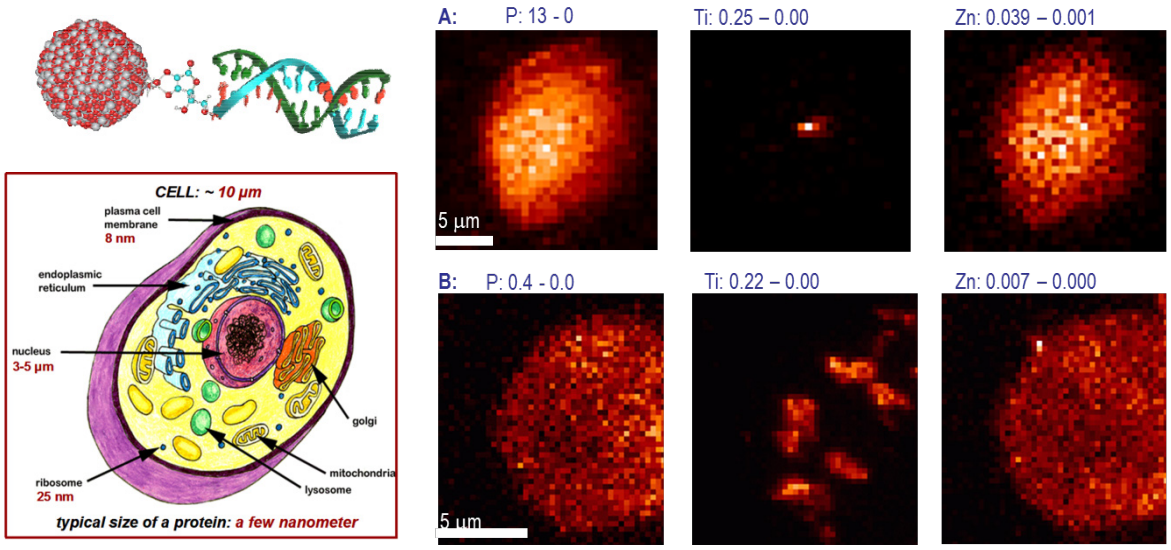


Figure 14: (Top Left) Schematic illustration showing a nanocomposite of a TiO_2 nanoparticle attached to DNA strand. (Bottom Left) Schematic of a cell with its internal organelles. (Right) X-ray fluorescence maps showing the elements distribution in freeze-dried biological cells, with the nanocomposite targeting nucleolus (top row) and mitochondria (bottom row). Data taken at APS with ~200 nm spatial resolution [28]. At NSLS-II the SRX beamline will provide higher x-ray flux in sub-100 nm resolution, addressing many key questions in nanobiotechnology and its potential applications in gene therapy.

through to the biosphere. Such ambition requires multi-disciplinary approaches with the coordinated access to beamlines and provision of appropriate support labs.

The Cell structure and dynamics: Understanding the organization and interaction of biological cells as well as their connections to bio-inorganic interactions (Figure 14) is an integrative research theme across structural and functional biology. In order to exploit to the fullest the potential for scientific discovery in this area it will be necessary to interpret crystallographic structures in the context of static and time resolved scattering data; correlation of the images from confocal and electron microscopies with scattering data across temporal and physical length scales.

Biological Imaging and Bioengineering

Bioinspired micro- and nano-fluidics: Nature has solved many problems that continue to vex engineers, understanding better the mechanisms developed by life offers the path forward for innovative approaches to problems we face. For example analysis of lepidopteran proboscises serves as a prototype of a new platform for micro and nanofluidic devices. Furthermore a shift toward fiber-based microfluidic platforms will provide devices with distributed actuation, sensing, and manipulation. Especially important are fiber-based probes which are able to absorb minute amounts of liquids, including chemical and biological aerosols, biofluids from cells and microorganisms, emulsion droplets, and the like, to transport and analyze them on the same sample. These fiber-based

microfluidic probes together with existing monolithic platforms are expected to push analytical chemistry and sensor engineering to a new level of resolution.

Evolutionary Biology: Unlike large (> 10 cm) animals, small animal physiology is generally not well-understood. The primary reason is that there is a lack of in-vivo visualization tools with the necessary features: sufficient temporal (< 100 ms) and spatial resolutions (1-10 um), sensitivity to soft tissue, and ability to penetrate the optically opaque exterior. As such, biologists rely on anatomy (generally obtained by dissection), measurements of the animal's interaction with the environment (*e.g.* gas exchange), and non-visual measurements such as internal pressure, electrical conductivity and temperatures to infer its physiology. Synchrotron x-ray phase-contrast imaging has been demonstrated to be an excellent imaging tool for in-vivo visualization of small animal physiology. Understanding small animal physiology is important for a variety of reasons: economic (agricultural), health (disease transmission), technology (biomimetics) and understanding fundamental evolutionary and genotype-phenotype links.

Paleontology and Paleobotany: Two major challenges in the study of ancient life include effectively examining the internal structure of fossils, and studying fragile or rare specimens embedded in matrix without destruction - in answering these questions synchrotron x-ray microtomography, which can provide exceptional resolution of internal structures and is non- destructive. The range of fossils that that can be served by synchrotron tomography is vast, ranging from early flowering plants to insects to dinosaurs to mammals, and the application of this technique to paleontology is in its infancy.

With NSLS-II, a beamline with a large field of view (6 cm x 1 cm) and spatial resolution at the 1-2 μm scale would greatly expand the range of life science-related animals and fossils that can be studied. With the expected photon flux at NSLS-II, 4D imaging (dynamics of 3D samples) can be attained. It will be possible, for example, to directly visualize a beating heart of a small animal in 3D in real-time. The potential impact of such live-animal studies is enormous. Much of the Cretaceous age fossil diversity, especially flowers and fruits, are larger than can be accommodated by current facilities. X-ray tomography will be an important tool in studying these fossils more thoroughly and in greater detail. Opening the study of invertebrate and vertebrate fossils where access to an instrument with a large field of view and high spatial resolution limits our capacity explore the origin and path of the evolution of our planet.

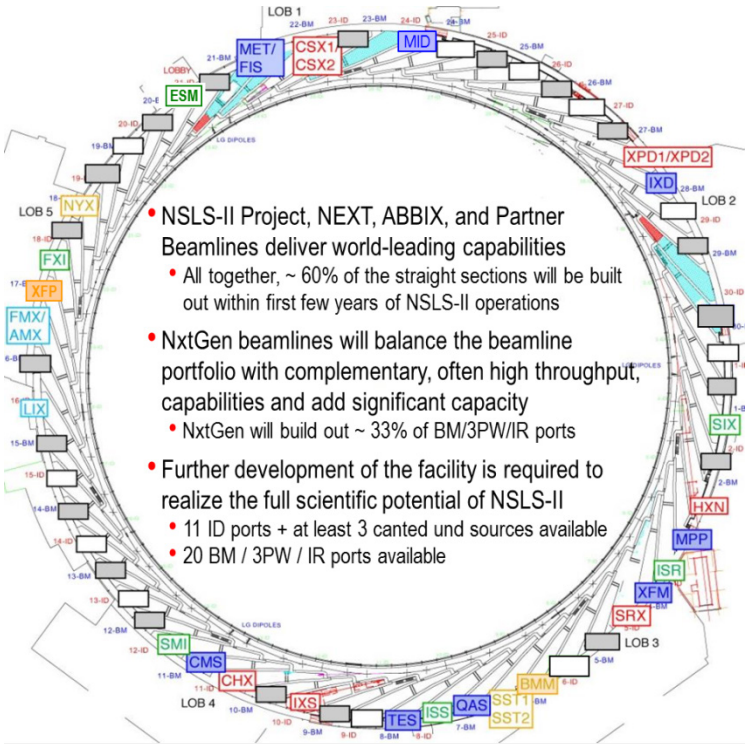
The unprecedented combination of flux density and collimation with make tractable crystallographic samples were previously unimaginable. Innovative sample delivery systems will enable dynamic process of transport to be revealed. Controlled substrate incorporation allows one to pursue femto-litre assays of enzymes reactions or substrate binding. As such, considerably more biological systems will become amenable to time-resolved crystallography approaches. This has the potential to dramatically expand the scientific scope of time resolved crystallography and, ultimately, to allow it to become an almost main-stream approach within the repertoire of Structural Biology. Moreover, it also presents the even more exciting possibility, with enormous theoretical and technological interest, of the production and analysis at room temperature of reaction intermediates *in crystallo* - the Holy Grail in the study of biocatalysis.

4. Strategic Developments for Next Five Years

As described in the last two Chapters, NSLS-II will complete the constructions of thirty beamlines in the next five years and is poised to make significant contributions and deliver high-impact science in a wide range of research disciplines. This constitutes an essential part of NSLS-II operations in the next five years.

It is important to note that NSLS-II will need to continue the development of new capabilities and new start-of-the-art beamlines, as well as other strategically important areas that require significant investments, in order to keep the NSLS-II facility at the leading-edge. In this Chapter, we outline five such development areas that NSLS-II plans to pursue, with planned resources in each area consistent with the current knowledge of funding guidelines for the next years.

4.1 Developing Additional NSLS-II Beamlines



The current NSLS-II beamline portfolio occupies ~60% of insertion device (ID) straight sections and ~33% of the BM/3PW/IR ports. Future development of additional beamlines is clearly needed to fully realize the scientific potential of NSLS-II. Among the remaining open ports, there are 11 insertion device straights plus 3 canted undulator sources, and 20 available BM/3PW/IR ports. It is understood that development of the majority of these new beamlines will require construction project funding, such as DOE major items of equipment, beyond the NSLS-II operating funds.

Given that the majority of the highly-demanded ID ports are already under development and the overall facility is more than half full, it is important to develop a high-level strategy for allocation of the remaining open beam ports. We have been actively engaging the PS SAC to discuss this topic in the past year. Based on these interactions, we have conducted the following analyses in order to make informed decisions on future strategic directions.

- Capabilities gap analysis of the current NSLS-II beamline portfolio based on the research needs of the scientific community
- Capacity estimates for both high-throughput beamlines as well as high-end beamlines in the current beamline portfolio
- Revisits of NSLS-II advantages and its community strengths and the effect of evolving synchrotron scene worldwide (outlined in Section 1.2.2)
- Strategic relevance to the NSLS-II science priority areas (outlined in Chapter 3).

The following sections summarize the analyses we have conducted to address the first two points while the other areas are already outlined in Section 1.2.2 and Chapter 3.

4.1.1 Capabilities Gap Analysis

Our capabilities gap analysis reconfirms that the 30 beamlines currently under development at NSLS-II will bring a broad range of leading capabilities to the scientific community. Looking at the complete picture, given the fact that each scientific community typically requires a complete suite of capabilities for their research, we see that our current beamline portfolio has the following capability gaps.

In nanoscale and mesoscale imaging, the current beamline portfolio is strong in hard x-ray scanning probes at nanometer (HXN), sub-micron (SRX), and micron (XFM) scale spatial resolutions, but the portfolio has the following capabilities gaps:

- There are no soft x-ray nanoprobes or soft x-ray full-field transmission microscopes for structural and chemical imaging of heterogeneous soft-matter, biological, or low-Z materials
- There is no spatially resolved grain-mapping microdiffraction beamline for engineering materials and energy storage devices
- There is no hard x-ray microtomography beamline for 3D imaging of engineering materials, biomaterials, and environments samples with larger field of view to complement the nanotomography capability provided by FXI.

In coherent scattering, the current portfolio of CHX and CSX-1 is strong in hard x-ray and soft x-ray photon correlation spectroscopy, with emphasis on dynamics with sufficient sampling volume, but

- The portfolio lacks beamlines dedicated to spatial imaging using coherent scattering, particularly in the ptychographic coherent imaging mode that enables studies of extended specimens in complex environment but requires more accurate positioning of the specimen.

In inelastic scattering, the current portfolio of IXS and SIX offer world-leading inelastic scattering capabilities with sub-meV in the hard x-ray and ~10 meV in the soft x-ray regime. The portfolio

- Lacks the capability of high-resolution (~10 meV) hard x-ray inelastic scattering for probing electronic excitations in heterogeneous hard condensed matter with nanoscale spatial resolution.

In structural biology, the current portfolio of FMX, AMX, LIX, NYX, XFP offers excellent world-leading structural probes for life science specimens in both crystalline and solution forms. However, currently

- There are no beamlines focusing on biological XAS studies of biochemistry of bio-macromolecules, nor beamlines using correlated spectroscopy and crystallography for combined biochemical structural studies.
- In addition, the novel sample handling method based on the innovative use of an acoustic droplet ejection system pioneered by PS staff has shown tremendous promise in enabling high-throughput room-temperature macromolecular crystallography data-collection at synchrotrons. A dedicated beamline at NSLS-II taking advantage of this innovation would open up completely new opportunities for combinatorial solution-based biochemical structural analysis of biomolecule complexes.

In in-situ and in-operando capabilities, the current portfolio lacks:

- Materials structural analysis under dedicated in-operando and extreme conditions (high pressure, high temperature, high radiation) that require large-scale dedicated experimental setups and infrastructure
- Beamlines with energy-dispersive XRD capabilities for engineering material systems and energy storage devices

- Beamlines in scattering, diffraction, and spectroscopy capable of handling rapid access tailored for industrial applications.

In addition, missing in the current beamline portfolio are beamlines that are tailored toward pump-probe time resolved studies, for example,

- Fast-timing capability with high-rep-rate and short x-ray pulses for in-situ studies of naturally existing, unclocked, irreversible processes in varieties of materials systems using the so-called 'pump-probe-probe-probe' approach.

4.1.2 Capacity Estimates

While accurately estimating the capacity for a brand new facility is challenging, we have considered several factors in our capacity analysis. First, several beamlines in the current suite of NSLS-II beamlines under development will provide cutting-edge world-leading capabilities. Therefore, by definition these beamlines will be among the very few beamlines worldwide to provide the cutting-edge scientific capabilities, potentially leading quickly to capacity issues during mature operations.

Second, being at the cutting-edge, multiple modalities (e.g. nano-XRF imaging and nano-XRD imaging) have been developed at these NSLS-II beamlines to serve diverse scientific communities. All capability modalities are developed to ensure world class performance, and this has attracted considerable demand from the community as evidenced in the First Experiments Proposal requests for the NSLS-II project beamlines. It appears that coherent scattering and high spatial-resolution spectroscopic imaging are the two areas where unique capabilities have attracted high demands. This observation is consistent with the evolving trends at other 3rd-generation SR facilities, such as at APS and ESRF.

Third, it is expected that such high user demands for cutting-edge capabilities will continue to grow from multiple scientific communities that often require specialized sample environments (e.g. in-situ battery cells vs cryo-preservation for biology), making efficient operations of such beamlines challenging. Thus the next phase of beamline development at NSLS-II will need to address this user demand issue, by considering building out additional 'high-end' beamlines with similar cutting-edge capabilities but tailored towards specialized sample environments for different communities.

Finally, there are clear indications that there exist considerable demands on the standard synchrotron techniques, such as x-ray spectroscopy, x-ray scattering, and x-ray microtomography, among the local and regional communities in materials engineering, catalysis, batteries, environment, and biological science areas. Therefore additional beamlines to meet the demands in these areas may be required at NSLS-II.

4.1.3 Strategic Directions for Future Beamlines

Taking into account all the above considerations and the discussion of NSLS-II strengths in Section 1.2.2 and science priority areas in Chapter 3, the NSLS-II strategy for the next 30 beamlines will be to complete its scientific capabilities portfolio by developing additional beamlines that

a) meet the unmet needs of the scientific and the industrial community aligned with one or more NSLS-II strategic priority research areas

b) provide additional cutting-edge in-situ capabilities with specialized sample environment and handling tailored towards specific communities

c) ensure NSLS-II's leadership role in developing science programs that meet the growing interest worldwide in high-resolution imaging and coherence

Based on these strategic directions, along with community input from prior rounds of calls for beamline development proposals and PS SAC feedback, we outline below a list of 20 beamlines as a *strawman* for possible development in the next phases of future beamline development. This list consists of both the beamlines for which funding is currently being sought (as indicated) as well as those beamlines with no clear funding routes at present. For the latter, NSLS-II plans to further engage the community and the SAC to identify the next steps for further developments. In addition, NSLS-II will issue calls for additional beamline development proposals to solicit new beamline ideas and concepts as well as to solicit updated proposals for the previously approved BDPs.

Beamlines for Nano-imaging and Coherence

- **X-ray Fluorescence Nanoprobe (XFN):** XFN will be located at 5-ID as an independent branchline to the SRX beamline. This beamline has been proposed to DOE-BER for potential funding in the near future. It will specialize in two- and three-dimensional element-specific imaging of biological materials with ~30 nm spatial resolution and attogram detection sensitivity. Simultaneous X-ray phase contrast imaging will be used to co-localize trace element chemistry with organelle substructures. X-ray absorption spectroscopy with the nanoscale beam will also enable the determination of elemental speciation from phosphorus through bromine.

- **Hard Inelastic X-ray Scattering Nanoprobe (HIX):** HIX would offer a high-resolution inelastic X-ray spectrometer with a world-leading 10 meV energy resolution in the energy range of 2.9 keV-15 keV, with a sub-100 nm beam spot size, for resonant and non-resonant inelastic x-ray scattering (RIXS and NIXS) studies of low-lying electron excitations in heterogeneous hard condensed matter. This would represent an order of magnitude improvement in resolution over similar instruments in the world today, and the first of its kind dedicated to the study of electronic excitations.

- **Scanning Microscopy Facility for Materials Science (SMF):** SMF would be an undulator-based soft x-ray spectromicroscopy facility at ~10 nm spatial resolution with polarization control, dedicated to the study of the nanoscale origin of macroscopic (electrical, magnetic and optical) properties of matter, and the evolution of such systems under relevant conditions.

- **Coherent Diffraction Imaging and Ptychography (CDI):** Taking advantage of the world-leading coherence at NSLS-II, CDI would be a state-of-the-art hard x-ray coherent diffraction imaging and ptychography beamline for 3D Imaging of nonperiodic materials structures and strain fields inside microcrystals on the nanometer scale, evolution of shape/strain under working conditions or manipulations, ptychographic imaging for extended objects and biological samples using phase contrast, and provision for cryogenic sample handling for diffractive imaging of biological cells, organelles and tissues.

- **Multiscale X-ray Diffraction (MXD):** MXD would be an undulator beamline with a variable x-ray beam size from 30nm to 3 microns for multiscale x-ray diffraction studies of heterogeneous materials with hierarchical multiscale features. It would offer a large working distance > 0.1m that enables different sample environments; UHV, diamond anvil cells with laser heating, and humidity and temperature cells.

- **Scanning Transmission X-ray Microscope (STX):** STX would be a BM-based high-throughput soft x-ray spectromicroscopy (STXM) beamline in an energy range of 250-2200 eV, and would consist of a STXM instrument extremely versatile and appealing to groups from a large variety of scientific disciplines including environmental science, energy research, soil science, geochemistry, microbiology and other biological research areas, as well as material science.

- **Soft X-ray Full-Field Transmission Microscope (TXM):** Soft X-ray transmission x-ray microscope has shown considerable promise in studying biological cells within the water-window of the soft x-ray range, revealing structures and organizations of subcellular organelles and their connections to cell function. Such a beamline would complement the existing fluorescence imaging capabilities at NSLS-II, and would be invaluable in the scientific theme of mesoscale biosciences.

Beamlines for Additional Capabilities & Capacities

- **Low-Energy Anomalous X-ray Diffraciton MX (LAX):** LAX would be an undulator beamline optimized for anomalous crystallographic diffraction experiments in the energy range from ~3 keV to ~7 keV. It would be located at 19-ID as an independent branchline to the NYX beamline. The LAX beamline will enable more accurate SAD and MAD phasing of increasingly more complex and challenging biological subjects – mammalian proteins, large multi-component complexes, integral membrane proteins, as well as many other biomolecular systems.

- **Infrared Imaging (IRI):** IRI will specialize in full-field, mid-infrared spectroscopic imaging (500 – 4000 cm^{-1}) at high spatial resolution of the chemical and structural properties of a wide range of biological materials. Coupled to an environmental chamber, the IRI beamline will provide unique capabilities for in vivo studies on time scales from microseconds to days with micromolar detection sensitivity and sub-micron spatial resolution. This beamline has been proposed to DOE-BER for potential funding in the near future.

- **Micro-tomography for Materials and Biological Sciences:** Microtomography for materials science would be a high-throughput micro-imaging beamline with a wide field of view at NSLS-II. It would allow 3D imaging of internal microstructures as well as crack formation and degradations in a wide variety of materials systems, including those structural materials such as concrete and light-weight alloys.

- **Correlated Spectroscopy and MX (SM3):** SM3 will support multidisciplinary studies of protein in solution and as single crystals. The fully-integrated experimental endstation will be optimized for nearly simultaneous, correlated measurements of macromolecular crystallography (MX), electronic absorption and Raman vibration spectroscopies. In addition, the beamline will offer solution-based x-ray absorption spectroscopy (XAS), which will also be correlated with optical spectroscopies. Indeed, because the x-ray diffraction and XAS processes often advance normal reaction cycles, these complementary techniques will provide structural and functional information from the same sample. This beamline has been proposed to DOE-BER for potential funding in the near future.

- **Soft X-ray Scattering and Spectroscopy (SSS):** SSS would be a BM-based, state of the art high resolution soft x-ray spectroscopy and scattering beamline capable of delivering both linearly and circularly polarized light from 100–2000 eV utilizing a bending magnet source is proposed. In addition to providing continuity of support to the strong existing soft x-ray

spectroscopy/scattering community, the beamline would provide significantly enhanced capabilities to enable research in the areas of condensed matter physics, material science, chemistry, environmental science and biophysics.

- **Biological X-ray Absorption Spectroscopy (XAS):** XAS would be a 3PW-based beamline for biological XAS research, and would address critical needs for the US metalloprotein user science community and represent an essential complement within the overall suite of XAS beamlines needed for NSLS-II, where other beamlines would be dedicated to more specialized needs that leverage specific NSLS-II properties or require specialized instrumentation. Being the only facility of its kind on the East Coast of the United States, it would be an invaluable resource to the continuity of service and transition of current high-impact scientific programs from NSLS to NSLS-II.

- **Industrial Small Angle X-ray Scattering:** This would be a high-throughput 3PW based SAXS beamline specifically tailored for studying the structures of polymers and other materials with high industrial relevance. The goal is to encourage the industry participations at the beamline from a strong regional community in the academia and the industry. It may also serve as a pilot project at NSLS-II for establishing a strong industry research program based on industry consortia.

- **High-throughput Combinatorial Macromolecular Crystallography (HTX):** HTX would be a dedicated beamline for room temperature high throughput in-situ crystal screening and data collection. The facility would aim to provide several powerful options to the structural biology community, including complete room temperature data sets from a single crystal without cryo-cooling the sample, combining partial data sets from multiple crystals that are challenging to cryo-cool, and the possibility to perform biochemistry screening for fast correlations between structures and associated biochemical conditions.

Beamlines with Dedicated Sample Environment

- **High Energy X-ray Diffract for Materials Engineering and Battery Research (HEX):** The HEX beamline would be based on a suite of high energy techniques, in particular, energy dispersive x-ray diffraction, with enhanced in-situ and in-operando endstation capabilities for attacking and solving fundamental and technological problems in engineering materials, as well as energy storage systems. It would enable time-resolved 3D mapping of materials phase, strain, and morphology in study of materials research challenges that are central to this nation's technological future.

- **Materials in Radiation Environment (MRE):** The MRE beamline will be a unique facility in the DOE light source complex that will allow in-situ studies of highly activated nuclear materials under realistic conditions. It will provide synchrotron x-rays techniques for investigating materials of interest for nuclear fission and fusion and national security at two endstations located in a separate satellite building. One endstation will focus on in situ and time resolved imaging/diffraction studies of radiation processes by combining NSLS-II capabilities with ion beam accelerators and ultrafast detectors. Another endstation will examine structural damage in previously irradiated targets and radioactive materials using x-ray diffraction, tomography and absorption techniques. This beamline has been proposed to DOE-NE for potential funding in the near future.

- **4-D Studies in Extreme Environment (4DE):** The 4DE would be a high-field wiggler beamline that would provide high-flux hard x-rays to study variety of materials with optimal control on high-pressure and high-temperature sample environment and to explore a broad

space-time range for high-pressure earth science community as well as materials science and engineering under extreme conditions.

- **Time resolved Studies in Extreme Conditions (TEC):** The TEC would be a high-brightness undulator beamline that would allow combination of x-ray diffraction, spectroscopy, and 2d and 3d imaging techniques to study materials in variety of extreme conditions such as pulsed laser driven and mechanical actuator (dDAC) compression, pulsed laser heating, pulsed internal heating, high magnetic fields, chemical reaction environment, and fast optical diagnostics of the sample properties in a pump-probe mode, with time-domain measurements to access the time-scales of micro- and macro processes in the materials under extremes.

Beamlines for Fast Timing Capabilities

- **Electron Beam Slicing for Ultrafast Science:** This beamline would potentially make use of the results from an ongoing accelerator R&D effort on electron beam slicing in the NSLS-II storage ring by cross-passing an ultrafast electron bunch from a separate LINAC. Such a beamline would in principle allow ultrafast studies on variety of materials and condensed matter systems without severe perturbations of regular operations of the NSLS-II storage ring.

The list of 20 new beamlines described above would nicely complement the current suite of 30 beamlines at NSLS-II, by contributing to a well-balanced techniques portfolio in scattering /diffraction, spectroscopy, MX, and imaging (Figure 15).

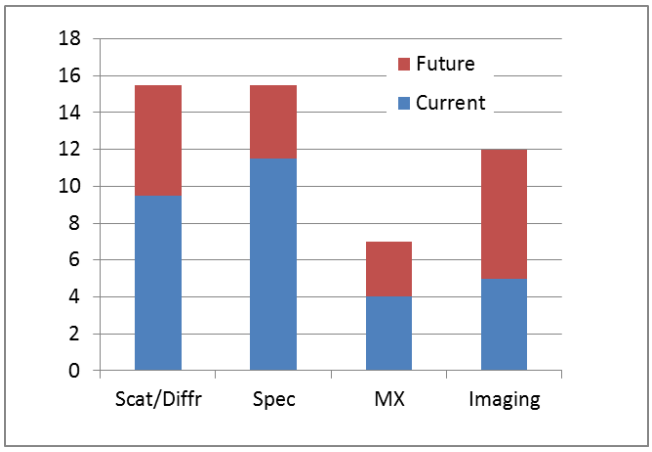


Figure 15: Number of NSLS-II beamlines in different techniques, with the 30 beamlines in the current portfolio (Blue) and additional 20 beamlines in the strawman list of future beamlines (Red).

4.2 Scientific Computing and Data Management

Data management and computing is an essential and important component of the NSLS-II strategy to enhance scientific productivity and impact of the NSLS-II facility. In this Section, we describe the data challenges that NSLS-II is facing, the approach that NSLS-II is taking and will take to address these challenges, and our plans to develop theoretical simulation and modelling in support of the user science at NSLS-II. While part of the essential funding is expected to be part of the NSLS-II operating budget, a large-scale data management and computing center will require additional funding through collaborative effort with other funding sources e.g. DOE Advanced Scientific Computing Research (ASCR).

4.2.1 'Big Data' Challenges at NSLS-II Beamlines

As the newest synchrotron facility with high-brightness and high-flux beamlines serving a broad and diverse scientific community, NSLS-II faces significant challenges in data management and scientific computing. These challenges primarily arise from three factors.

First, many of the NSLS-II beamlines support cutting-edge scientific capabilities that make use of the most advanced systems for specimen positioning and manipulation as well as photon detection. In order to ensure all experimental techniques are conducted in the most optimal way and not constrained by a 'standard' data acquisition system, NSLS-II has adopted, by design, the strategy that the data acquisition system at each beamline is developed to match the intrinsic data collection needs dictated by the specific experimental technique in sample and photon beam manipulation as well as in photon detection method. As such, the data structures and formats may be complex and can vary substantially from beamline to beamline, making follow-up visualization and analysis of the data challenging. This is the *data complexity* issue of the NSLS-II data challenge.

Second, high brightness and high flux available at many of the NSLS-II beamlines coupled with advanced high-speed megapixel detectors will drive much higher data rates and volumes compared to situations at most existing synchrotron beamlines. Indeed, all synchrotron disciplines are increasingly using multi-element detectors to efficiently measure and record the results of the experiment, and certain techniques often utilize detectors that can produce multi-megapixel images with frame-rates in the kilohertz range. The volume of data associated with an experiment may now exceed several tens of terabytes so simply moving data from one location to another is prohibitive. As such, it may not be possible for external users to take a copy of all the data on portable media or to transfer over the internet. Thus it will require high-performance data storage systems and front-end processing facility to allow users to access the data both during- and post-experiments. This is the *data management* issue of the NSLS-II data challenge.

Finally, broad uses of new megapixel detectors in new techniques drive a new paradigm for data processing and analysis at NSLS-II and at synchrotron sources worldwide, where individual users are often unable to write the sophisticated algorithms required to process, analyze, visualize, interpret or otherwise extract the important information from raw detector data. In addition, visualization and analysis of 3D or multi-dimensional data are intrinsically more difficult, particularly if one wants to extract out scientifically relevant information from a multi-dimensional dataset, often requiring specialized data reduction and manipulation algorithms and routines not readily available and/or not available to individual users. This is the *data mining and analysis* issue of the NSLS-II data challenge.

4.2.2 NSLS-II Plan to Address the Data Challenges

Recognizing the challenges in data management and computing, NSLS-II has been working closely with other groups in BNL and in other laboratories and developed the NSLS-II data management plan that consists of the following key elements:

Flexible Modular Data Acquisition Architecture: NSLS-II beamline data acquisition system is built to provide an essential infrastructure that can grow and evolve over the life of the facility. It not only supports the new detectors and new techniques as they continue to evolve, but also allows the analysis of the quality of the data as being collected and the performance of the beamline. The software architecture is built as a set of tools that use standard Application Program Interfaces (APIs), taking full advantage of the tools and standard communication protocols that exist in the Experimental Physics and Industrial Control System (EPICS). This architecture supports all data handling from the detector and other instrumentation, through analysis, visualization, and storage at each phase.

Data Stores and Data Broker Application Interface: At the heart of the NSLS-II data acquisition and data management system is an essential set of flexibly structured *data stores* that store all data and

metadata related to an experiment, and a *data broker* application interface to retrieve and manage data and metadata from a distributed set of data stores. The set of data stores are tailored for specific types of experiments, and store not only the raw data from a detector, but also requires additional data from the beamline, information from the accelerator complex, logbooks, and administrative information (such as metadata from user experiment proposals and safety reviews). The data broker is the key piece of data handling interface software to enable the development of data analysis pipelines for visualization and analysis of the real-time data to allow decision making, and for post-processing of all data after the actual experiment.

Two-tier Data Management System: To be able to accommodate high data-rate and high data-volume data at beamlines, NSLS-II will implement an essential two-tier data management system to ensure efficient and adequate data storage for complex experimental data from beamlines. (1) Each beamline will implement a local data storage and data management system at the beamline as part of the beamline data acquisition requirements, allowing on-demand fast data recording from detectors and data access for immediate visualization and analysis for feedback on the experiment. The data will be stored for a limited duration at the local system as determined by the beamline techniques until replicated elsewhere. (2) Data from each beamline will be replicated and archived at a centrally managed data center for longer-term storage, where same visualization and analysis tools for evaluating and processing are made available. This centrally managed data center will be established in close coordination with other computing sources at BNL such as Computational Science Center and RHIC and ATLAS Computing Facility.

Functional Library of Analysis Software Tools: Based on the data architecture and the data broker interface, a library of software routines and tools will be developed within the two-tier data management system by experienced staff as well as by some expert users for data visualization, reduction, analysis, processing, phase-retrieval, and extractions of scientifically relevant information

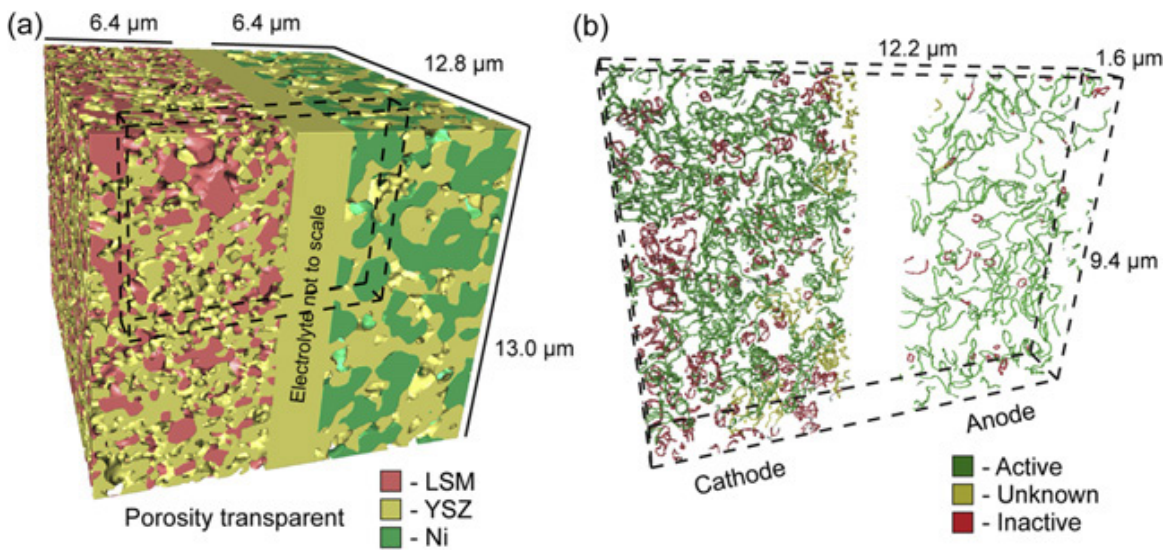


Figure 16: Example of extracting scientifically relevant information from processed and reconstructed complex experimental data [29]. In this case, the density of triple-phase-boundaries (TPBs) is obtained for the entire active region in a SOFC reconstructed from four sets of 3D rendered volumes [shown in (a)] at four different x-ray energies around the Ni K-absorption edge, each dataset consisting of 1441 2Kx2K TXM projection images. This analysis reveals the dramatic difference in TPB activities between the cathode and the anode [shown in (b)].

(see example in Figure 16). These essential tools will be tailored to meet the specific needs of specific type of technique, experiments, and scientific disciplines. Recognizing the large effort required to meet all the needs from the diverse community, NSLS-II plans to develop the analysis tools in a phased approach consistent with the NSLS-II beamline development timeline. Supported by several BNL LDRD projects, developments of data workflow and data visualization and analysis tools for the NSLS-II Project beamlines are already ongoing with substantial input and coordination in supporting the needs from other beamlines. In addition to coordinated effort within BNL, NSLS-II is an active participant in joint pilot projects with ANL and LBNL on data reduction and analysis in coherent scattering and ptychography. These coordinated efforts will continue in the future.

Post-Experiment Data Processing Facility: Anticipating the greater need for post-experiment data mining and processing, NSLS-II will work with other stakeholders on computing within BNL to develop and operate a central data processing computing facility as part of the two-tier data management system. The main goal of this facility is to provide front-end computing on top of the centralized data storage/archiving system for NSLS-II users to access their data on-site during experiment and/or remotely from their home institutions for post-experiment processing and analysis. The archived data are made available to remote users for a length of time that is largely determined by policy and resource constraints. It is anticipated that such a post-processing facility on archived data will be an important component of the NSLS-II scientific capabilities portfolio to enable effective and efficient workflows from experiments data to publications and solutions for high scientific productivity and societal impact.

4.2.3 Theory Simulation and Modelling

As synchrotron experiments become more and more sophisticated, there exists an increasingly greater need for adequate theoretical modelling and simulations. This is particularly desirable for certain high-end experiments at NSLS-II beamlines, in two aspects. First, in high-end experiments depending on high degree of x-ray beam coherence, the experimental results have a greater dependence on coherent properties of the beamline optics and beam defining apertures. Therefore, better understanding of how a complete experiment works including the effects of optics is important to being able to interpret the experimental data correctly. NSLS-II plans to address this issue by working with the community and exploring the development of a complete "start-to-end" simulation chain from radiation sources through beamline optics and sample to detectors for certain experiments. This would ensure more optimized experimental design with correct matching of different links in the experimental setups, including source, optics, sample, detector and data processing, leading to most efficient use of resources and beamtime at beamlines and timely and correct interpretations of experimental results.

Second, new and enhanced experimental capabilities at NSLS-II will lead to new experimental results that may require new theoretical development and interpretations. Therefore, there will be greater needs for theoretical modelling and analysis to lead to high-impact and scientifically relevant conclusions. NSLS-II will work closely with the scientific community to tackle this challenge, through collaborative efforts on *joint research projects* with key members of the community and through forming *targeted initiatives* to outreach to specific expert groups in the community. A current example of the latter is an ongoing discussion with the materials degradation theory group at MIT on modelling materials fatigue and crack formation mechanisms at the mesoscopic length scales of a few grains in the context of future experiments at the XPD, HXN, and future MRE beamlines.

Together these theory simulation and modelling effort will greatly enhance the NSLS-II capabilities in experimental planning and design, in interpretations of experimental data, and in arriving at research results with a greater impact on the research activities in variety of scientific disciplines.

4.3 Advanced R&D and Support Laboratories

It has been well-recognized in the light source community that advanced R&D in X-ray optics, detectors, and precision engineering, as well as the development and operations of a suite of support laboratories, is a crucial and necessary component of any modern light source facility. This is particularly true for NSLS-II. As the newest high-brightness and high-coherence synchrotron facility, achieving the full scientific potential of NSLS-II very much requires strategic developments in these areas that will often reach beyond the current state-of-the-art.

Leveraging upon the experience gained and infrastructure already existing at BNL as well as established during the NSLS-II construction phase, we plan to pursue advanced R&D and engineering using the following strategy:

- Define mission-driven R&D directions: To ensure efficient and effective utilization of resources, NSLS-II R&D program will focus on those targeted areas that are required to achieve certain strategic objectives in the NSLS-II mission;

- Encourage and develop collaborations and partnerships: To leverage expertise, developments, and resources elsewhere in academia, industry, and other national laboratories, NSLS-II will pursue R&D in coordination with the community and our sister facilities;

- Adopt integrative systems engineering approach: NSLS-II will use a goal-oriented systems-engineering approach to pursue R&D. This approach ensures development and integration of all required subsystems (optics, detectors, nanopositioning, environment, and controls) to meet the NSLS-II R&D goals.

This section describes three strategic R&D areas plus a suite of support laboratories that are critical to enable the NSLS-II beamlines to achieve their best-in-class performance and capabilities.

4.3.1 Advanced X-ray Optics

Many advances in synchrotron beamline technology, and consequently in the range and quality of scientific applications, continue to be driven by advances in X-ray optics. Optics developments over the preceding decade have encompassed improved performance from existing optics such as mirrors, increasing use of multilayer coatings, and the development of new X-ray optical elements such as refractive and multilayer Laue lenses. This trend is expected to continue in the future, as driven by the demands of the high brightness of the third generation sources and by increasing performance required by scientific experiments [30]. At NSLS-II, meeting our strategic objective to establish and retain NSLS-II leadership in high-spatial-resolution imaging, in high-coherent-flux scattering, and in high-energy-resolution inelastic scattering, requires development and characterization of a number of advanced X-ray optics that are not available today. Therefore, an essential and integral part of the NSLS-II strategic plan is to develop novel X-ray optics and the associated tools to characterize and utilize them. Our plan focuses on the following three critical optical areas.

Nanofocusing X-ray Optics: We plan to continue to advance the essential nanofocusing X-ray optics R&D towards achieving the ultimate goal of nanometer spatial resolution. Owing to its excellent structural, elemental, and chemical sensitivity and sufficient penetrating power, hard X-ray microscopy attracts enormous attention in recent years in the synchrotron community. Existing hard x-ray microscopy tools offer spatial resolution down to a few tens of nanometers, still not adequate for addressing a wide variety of scientific problems that require the understanding of the interplay between materials' properties and their functionality at nanometer level. This strong demand fuels the driving force toward achieving hard x-ray focusing well into the single-digit nm regime.

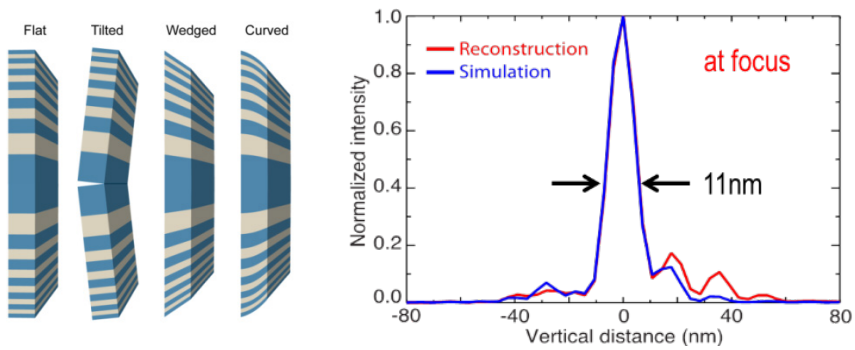


Figure 17: (Left) Four different types of multilayer Laue lenses (MLLs). Each type has a different way of utilizing dynamical diffraction effects, occurring within the lens. (Right) Comparison of simulated and measured focal spot intensity profiles based on 2D ptychography measurements on a Au grating sample, indicating an 11 nm focus at 12 keV for a tilted MLL optic with 4 nm outmost zone width [31].

Two complementary nanofocusing optics approaches will be pursued at NSLS-II in the next 5 years.

- **Development of large-aperture tilted and wedged multilayer Laue lenses (MLL):** Leveraging several critical advances on the novel multilayer Laue lens (MLL) optics (Figure 17) development made during the NSLS-II construction project, we will continue to develop and advance the necessary thin-film deposition including materials selection for large-aperture MLLs, sectioning and polishing techniques, and characterization and analysis methods to fabricate and implement tilted and wedged MLLs (Figure 16) and their associated mechanical systems to achieve 5 nm focus in the 10-20 keV range.

- **Collaborative development of large-numerical-aperture multilayer (ML) mirrors:** We will pursue collaborative efforts with other Laboratories (e.g. APS) and interested industry partners to develop novel fabrication techniques for multilayer focusing mirrors based on combination of profile ML coating and controlled ion beam figuring with in-situ optical metrology. Our goal here is to develop and implement Kirkpatrick-Baez (KB) mirrors producing focal spots down to 10-20 nm for larger working distance spectroscopic imaging applications.

It has been widely recognized by the community that these two approaches – multilayer Laue lens (MLL) and multilayer KB mirrors, are the most promising ways to ultimately achieve nanometer-scale spatial resolution with high optical efficiency for hard x-rays. While our main emphasis will be to continue to drive and advance the MLL technique, our strategy to supplement this main focus with a collaborative effort with APS on ML mirrors will ensure NSLS-II to stay at the cutting-edge in hard x-ray nanofocusing capabilities.

Coherent X-ray Optics Metrology and Development: Many of the high-impact scientific opportunities at the nanoscale afforded by NSLS-II, such as coherent X-ray imaging, nano-diffraction, and nano-spectroscopy, require maximum intensity in the focus and minimal wavefront distortion. These applications require X-ray mirrors with $\leqslant$0.5 nm rms height errors and sub-100 nrad slope

errors for surface spatial frequencies ranging from 100 microns to the full optical aperture of the optic. These characteristics are extremely close to the present noise floor for short flat mirrors and are beyond the state-of-the art for highly curved mirrors.

To fully meet these R&D needs and challenges requires concerted and coordinated efforts in the synchrotron community and targeted efforts in close collaboration with optics manufacturing industry. Leveraging the unique expertise and the cutting-edge optical metrology capabilities acquired through the NSLS-II construction project, our strategy is to identify and pursue a number of targeted initiatives where NSLS-II will continue to play a significant leadership role in the development and metrology of advanced X-ray mirrors for coherent applications. These initiatives include:

- **Development of next generation of metrology tools and techniques:** This is essential to enable measurements of figure errors at sub 100-nrad levels. This will be done by combining upgraded instrumentation in the existing NSLS-II optical metrology laboratory with a new at-wavelength measurements capability to be established at the Metrology and Instrumentation Development (MID) beamline at NSLS-II. The at-wavelength wavefront characterization techniques will open up perspectives, for instance, in the in situ optimization of adaptive optics or correction of reflective optics and could also be used as an online setup permitting focusing optimization, for example, by assisting in the alignment of critical x-ray optical components or compensating for the astigmatism of an incoming beam or mechanical deformation due to heat load or mounting stress.

- **Development of advanced analysis and simulation tools:** This is essential to enable quick feedbacks on optics fabrication and characterization as well as forward simulations of coherent wave propagation of combined optical effects, with imperfections, that directly influence targeted experiments. This includes the implementation of efficient analysis codes for phase retrieval and reconstructions of wavefronts based on at wavelength measurements of X-ray optics.

- **Development of targeted partnerships with optical manufacturing industry:** Very few optical manufacturers have the expertise necessary to perform the surface metrology required to produce ultralow slope-error optics. For various reasons, this is particularly true for US manufacturers. Therefore it is important to promote partnerships with optics fabrication industry in the northeast of US by developing the next generation of metrology instrumentation and making them available to those companies in the US who are willing to develop cutting-edge optics. Specifically, we plan to explore potential collaborations with the regional optics manufacturers alliance that already exists in upstate New York, with its own trade organizations – New York Photonics and the Rochester Regional Photonics Cluster – centered in the Rochester area, and with APOMA (American Precision Optics Manufacturing Association) that has an existing track record in developing new techniques to help the optics industry. Partnering with these organizations and New York State may lead to establishment of an advanced polishing laboratory to perform the necessary R&D geared to producing ultra-precise aspheric optics utilizing these novel fabrication techniques. Such a laboratory would also provide education and training opportunities for optical technicians to be skilled in the technologies that are needed for ensuring a supply of high quality synchrotron radiation optics for the community.

High Resolving-Power Spectrometers for Soft and Hard X-rays: Owing to the unique dependence and sensitivity on energy, momentum, and polarization, resonant (RIXS) and non-resonant inelastic x-ray scattering (IXS) have become increasingly important techniques for studies of low-energy

excitations in complex correlated electronic materials, and weak excitations due to micro- and nanoscale heterogeneities in solid state and disordered systems. Increased the energy resolutions in both soft x-ray RIXS to meV range and hard x-ray IXS to 0.1 meV range will be essential to keep NSLS-II at the leading-edge in IXS and RIXS, and would dramatically enable a wide range of studies that are not possible today at synchrotrons.

To meet the NSLS-II strategic objective on leadership in high energy-resolution inelastic scattering, we plan to continue develop and advance high resolving-power spectrometer systems for both soft and hard x-rays. Our strategy includes the following:

- **Developing world-leading RIXS and IXS beamlines with flexibility for future upgrade:** Two beamlines currently under construction, IXS at 10-ID and SIX at 2-ID, will have best-in-class performance when starting operations, with <1 meV resolution with sharp-resolution-tails at 9.1 keV at IXS, and ~15 meV resolution at 1 keV at SIX. Anticipating the advances in the coming years in high-resolution crystal optics and surface gratings, these two NSLS-II beamlines are designed and constructed with large experimental hutches that can accommodate long spectrometer arms, 10m for IXS and 15m for SIX. This ensures the flexibilities for future spectrometer upgrades when higher-resolution optics become available. Furthermore, the spectrometer designs allow straightforward upgrade to multiplexing multiple spectrometers to enhance signal throughput covering a desired range of momentum transfer or inelastic energies.

- **Working with LBNL and potential industry partners to promote development of high-density-gratings:** We plan to work closely with our colleagues at LBNL and potential industry partners to support the development of high-resolving power, high-density grating optics with low slope and line ruling errors for soft x-ray applications. We will monitor closely the multiplexing schemes that have been proposed by our colleagues at LBNL for the purpose of improving energy resolution and/or throughput of the soft x-ray spectrometer at SIX beamline.

- **Developing dispersive crystal optics for hard x-ray spectrograph at 0.1 meV resolution:** The asymmetric back-reflection dispersive crystal optics (CDW) scheme that NSLS-II has adopted, based on the original idea of Shvydko [32], offers a unique opportunity to develop a hard-x-ray version of a spectrograph by imaging the highly dispersed scattered x-rays onto a spatially resolving area or linear detector, whose pixels act as multiple 'exit slits'. This inelastic scattering imaging approach was conceptualized during the early R&D phase of the NSLS-II project. The achieved resolution of <1 meV on the IXS CDW prototype instrument tests (Figure 18) makes it possible to further develop and implement the imaging approach. Therefore, NSLS-II plans to exploit and pursue this

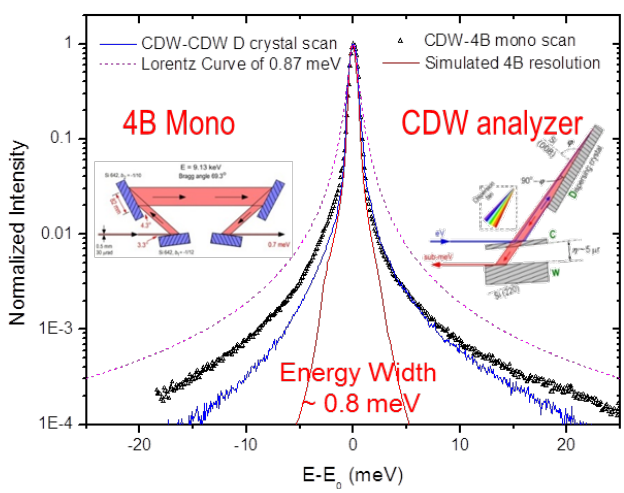


Figure 18: The IXS high-resolution x-ray optics test result shows 0.8 meV energy resolution at 9.1 keV using the combination of a 4-bounce monochromator and a CDW analyzer [33]. It is expected that such optics can be expanded to incorporate a spatially resolved multi-pixel detector system to achieve improved energy resolution, ultimately to 0.1 meV.

spectrograph concept to improve the energy resolution at IXS to its ultimate target value of 0.1 meV.

4.3.2 Nanopositioning and Nanometrology

Nanopositioning and nanometrology is an essential key element of the NSLS-II integrative systems engineering approach for mission-oriented R&D, as nanoscale motion sensing and control, positional and angular stabilities often determines the ultimate performance of a cutting-edge x-ray optical element. In addition to x-ray optics, all related experimental subsystems, such as sample positioning and beam-defining apertures, will also require high-precision positioning and stability in order to take full advantage of the cutting-edge x-ray optics or advanced coherence techniques such as ptychographic imaging.

In order to meet such needs, NSLS-II has established a cutting-edge nanopositioning laboratory during the NSLS-II construction project to pursue R&D in precision positioning platform, monitoring, feedback, and controls. Such R&D effort has been very successful, leading to a pioneering design of a precision MLL nanopositioner with five degrees of freedom, and the world's first implementation of a compact diode-laser interferometer system in an x-ray microscope with sub-nm precision positional sensing and feedback controls. These novel accomplishments formed the foundation for the development of an initial 10nm MLL microscope (Figure 1), which has been successfully tested [7] at the Diamond Light Source and is being installed at the Hard X-ray Nanoprobe beamline at NSLS-II.

Building upon the experience and expertise acquired during the NSLS-II project, we plan to further research and development of advanced capabilities for positioning, actuation, manipulation, sensing and control at the nanoscale, with the overall goal to (a) establish the next-generation nanopositioning platform in support of NSLS-II strategic objective toward a 1-nm hard x-ray nanoprobe, and (b) expand the nanopositioning and nanometrology R&D and support to enable broad range of mission-critical capabilities at NSLS-II. Specific development areas include:

- **Further development of laser interferometry sensing:** This is critical for advancements of microscopy capabilities at NSLS-II. The development will target improvement of background noises, environmental compensation of background drifts, smaller laser focal spot size, and ability to encode cylindrical or spherical surfaces using interferometers or other optical techniques. All these advances directly benefit instrumentation development suitable for fluorescence, diffraction, Bragg CDI, TXM, and ptychography imaging at nm-scale.

- **Nanoscale precision positioning, actuation, and associated controls:** This is a key component to any microscopy and imaging system, including both coarse motion based on stick-slip, piezo crawling, ultrasonic, mechanical systems, and fine motion based on piezo actuators, piezo scanners equipped with flexure amplification to increase the range of motion. Development of stiffer, more robust and stable stages with minimal heat dissipation due to motion or encoding is of prime importance for microscopy advancements at NSLS-II, particularly important for advanced capabilities that allow regulation of sample environment, e.g. temperature adjustment, application of magnetic and/or electric fields, etc..

- **Development of novel techniques such as MEMS:** This may be required for positioning at the nanometer scale and therefore must be considered as an option for instrumentation used in nm-scale imaging experiments. Specially designed and fabricated Micro Electro Mechanical Systems (MEMS) devices will need to be developed for nanofocusing MLL optics

manipulation and alignment, stacking of various focusing optical elements, and development of adaptive X-ray optics.

4.3.3 Advanced X-ray Detectors

As recognized in a recent DOE-BES report *Neutron and X-ray Detectors*, as the synchrotron source characteristics continue to improve over the years, areas of scientific investigations at these sources are increasingly limited by the detectors in certain experiments [34]. This is particularly true for a new synchrotron facility like NSLS-II. Therefore, one of the important strategic R&D directions at NSLS-II is advanced X-ray detector development.

Given the broad range of detector improvement needs in the scientific community, our plan is to coordinate and collaborate with other DOE facilities to ensure that resources are well directed towards targeted strategic areas, benefiting the broader community well beyond the NSLS-II. We are also leveraging the resources available at the Instrumentation Division of BNL such as clean laboratory for prototype sensor and/or ASICs fabrications. Through this approach and taking into account the NSLS-II strategic strengths, we have identified the following detector development projects to pursue.

X-ray Fluorescence Pixel Detector MAIA: MAIA is an award-winning x-ray fluorescence microprobe system which has transformed the way such measurements are made. It is a massively parallel detector system (~400 independent detectors) with unique custom computing elements which provide real-time analysis of the elemental makeup of a sample. The system is under continuous development which is essential to retain our leadership. Our current emphasis is on improving the energy resolution of the detectors by (a) making a new readout integrated circuit with better noise figure and (b) developing an x-ray sensor array presenting a lower capacitance to the amplifier, again improving noise performance.

In the future we expect to move towards systems with even more (by a factor of at least 10) elements, each smaller than the current devices. This provides the dual advantage of allowing a higher aggregate throughput and a lower capacitance sensor. This change would also move us away from the current wire-bonded package towards a more modern bonding technology.

VIPIC for X-ray Correlation Spectroscopy: A prototype of a detector optimized for X-ray correlation spectroscopy (XCS) experiments is essential for accessing micro-second time regimes. The

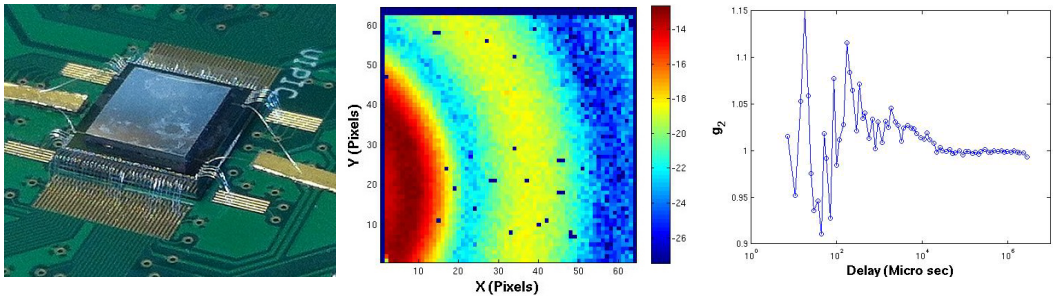


Figure 19: (Left) Picture of the VIPIC prototype detector - a two-level microchip design that provides twice the area per pixel and allows more on-detector, real-time, processing. (Middle) Reconstructed image corresponding to a few seconds data collection in a test run using the VIPIC prototype. (Right) Autocorrelation function derived from the data, indicating such detector will enable dynamic studies at ~10 us level [Ref. 35].

VIPIC (*Vertically Integrated Photon Imaging Chip*, Figure 19) is a unique design, based on the most advanced CMOS technology, and proving the viability of this technology for x-ray and HEP detectors. The prototype was funded by a DOE FWP. We are currently developing a plan to make a full-scale (i.e. 1 megapixel) version of this detector. It is anticipated that this will be a two or three-year project with additional funding by DOE-BES. At the same time we are working on prototyping the next generation of such a detector. It will improve the time resolution by a factor of at least 100 compared with the prototype, i.e. from 10 us to 100 ns. That requires testing out some circuit ideas. The first submission of a test device for manufacture is in process. We anticipate that a small, fully functional prototype is probably three years away, and a full-scale device another two years beyond that.

HEXID (High Energy-resolution X-ray Imaging Detector): This is a prototype detector which provides full spectral information for every pixel, i.e. a true "color" x-ray camera that is essential for spectroscopic X-ray imaging. The device takes ideas from the Maia detector and compacts it into an area on the integrated circuit which is the same size as the sensor pixel. The sensor can then be bump-bonded to the circuit to form what is now known as a hybrid detector. The first prototype integrated circuit of such a device has just now been received and is undergoing tests. We are also developing the technology to bond the chips to the sensor In the future it could become the replacement for Maia in an x-ray microprobe and we are pursuing that path. A full-size version will also be useful for full-field x-ray fluorescence imaging and Laue diffraction. Neither of these techniques is much utilized at the moment, primarily because of the inadequacy of existing detectors.

Segmented Germanium Detectors: Development of monolithic segmented germanium detectors. We have built a detector based on a 64-element sensor fabricated by our German collaborators, Semikon Detectors GmbH, and on integrated circuits developed here at BNL. The sensor has 64 strip-shaped pixels, each one 0.5mm x 5mm, and was read out by two of our 32-channel readout chips. This device has shown that our ASICs can function properly in a cryogenic environment, and that the segmented germanium sensors produced by Semikon are of high quality. In order to have this information quickly, we used simple electronics which could only provide spectra from one channel at a time. We are now in the process of building a fully spectroscopic version based on the Maia readout system. The limitation of that chip set is that it cannot handle energies much higher than 60 keV, and so we are designing a new chip which will be capable of working up to 200 keV. We hope to have samples of that design in a few months. At that time, assuming a successful outcome, we will retro-fit the sensor with it and it will be used at 6-BM at APS as part of a NSLS-II/APS collaboration on energy-dispersive diffraction experiments, where it is anticipated it will bring a factor of 20 or so improvement in data collection time.

The next step in this project is to implement a microstrip detector for high-energy monochromatic powder diffraction, specifically for use on the XPD beamline at NSLS-II. The sensor is on order and should be delivered soon. Also, in collaboration with APS we will equip that sensor with full spectroscopic readout using essentially the same system.

Other projects: Detector R&D will also support NSLS-II beamline science in smaller projects that make use of the technology we have developed. This is an important part of NSLS-II operations. We have built a custom microstrip detector for use on the HXN beamline, and are working on a high-spatial resolution 1-D hard x-ray detector for application in a Von Hamos geometry energy analyzer for use on the ISS beamline. For the XPD beamline we have developed a detector based on the high-Z detector material CZT. It will be used to detect the x-rays arriving from a multi-crystal analyzer array. It has 8 channels, matching the number of crystals in the analyzer. It is expected that there will be more such development projects as NSLS-II becomes operational and experimenters realize the advantages of customized detectors for their experiments.

4.3.4 Support Laboratories

In addition to R&D laboratories, NSLS-II has developed and will continue to develop a suite of laboratories in each of the five Laboratory and Office Buildings (LOBs), which are an essential part of the user support infrastructure at NSLS-II. At present, there are twenty such functional laboratories in LOB1 and LOB3, and the expected build-out schedule for the remaining laboratories in the other LOBs is discussed in Chapter 6.

While on average the ten laboratories in each LOB are expected to serve six beamline Sectors or about twelve beamlines, each such laboratory will be setup for specific functions and will be shared among multiple beamlines. Most of the intended usage of the laboratories will be for those support activities directly related to an experiment at a beamline, such as sample mounting and preparation, instrument testing, and auxiliary measurements in support of an ongoing experiment. To ensure proper coordination of the laboratory access, NSLS-II will include the laboratory usage in user proposal requests and as part of the scheduled user visit during beam time allocations.

We envision the following standard support laboratories in each of the LOBs:

- Standard dry-labs for specimen preparation, mounting, viewing, and characterization
- Standard chemistry labs for specimen preparations and manipulations that require a chem-hood
- Set-up lab for preparation and testing of a large piece of equipment such as a roll-in diffractometer or vacuum chamber
- Clean assembly lab for assembly of clean optics and precision equipment
- Electronic lab for testing of electronics and motion control systems.

Taking advantage of the synergies among beamlines and techniques, and capitalizing on the science village concept, we plan to provide a suite of specialized support capabilities shared for the entire facility, in addition to the suite of standard laboratories listed above. These specialized laboratories include:

- Biochemistry laboratories for biochemical specimen preparation and handling
- Cold room-partition for sample handling for macromolecular crystallography
- Battery laboratory for preparation of in-situ battery samples and associated ancillary measurements
- High-pressure laboratory for high-pressure sample mounting and pressure characterization
- Soft matter laboratory for preparation and characterization of soft matter samples
- Advanced materials characterization laboratory with specialized high-power microscopes
- Environmental science laboratory for handling of earth and environmental specimens
- In-situ catalysis laboratory for handling of special specimens that require a HEPA filter.

Finally, NSLS-II will investigate the possibility of installing an in-situ catalysis research laboratory on the experimental floor, in the close vicinity to the ISS, QAS, and TES beamlines. Providing such laboratory space for pre-staging of experiments, sample preparation, and screening is essential to accommodate the needs of in-situ and operando experiments, and to maximize experimental throughput built upon the enhanced flux and sample environment infrastructures at these world-class beamlines. In order to serve the users in the fields of heterogeneous and biological catalysis, battery research and thin film fabrication, ISS beamline has developed sophisticated transfer methods that will allow transport of samples under controlled conditions from preparation area (e.g., glovebox) to the experimental station. In this context, special emphasis will be placed on fully automated sample

transfer to allow remote operations of the beamlines. To meet these needs, we envisage the sample preparation enclosures located on the experimental floor immediately next to the beamline user area. Such an enclosure will permit user groups from different disciplines to operate under conditions best suited for their samples preparation techniques. Designated glove boxes will be provided for biological materials, catalysts and batteries (with latter being argon-filled). Extensive infrastructure for pre- and post-measurement sample characterization, including optical and vibrational spectroscopy will be made available (building upon on-going collaboration with Synchrotron Catalysis Consortium). In addition, the sample treatment capabilities (elevated pressure and temperature, exposure to gas and vapor mixtures) available at the ISS sample chamber will be replicated in the sample preparation enclosure to allow users to prototype experiments off-line, or pretreat the samples (as often required for catalysts).

4.4 Accelerator Science and Technology

Much of the NSLS-II scientific portfolio depends critically on the high-brightness and high-flux sources as well as their stability and reliability provided by the NSLS-II accelerator system and insertion devices. For the next five years, the main strategic objectives for the NSLS-II accelerator facility will be four-fold:

- accomplish the full design capabilities of the NSLS-II storage ring and mature its steady-state operations in reliability and availability
- support the development and implementation of NSLS-II beamlines
- continue to improve accelerator performance in photon beam brightness, flux, stability, and timing
  develop ideas and concepts for a possible future lattice upgrade into a fully diffraction-limited storage ring

4.4.1 Full Design Capabilities Ramp-up of NSLS-II Storage Ring

It is essential to ramp-up the NSLS-II storage ring to its full-design capabilities as rapidly as possible. At the time of this report, the NSLS-II storage ring has demonstrated accelerator performance of stored electron beam current of 50 mA at the electron beam energy of 3 GeV, meeting one of the key performance parameters at the start of the NSLS-II accelerator operations. To reach the full design capabilities that support the routine operation of an experimental user program will require continued ramp-up and improvements on various accelerator subsystems over the first two to three years of NSLS-II operations, with the following main objectives:

- Accommodation of insertion devices and beamline front-end operation into beam operations thereby delivering photons to beamlines
- Improve beam quality to reach design beam emittance
- Provide high beam stability
- Achieve large beam intensity 500 mA
- Enable top-off injection mode
- Achieve high operational reliability and availability of the machine for user operation.

NSLS-II accelerator will be progressing towards these goals in a steady, step-by-step manner. During the first several years installation and commissioning of IDs and FEs will become routine practice. Installation of the 2nd RF cryo-module will enable high-current operation of the Storage Ring. Early

implementation of the top-off injection mode will insure stable beam operations and, thus, accelerate the process of the beamline commissioning. Gradual increase of circulating current will be interleaved with studies of machine performance in intermediate points to mitigate risks of overheating vacuum chambers.

The planned future improvements and upgrades outlined below are important parts of maturing the NSLS-II facility. While great efforts and insight were invested in the accelerator design prior to its construction, commissioning and operations may reveal opportunities for modifications and improvements of the machine components to maintain steady progress in approaching and exceeding the design performance.

4.4.2 NSLS-II Accelerator Improvements

Diagnostics and Instrumentation improvements: NSLS-II beam position monitors (BPMs) are recognized as the most accurate and stable instruments for monitoring beam position. Advancing the BPM electronics even further will be desirable and will retain NSLS-II leadership in this area and match the requirements of the next generation light sources. Future plans for developing X-ray diagnostics include development of a high resolution electron beam size measurement system. Implementation of advanced systems with several slits, as well as installing the second X-ray diagnostics set-up at a location with significant dispersion will permit simultaneous high-resolution measurement of the beam emittance and energy spread. Monitoring of these major beam qualities will provide major insight in maintaining high brightness of the NSLS-II sources for users between the beam studies.

Similarly, developing additional photon BPMs in Front-Ends and user beamlines will provide additional monitors of the X-ray beam position on their way to user end stations. These monitors will be included in the local feedback loops further increasing positional stability of small X-ray beams on user samples.

Reaching high positional stability: Addressing the need for reaching and maintaining high e-beam stability, NSLS-II by design implemented and planned ahead many solutions focused on minimization of beam jitter at the beamline source points. These solutions include design of the storage ring girders with suppression of all vibrational harmonics at low frequency range, a number of feedbacks (Slow and Fast) for stabilizing transverse beam motion, using modern X-ray BPMs for future development of local (per beamline) feedbacks.

During NSLS-II commissioning we accumulated initial data on the orbit motion and slow jitter. The measured data indicate that the “natural”, i.e. without any feedbacks, jitter is very small, below 4 μm and 2 μm RMS in X and Y planes correspondingly. While jitter in X plane is below the requirement already, the vertical jitter is still much larger than the limit set by 10% of the RMS beam size. In R&D focused on achieving high positional stability, we will characterize sources of jitter in the beam orbit (RF, girders, power supplies, BPM noise) and then will work out local solutions to quiet down the harmful noise harmonics. Another set of activities will pursue development and commissioning of new orbit feedbacks, such as tune feedback, longitudinal damper, local beamline feedbacks, etc.

Besides the extensive use of different feedback methods and systems, we will ensure availability of high-accuracy feed-forward systems for every insertion device. These systems will maximally compensate “deterministic” perturbations to the electron beam closed orbit occurring at variation of undulator magnetic gaps (for IVU and EPU) and shifts of magnet arrays (for EPU).

Improvements in accelerator pulsed magnets: Increasing reliability of, and reducing the transient induced on the stored beam by, the injection kickers is essential to reducing the probabilities of operational downtimes of the NSLS-II storage ring and injector. Our recent commissioning experience clearly indicates a need of upgrade for all three kicker families. Their modulators, while maintaining high quality of the beam delivered to the storage ring, are requiring constant tuning by the pulsed magnet experts. The kicker upgrades include replacing switching elements and auxiliary power supplies, implementing advanced monitoring of the circuit performance on the subsystem levels and high precision control of the current waveforms. The end goal of the upgrades is two-fold: a) to reach the level of high reliability of the kicker operations and b) to decrease the injection transients on the stored beam below 30 μm. The latter will enable more transparent injection process critical for "not-perturbation" top-off operations.

4.4.3 R&D on Storage Ring Lattice Modifications

Improving Source Brightness in High-β Straights: The beam envelope function (or β function) describes the variation of beam size around the storage ring. In the NSLS-II storage ring, the beam envelope has a local minimum in the middle of the insertion straight sections. There are two kinds of straight sections: A long straight section with a length of 9.3 m and a short straight section with a length of 6.6 m. The design values of the horizontal (x) and vertical (y) β functions in the center of the straights are: β_x = 3 m and β_y = 1 m in short straight, and β_x = 20 m and β_y = 3 m in long straight. The large value of the horizontal beta function in the long straight helps to provide optimum conditions for injection, which is located in 30-ID, a long straight section.

A study has been performed to explore various configurations with the large horizontal beta function reduced to a significantly smaller value in the high-beta straights. This would increase the usefulness of long straight section for placing insertion devices. It will provide brighter photon beams and will reduce the sensitivity of the electron beam to the fields and imperfections of the insertion devices.

NSLS-II plans to pursue this important concept by further developing the lattice configuration designs, selecting one of the possible configurations, and optimizing the resulting dynamic aperture by e.g. introduction of more sextupoles per pentant. Once the design is matured, the chosen configuration will be tested and empirically optimized by beam studies, and implemented as needed at up to 9 long straight sections.

Future Multi-bend Lattice Upgrade: In the quest to reach lower, and ultimately, fully diffraction limited emittance, the NSLS-II team is considering a future upgrade of the storage ring optics. Currently the NSLS-II storage ring lattice design is based on the robust and well-tested Double-Bend Achromat lattice. With this lattice, NSLS-II will produce diffraction-limited beams in the vertical direction up to energies of ~ 10 keV and in the horizontal direction up to energies of ~ 500 eV.

A potential upgrade path to achieve even higher levels of photon brightness at NSLS-II is to design a new lattice based on the Multi-Bend Achromat principle. The essential property of the MBA lattice is to split the bending magnets into several ("multi") cells, which helps to decrease emittance since the latter depends on the number of bends (N) as N^{-3}.

Any future MBA lattice upgrade would need to preserve the existing beamline arrangements as much as possible. Designing and implementing an MBA lattice would require careful and extensive analysis.

NSLS-II intends to pursue an R&D program on MBA (or other) lattice upgrades to identify future options for upgrades to the storage ring.

4.4.4 Developing Novel Insertion Devices

Cryogenically-cooled permanent magnet undulator (CPMU): A CPMU device represents a direct upgrade of a hybrid in-vacuum undulator (IVU), and offers a substantial increase in magnetic and spectral performance over IVU, thanks to operation at cryo-temperatures, when both the remnant magnetization (B_r) and coercivity of permanent magnet materials increase quite significantly: e.g. the increase in B_r can be by ~30-40%, allowing to reach $B_r \approx 1.45$ T in the case on NdFeB material, and even higher value, ~1.6 T in the case of PrFeB material. This makes it possible to reduce period length of in-vacuum undulators and reach hard X-ray spectral range at lower harmonic numbers at medium-energy storage ring sources (such as NSLS-II), and obtain a considerable gain in spectral flux and brightness. For NSLS-II, we have developed a few prototype PrFeB arrays and confirmed that bake-able CPMU running at 77K was possible to fabricate. Continuing this development and realization of actual CPMU devices will help to keep NSLS-II at the cutting-edge of spectral brightness and flux for a variety of applications.

Superconducting undulator (SCU): The clear advantage of SCU over room-temperature IVU and over CPMU is the promising higher magnetic performance. However, because of relatively high technological complexity, important constraints related to the required low thermal budget, difficulties of realizing shimming / magnetic field corrections, and sometimes lack of good engineering support, the progress in this area was relatively slow, until very recently. In 2013, APS demonstrated successful in-house design, construction, and reliable everyday operation of a short (~0.3 m) SCU for one beamline. Currently, the work is in progress at APS on a 1.2 – 1.5 m long device, which represents big practical interest for many beamlines. The work on a potentially even higher performing SCU, based on a more complicated niobium-tin wire technology (compared to the standard niobium-titanium) is currently in progress at LBNL. It is important for NSLS-II to pursue R&D in this area. NSLS-II will coordinate with these facilities and develop the SCU R&D activity at BNL, taking advantage of the expertise and infrastructure already existing in the Superconducting Magnet Division of BNL, with a longer term goal of in-house production of SCUs for NSLS-II.

Segmented adaptive-gap undulator (SAGU) concept: A novel concept of a segmented design of an IVU allowing different tunable gap in each segment has been developed by O. Chubar of NSLS-II [36]. Calculations show that important magnetic and spectral gains, comparable to those attributed to the use of a superior undulator technology, can be reached simply by using a segmented undulator design approach and allowing different segments to have different magnetic gaps and periods (yet selecting the periods so that all segments produce undulator radiation at the same photon energies of harmonics). NSLS-II will continue this important development, towards the development of a conceptual design of an SAGU which may be eventually implemented at NSLS-II beamlines.

Improvement of insertion device magnetic and spectral calculations methods and tools: To a large extent, the progress of R&D on insertion devices depends on the accuracy and level of details of simulations that can be provided by dedicated computer codes. Various optimization methods will be investigated to improve design efficiency.

4.4.5 Timing Modes and R&D on e-beam Slicing

Storage ring bunch patterns for timing applications: Some of the experiments on the NSLS-II beamlines plan on carrying out pump-probe experiments. The essential technique of such irradiating a sample by a powerful laser pulse (pump pulse) and then scanning evolution of a chemical process that have been excited by the pump pulse using a single or several X-ray pulses separated by several nanoseconds (probe pulses). To address the needs of the pump-probe experiments at NSLS-II, it is important to develop and implement flexible bunch patterns in NSLS-II storage ring operations. Possible storage ring bunch patterns includes:

- camshaft bunches, separated by n·2ns intervals
- m bunch trains consisting of l bunches per train
- combination of two patterns above
- uniform fill

Implementation of the above bunch patterns requires optimization of the NSLS-II performance to a high degree of flexibility. Achieving high current in the camshaft bunches will be a subject of beam studies and optimization of bunch-by-bunch feedback focusing on reducing single bunch instabilities that limit peak current. Development of the bunch cleaning system in the ring is planned to warrant sharp edges of the storage ring bunch pattern and keep electrons out of the empty buckets.

Electron beam slicing: F. Willeke and L.H. Yu (*https://accelconf.web.cern.ch/accelconf/IPAC2013/papers/tuoab201.pdf*) have proposed a new method for generation of ultra-short x-ray pulses using focused short low energy (5-10MeV) electron bunches to create a short X-ray pulse from the circulating electron bunches in a storage ring. When the low- and high-energy electron bunches cross in proximity of each other, its coulomb force will kick a short slice from the core of the storage ring (high-energy) electron bunch. The separated slice, when passing through an undulator, will radiate ultra-short x-ray pulses at about 150 fs.

This method exhibits the following advantages of when it is compared with other schemes respectively:

- When compared with crab cavity method, it needs much smaller space in storage ring for interaction point, and its pulse length (150fs) is much shorter.
- When compared with laser slicing method, the flux per pulse may be increased significantly, by a factor of from 6 to 10, and the repetition rate can be much higher while the pulse length is comparable.
- When compared with LCLS SASE x-ray free electron laser, its repetition rate can be 10^3~10^4 of orders of magnitude higher, and it is much more stable, even though the single shot pulse energy is many orders of magnitude lower.

The potential implementation of this technique will enable generation of ultra-short x-ray pulse sources at several of NSLS-II beamlines to allow ultrafast time-resolved investigations of materials. It is therefore desirable to continue to pursue R&D in this area to allow refined understanding of X-ray photon characteristics for ultrafast applications.

4.5 Managing the NSLS to NSLS-II User Transition

NSLS at BNL has been an outstanding synchrotron facility serving a broad scientific user community for the past three decades with tremendous scientific productivity and technological and societal

impact. For the past number of years, NSLS has consistently served over 2300 unique users annually in materials physics and engineering, chemistry, environmental and life sciences, and industry, leading to about 900 publications per year. This user community at NSLS constitutes a substantial portion (about ~23%) of the US light source community. Thus the planned closing of NSLS at the end of September 2014 – loss of capabilities and capacities until NSLS-II is substantially built-out, will cause significant changes in how the existing NSLS user community will conduct their research and eventually transition to NSLS-II.

Recognizing this fact, PS has taken the initiative to develop and implement a multi-facet plan for mitigating the NSLS to NSLS-II transition period. Our plan includes the following four elements:

- Build out NSLS-II as rapidly as possible, including transfers of NSLS beamline components to NSLS-II bend magnet and 3-pole wiggler beamlines to increase early capacity (NxtGen)
- Work with specific user groups at NSLS to identify and establish critical beamline capabilities and long-term partnerships at appropriate beamlines at NSLS-II, and make interim arrangements at the early suite of NSLS-II beamlines if necessary
- Coordinate with other DOE facilities to identify and communicate to users similar capabilities at ALS, APS, and SSRL, and potential for increased capacities for certain techniques at these facilities
- Develop and implement specific user support and coordination plans at a set of specific beamlines at ALS, APS, SSRL, as well as at other SR facilities such as CHESS and CLS, to accommodate existing NSLS users in areas that are strategically important to NSLS-II.

The first area has been covered in the previous beamline sections, and the following sections will provide more details on the latter three areas.

4.5.1 Transitioning User Programs to NSLS-II Beamlines

NSLS-II has been working with the scientific community in developing new beamlines at NSLS-II, and this includes working with existing communities at NSLS to establish beamline programs that will provide improved and enhanced capabilities to meet the specific community's research needs. NSLS-II also welcomes and encourages close participations from various segments of the community in the forms of beamline development proposals, beamline advisory teams, and beamline partner users, as strong involvements by the community are important to the long-term future of the scientific programs at NSLS-II. Based on this principle, NSLS-II has been working with all the major groups in the NSLS user community to identify and pursue partnerships in the form of active general users and/or partner users at NSLS-II beamlines. Among the 30 beamlines currently under development at NSLS-II, these arrangements include:

- Center for Functional Nanomaterials (CFN): CFN is a Contributing User (CU) at three NSLS beamlines X9, X1A1, and U5UA. CFN played a leadership role in the beamline development proposals that led to the development of CMS and SMI beamlines as well as the ambient pressure photoelectron spectroscopy program at the CSX-2 beamline. Three partner user arrangements have been made at three beamlines with CFN.
- Synchrotron Catalysis Consortium (SCC): SCC is a CU at three NSLS beamlines X18A, X18B, and X19A. SCC led the beamline development proposal for the QAS beamline and played a major role for the TES beamline. Two partner user arrangements have been made at these beamlines with SCC.

- GeoSoilEnviro CARS (GSE-CARS): GSE-CARS operates a PRT beamline at NSLS X26A and is a CU at X27A. GSE-CARS played a leadership role in the development of SRX and XFM beamline development proposals, and a partner user arrangement has been made at the XFM beamline.
- Protein Crystallography Research Resource (PXRR) and East Coast Structural Biology Consortium: These consortia operate six NSLS structural biology beamlines X25, X29, X12B/C, X26C, and X6A. NSLS-II FMX and AMX beamlines are being built based on the beamline development proposals developed by this community, who will access these beamlines as general users.
- NY Structural Biology Center (NYSBC): NYSBC operates two PRT beamlines X4A, X4C at NSLS, and is constructing an undulator beamline NYX at NSLS-II based on their beamline development proposal for NYX. The partner user proposal has been approved for the NYX beamline.
- Case Center for Synchrotron Bioscience (CSB): CSB operates three PRT beamlines X3A, X3B, X28C for Bio-XAS and X-ray footprinting research and is a CU for macromolecular crystallography at X29 at NSLS. Partner user arrangements have been made at the FMX, AMX, and ISS beamlines to accommodate the CSB community interests in protein crystallography and bio-XAS. In addition, the CSB is constructing the XFP beamline based on their successful beamline development proposal for XFP.
- Consortium for Materials Properties Research in Earth Science (COMPRES): COMPRES has CU programs at four NSLS beamlines U2A, X17B2, X17B3, and X17C. Partner user arrangement has been made at NSLS-II XPD beamline to accommodate the angle-resolved XRD program. Three additional NSLS-II beamlines proposed by the COMPRES community have been approved by PS, with the FIS beamline under development of part of the NxtGen project and the 4DE and TEC beamlines among the next suite of beamlines for possible future development.
- Energy Dispersive XRD for Materials & Battery Research: This consortium operates a CU program at the NSLS X17B1 beamline. The HEX beamline proposed by this community for NSLS-II has been approved by PS and is among the next suite of beamlines for future development.
- National Institute of Standards & Technology (NIST): NIST operates three PRT beamlines at NSLS, U7A, X24A, and X23A2. NIST is constructing three beamlines, SST-1, SST-2, and BMM at NSLS-II based on the corresponding beamline development proposals that have been approved by PS. A partner user arrangement will be formalized for the operations of these beamlines.
- Center Emergent Superconductivity (CES): CES operates PRT beamlines U13UB and X22C and is part of the PRT program at X1A1 at NSLS. CES played a major role in the beamline development proposal for ESM, which is now under construction as part of the NEXT project. The X1A endstation was transferred to the NSLS-II beamline CSX-1 under a partner user agreement while the resonant scattering program from X22C will be accommodated on the NSLS-II beamline ISR.
- Radiation Detectors Research (BNL-NNS): The BNL radiation detectors group operates a PRT beamline X27B at NSLS. The group has established a partner user arrangement at the MID beamline.
- Rapid Acquisition PDF (BNL-CMP): The PDR group has a CU program at the NSLS X17A beamline, and played an important role in the development of XPD beamline program at NSLS-II. A partner user arrangement has been made for the group at the XPD beamline.
- Chemistry XRD Consortium (BNL-Chem): This group operates a PRT beamline X7B at NSLS. A partner user arrangement has been made for the group at the XPD beamline at NSLS-II.

- Liquid Surface Science (LSS): This group operates a PRT beamline X22B at NSLS and played an important role in the development of the SMI beamline at NSLS-II. A partner user arrangement has been made for the group at the SMI beamline.
- X-ray topography (SBU-MSE): This group operates a PRT beamline X19C at NSLS. The beamline development proposal for high-resolution x-ray topography at NSLS-II proposed by this group has been approved by PS, and the program is being implemented at the MID beamline at NSLS-II.
- Microelectronics R&D (IBM): IBM operates two PRT beamlines X20A and X20C at NSLS. IBM played a leadership role in the development of the MPP beamline development proposal, and the MPP beamline is currently under construction. A partner user arrangement is expected to be made at the MPP beamline.
- Infrared program: Infrared user community has four IR beamlines U2A, U2B, U10B, and U4IR at NSLS. This community led the development of four beamline development proposals – FIS, MET, AIM, and IRI for NSLS-II. These proposed programs are being implemented at the FIS/MET and IRI beamlines, with FIS/MET under construction, and the expected funding for IRI from DOE-BER.
- Transmission X-ray Microscopy (TXM): The TXM program at the NSLS X8C beamline was established using ARRA fund and started ramping up user operations in 2012. It is among the newest user programs at NSLS, and a large diverse community has been quickly established in the past couple of years. This community played a leading role in the development of the FXI beamline development proposal. The FXI beamline is under construction and will be the long-term home of the TXM program at NSLS-II.

4.5.2 User Program Coordination with Other Facilities

While clear transition plans for NSLS major user groups have been identified and are being implemented at NSLS-II beamlines, we recognize that for certain existing science programs there are availability and capacity gaps of one or more years during the NSLS to NSLS-II transition period. To mitigate such gaps, we have been working closely with other DOE synchrotron facilities to identify existing and/or additional beamline capacities at the other facilities that can be used by NSLS users.

This effort was kicked off at the 2012 NSLS Users Meeting, where a special User Transition Forum was held at BNL, organized jointly by PS and PS User Executive Committee, with participations by representatives from APS, ALS, SSRL, as well as DOE SUF. At the forum, a careful analysis of the beamline capacities at APS, ALS, and SSRL in the main techniques categories – scattering, spectroscopy, and imaging was discussed and presented to the NSLS user community. A set of matching beamlines at these other facilities for specific techniques was identified as potential resources where NSLS users can conduct their research before the corresponding NSLS-II capabilities become available.

Following the 2012 NSLS User Transition Forum, we have been closely coordinating with other facilities to provide the necessary information that led to increased capacities at some of the identified beamlines at these facilities. This includes the following:

- At APS: Increase in beamline capacity at 1-BM for topography, 12-BM spectroscopy and diffraction, 2-BM micro-tomography, 17-BM powder diffraction, 9-BM spectroscopy, 32-ID transmission x-ray microscopy, and 6-BM white beam energy dispersive diffraction,

- At ALS: New IR front end and optics increasing total IR capacity by 50%, repurposing and upgrading BL 3.3.2 for detector testing, and reopening of BL 3.3.1 operations for X-ray footprinting,
- At SSRL: Reopening of BL 2-2 operations for X-ray spectroscopy and BL 14-1 for macromolecular crystallography, and relocating the advanced spectroscopy program from BL 6-2 to another beamline to increase the beam time available to the TXM at BL 6-2.

We have set up a transition webpage to inform the user community about the identified beamlines at the other facilities along with the information on user proposal submission cycles and due dates. This helps encourage and assist the existing NSLS users to plan ahead in their research so that they can continue their scientific programs during the transition period.

4.5.3 Establishing User Support Programs at Other Facilities

In addition to informing the user community about the opportunities at other facilities, NSLS-II has identified several strategic areas where the existing NSLS user groups have been productive and/or will be strategically important to the science programs at NSLS-II. For these select set of programs, NSLS-II plans to actively coordinate with other DOE facilities to make specific near-term arrangements, with committed significant resources and staffing, to support existing NSLS users at the appropriate beamlines at these other facilities. These arrangements include the following:

Energy Dispersive X-ray Diffraction Program at APS Beamline 6-BM: NSLS-II has formed a collaborating access team (CAT), with COMPRES and APS as partners, to operate the 6-BM beamline at APS as a mini-CAT. The beamline consists of two white beam hutches, 6-BM-A and 6-BM-B, with the 6-BM-A accommodating the materials engineering and battery research program and the 6-BM-B accommodating the COMPRES program. The mini-CAT will be co-Directed by BNL-PS and COMPRES, with scientific staff among all partners providing user support. Beam time allocation will be through the APS proposal system with input from the BNL-PS and COMPRES co-Directors.

Materials Engineering Program (APS Beamline 6-BM-A): The program at 6-BM-A uses high-energy polychromatic x-rays above 50 keV from a bending magnet source for energy-dispersive x-ray diffraction (EDXRD). Two solid-state germanium detectors capture diffracted x-rays in a transmission geometry (at angles of 5-10 degrees) allowing simultaneous capture of scattering vectors in the horizontal and vertical directions. Variable incident and diffracted slits of typical size 0.1mm are used to form gage volumes of approximately 0.1x0.1x1.4 mm^3.

This probe allows significant penetration (several mm) into engineering materials to quantify phase evolution, orientation distribution, and stress field in them. Large sample coverage will be provided by XYZ translations (several cm each) and 3-axis tilt/rotations, including full 360 degree vertical rotation. Additional hardware includes an Arbin BT-5HC 2-channel battery cycler with hardware/software interface for visualizing simultaneous battery charge discharge curves and EDXRD. Arbin MITS Pro battery testing software provides comprehensive tools for testing batteries, super-capacitors, electro-chemical cells and others. This instrumentation is optimized for industrial and academic groups involved in engineering and energy storage research.

High Pressure Program (APS Beamline 6-BM-B): The high-pressure program at the 6-BM beamline at APS will feature a DDIA apparatus capable of generating pressure of 15 GPa and temperatures of 2000K as the sample is loaded in a uniaxial stress field of up to 5 GPa. A detector array enables the diffraction vector to sample grains over a range of angles relative to the applied stress field, yielding a

precise measure of the stress (10 MPa resolution). Imaging the sample allows measurement of changes in dimensions (strain resolution of 10-4). The stress field can be varied with time or applied uniformly over long periods of time. This system allows measurements of the quantitative rheological properties of materials under a variety of P-T conditions. This has attracted a large Earth science community interested in the deformation properties of the Earth. Time varying stress and temperature fields allow measurement of dynamic properties such as anelasticity, elastic dispersion, kinetics of phase transitions, and thermal diffusivity at conditions of elevated P and T.

Infrared Spectromicroscopy Program at ALS Beamlines 1.4 and 5.4: NSLS-II has established a 3-year Approved Program at the ALS beamlines 1.4 and 5.4 for 15% of the available beam time on each beamline. Perspective users will go through the NSLS-II PASS system to gain access to this allocated time, with user support provided by PS staff during the experiments. The infrared spectromicroscopy programs at ALS Beamlines 1.4 and 5.4 feature Thermo Nicolet infrared spectrometers and microscopes for single-pixel spectromicroscopy and mapping. The endstations are essentially identical to the equipment at NSLS beamline U2B spanning a spectral range from 650 – 4000 cm^{-1} with a diffraction-limited spatial resolution of 3 – 10 μm in the mid-infrared spectral region. Scientific applications span from biological samples, environmental samples, novel compounds, forensic studies, laminates, polymers, fibers, particulate contamination, and materials science applications.

Transmission X-ray Microscopy Program at SSRL Beamline 6-2 and at APS: The transmission x-ray microscopy (TXM) program at SSRL beamline 6-2-C is being arranged as a collaborative access program (CAP). Beamline 6-2-C is a multi-pole Wiggler insertion device beamline and provides much higher intensity beam compared with the NSLS X8C bending magnet source with the energy range 5-11keV for TXM applications. The TXM instrument at BL 6-2-C is a very similar instrument running at NSLS and provides absorption and phase contrast modes with 30 um field of view and 30nm spatial resolution. XANES capability for chemical mapping as well as nanotomography is available. In addition, NSLS-II plans to relocate the cutting-edge TXM instrument from NSLS X8C to a bending magnet beamline at APS or at another facility. This is being actively pursued in close collaboration with staff and management at the other facilities. We expect to finalize this arrangement in the next few months.

Hard X-ray Spectroscopy Program at SSRL BL 2-2: NSLS-II has established a collaborative access program (CAP) in X-ray Spectroscopy for 80% of available beam time at the SSRL BL 2-2, in collaboration with the Synchrotron Catalysis Consortium (SCC) and the Case Center for Synchrotron Biosciences (CSB), with coordinated scientific staff efforts providing user support at the beamline. In addition to staffing, PS plans to bring operating equipment to BL 2-2, including sample cells, detectors, and gas handling apparatus for catalysis research. Perspective users will go through the NSLS-II PASS system to gain access to this beamline, with user support provided by PS and partner staff during the experiments.

Macromolecular Crystallography Program at SSRL BL 14-1 and ALS: NSLS-II has established a collaborative access program (CAP) in Macromolecular Crystallography for 50% of available beam time at the SSRL BL 14-1, with a PS scientific staff member providing user support at the beamline. The PS staff will also coordinate with the Berkeley Center for Structural Biology at ALS to provide support to NSLS users at the structural biology beamlines at the ALS. Perspective users will go through the SSRL and ALS proposal systems for accessing the beam times, with the PS staff providing the beam time allocation for individual NSLS user groups within the allotted time.

These specific user support plans at other DOE facilities will be essential in meeting the community and stakeholders expectations and keeping the community together with BNL Photon Sciences, as well

as to help the community in accomplishing their research objectives and sustaining their on-going programs. We plan to continue our outreach efforts to the existing NSLS community to inform and update the community about our coordination plans with other facilities. This will be done through updated transition website, by broadcasting email messages, and through the explicit listings of available beamlines at other facilities within the on-line user beamtime request system – NSLS-II Proposal Application Safety Scheduling system (PASS).

5. Initiatives to Enhance Productivity and Impact

NSLS-II recognizes that development of cutting-edge synchrotron beamlines and enabling capabilities is only one necessary ingredient of producing discovery-class and high-impact science at NSLS-II. Scientific research in the 21st century has become increasingly interactive and interdisciplinary, and often relies on a larger team of researchers with complementary expertise to achieve the best possible research objectives. This is the chief reason that, as stated in Section 2.1, two elements of the NSLS-II four-fold strategy involve *people* – creating a vibrant environment to attract the best researchers (staff and users) to the facility, and facilitating university-industry-government partnerships to catalyze innovation in support of the discovery to deployment theme. In this Chapter, we outline our list of strategic initiatives to leverage the intellectual power and resources in the community to enhance scientific productivity and impact of NSLS-II.

5.1 Research Consortia and Partnership

5.1.1 Nanoscience Partnership and Synergy with CFN

One of the strengths of BNL Photon Sciences is its long-time cooperative partnership with the Center for Functional Nanomaterials (CFN), which is one of the five DOE nanoscience research centers located in BNL. The primary mission of the CFN is to explore the unique properties of materials and processes at the nanoscale through a variety of materials synthesis, modelling, and characterization techniques, including nanofabrication, nanomaterials synthesis, advanced electron and optical spectroscopy and microscopy, proximity probes, advanced X-ray probes, and theory and simulations. Recognizing the considerable synergy between CFN and Photon Sciences at BNL, CFN and NSLS have built a strategic partnership and established a mutually beneficial relationship through CFN investments in state-of-the-art research tools at three endstations with targeted staff hires. These have been key resources for CFN and NSLS users, as well as for CFN's scientific programs, leading to a steadily growing number of users requesting coordinated access to both conventional CFN techniques and X-ray based capabilities at NSLS.

Building upon this highly successful synergy, NSLS-II and CFN plan to continue and strengthen our strong strategic partnership to play more important respective roles in coordinating the formation of integrated research centers at BNL targeting specific scientific areas with emphasis on nanoscience applications. The enhanced partnership will include the following strategic elements: co-investments in instrumentation, co-development of staff expertise, coordinated streamlined access mechanisms, and joint research and development projects. Specifically,

- CFN and NSLS-II are establishing Partner User Agreements to develop four endstations at NSLS-II. Taking advantage of the enhanced brightness, coherence, and focusing at the new light source, these joint ventures will establish world-leading capabilities in X-ray scattering, photoelectron microscopy, and in-operando spectroscopy.
- CFN capabilities and expertise will be instrumental for the build-out of NSLS-II over the coming decade. The nanofabrication facility, for instance, will be utilized to nanostructures needed to develop new photon scattering and spectroscopy methods.
- Beyond the formal partner user agreements, NSLS-II and CFN will establish joint projects with staff and users, for example, projects that exploit the complementary properties of X-rays and electrons to image the same catalyst under the same high-pressure and elevated-temperature conditions.

- NSLS II and CFN plan to develop a joint electronic user-proposal system that will make seamless the experience of users carrying out projects that utilize both facilities.
- NSLS-II and CFN will collaborate to develop software management of large data sets collected in synchrotron-based and electron-microscopy experiments. They will benefit from the data-management expertise accumulated through the years at BNL by the Computational Science Center, and the Relativistic High Ion Collider facility and the ATLAS project in high-energy physics.
- NSLS-II and CFN will continue to jointly engage the communities and support the creation of Integrated Centers for Energy Sciences at BNL to enhance the impact of large facilities and core research programs in key topical areas, e.g., by targeted development of new techniques, tools, facility expertise and user support, and by facilitating access and productivity of novice users in those areas. One of such centers or consortia would focus on catalysis science (see next Section), which will leverage in-operando catalyst characterization and computational resources at the CFN, advanced scattering and spectroscopy beamlines at NSLS-II, together with scientific expertise in BNL Chemistry department to create an integrated research environment for staff and external users.

5.1.2 Integrated Catalysis Consortium

Developing new generations of catalysts for challenging energy production and conversion processes required expertise in synthetic techniques, catalytic testing and characterization, and modelling. The catalyst should be characterized under realistic reaction conditions (*in situ*) and, whenever possible, structural and chemical transformation in the catalytic material during the reaction should be correlated with its chemical activity and selectivity (*operando*). Clearly, NSLS-II with its high brightness and flux as well as a comprehensive set of in-situ and operando experimental tools is in an excellent position to promote and enhance in-situ catalysis investigations for the community.

A success story in this area is the existing Synchrotron Catalysis Consortium (SCC), which is a consortium organization at NSLS that promotes catalysis research, develops unique in-situ specimen cells, and provides operations staff for training and support of catalysis users at NSLS beamlines. The SCC has been tremendously successful in establishing a well-recognized catalysis program at NSLS, and will continue to be a major Partner User for NSLS-II QAS and TES beamlines.

Building upon such success, NSLS-II plans to work with the SCC to expand the effort in catalysis research by working with other BNL departments, in particular the Chemistry Department and the CFN, to establish an Integrated Catalysis Consortium. Central to this integrated consortium is to facilitate interactions among the national and international catalyst communities, both industrial and academic, and to promote access to experimental and theoretical tools tailor-made to address emerging issues. Integrating together the SCC effort in outreach and education, the in-situ and in-operando capabilities at NSLS-II, the electron microscopy facility at CFN, and the computational resources in the Chemistry Department, the Consortium will jointly pursue and promote research in the following areas:

- *In-operando* investigation using multi-techniques. Applying multiple characterization methods to the catalyst, simultaneously or sequentially, allows to detect relevant changes on various length scale from individual atoms to micron-sized particles

- Development of spatially resolved (2D and 3D) characterization tools, enabling analysis on a single-particle/single-site level. Through recent technological innovations, many techniques can

be operated in space resolved manner, allowing unprecedented insight into catalyst structure under reaction conditions

- Improving and extending time-resolved capabilities of analysis methods. Various time scales can be covered at NSLS-II, from nanoseconds to minutes and hours. Not only more accurate structure/function correlations can be obtained, but also the throughput can be dramatically increased, which is of particular relevance for industrial applications

- Strengthening the link between experimental and computational channels. Experimental results coupled with theoretical modelling lead to an efficient flow of information, facilitating catalyst development and optimization, and help to shape rational design principles for new generation of catalysts.

5.1.3 Energy Storage

The Department of Energy (DOE) report, "*Basic Research Needs for Electrical Energy Storage*", made clear the need for innovative technologies for electrical energy storage, both to transform the renewable energy usage in the electric grid as well as to provide electric vehicles with sufficient range. Major public and private investments have focused on electrochemical performance, with emphasis on energy and power density, as well as safety and lifetimes of energy storage materials and systems. One of the major challenges is advancing the energy storage technology is the ability to characterize the materials and device performance in situ and in operando and obtain the necessary structural and electrochemical information at multiple length and time scales.

There is already a strong scientific and industrial community within and around BNL working with Photon Sciences focusing on many aspects of energy storage research. Among the premier industrial companies, General Electric Global Research has been a long time user at NSLS and has employed in-operando XRD to study and improve their commercial NaMH batteries for heavy duty transportation. The Advanced Energy Research & Technology Center at Stony Brook University is a new energy research center in partnership with NY State and BNL. Two of the newly funded 2014 Energy Frontier Research Centers in energy storage research are led by State Universities of NY, Center for Mesoscale Transport Properties (m2M) led by Stony Brook and BNL, and the NorthEast Center for Chemical Energy Storage (NECCES) by Binghamton; both are in collaborative partnership and/or are conducting joint research with Photon Sciences.

As a premier synchrotron facility, NSLS II will continue to work with the community to form and participate in research alliances in energy storage and provide the most advanced characterization tools to enable in-situ and in-operando studies of energy storage systems in action. The relevant scientific capabilities at NSLS-II include:

- in-operando studies of electrochemical reaction fronts during charge and discharge cycles in real battery cells by spatially resolved X-ray powder diffraction and X-ray spectroscopy,
- in-situ nanodiffraction studies of grain refinement in active materials and possible formation of quasi-amorphous phases due to multiple charge/discharge cycles,
- in-situ sub-micron X-ray spectroscopic mapping of the oxidation state of the active battery materials with sub-100 nm resolution, and
- in-situ 3D nano-tomography for imaging micro-morphological and chemical changes of active battery electrodes during electrochemical cycling.

In addition to conducting and supporting collaborative research using the advanced capabilities, NSLS-II plans to strengthen the efforts to promote informational exchanges and outreach to additional research groups in academia and industry. To accomplish this, NSLS-II will encourage the formation of an informal energy storage research interest group among the interested PS staff and users. This group will

- hold periodic seminars on topics in energy storage research that are relevant to PS activities,
- send representatives to topical society meetings and report back on the latest developments in the community,
- brain-storm and discuss any technical issues and enhancement related to energy storage research at NSLS-II, and
- promote workshops and user participation on energy storage topics at the PS Users Meetings.

5.1.4 High Pressure Research

High pressure research has been a strong component of the user science program at NSLS, led by the *Consortium for Materials Properties Research in Earth Sciences (COMPRES)*, a community-based consortium whose goal is to enable Earth Science researchers to conduct the next generation of high-pressure science on world-class equipment and facilities. COMPRES facilitates the operation of beamlines at NSLS, the development of new technologies for high- pressure research, and advocates for science and educational programs to the broader community and the various funding agencies. At present, the COMPRES community is comprised of researchers from 60 US member Institutions and 46 foreign affiliated Institutions.

High-pressure science is represented across the full breadth of the physical sciences and materials sciences. Mineral Physics is a frontier area of high-pressure research focused on the Earth and other planetary interiors. The key to much of experimental high-pressure research is the establishment of synchrotron beamline capabilities dedicated to experiments at extreme pressure and temperature conditions. Indeed, these facilities at national and international synchrotron sources over the past three decades have profoundly extended our understanding of the interiors of planets and their satellites in our solar system. Furthermore, studies on solid Earth mineral and melt structures and their phase transformations are essential for a better understanding of earthquakes and volcanic activities that directly affect our environment and climate.

More recently, there is considerable renewed interest in research on the Earth's critical zone, which is the near surface environment characterized by complex interactions of the atmosphere, fluids, rocks, soils and organisms. Human society is directly interacting with the Earth's critical zone and affected by the processes in this region. The most active research programs associated with the Earth's critical zone are focusing on the above-ground surficial region, especially the highly dynamic interplay of weather, atmospheric chemistry, water quality, and natural hazards. As such, the scientific challenges in below-ground region of the Earth's critical zone are manifold and cover topics closely related to our environment, energy security and sustainability, as well as element cycling such as CO_2 sequestration.

NSLS-II views the high pressure research led by COMPRES as a strategically important component of the overall NSLS-II science programs, and will work with the community and COMPRES to establish a world-class high-pressure research portfolio at NSLS-II. Our strategic approach in this area for the next 5-10 years includes:

- Promote and encourage participation of the COMPRES community in the early operating beamlines at NSLS-II through specific partner user arrangements and/or collaborative research projects.

- Broadly promote the usage cutting-edge NSLS-II beamlines by the COMPRES community, especially new enabling capabilities such as high-resolution inelastic scattering at IXS for studies of collective dynamics at high-pressures,
- Develop the Frontier Infrared Spectroscopy (FIS) beamline at NSLS-II for dedicated high pressure research.
- Work with COMPRES and its community as well as potential funding agencies to establish dedicated beamlines, 4DE and TEC in particular, as high-pressure research hubs and resource for the entire high-pressure research community.

5.1.5 Polymer Research Consortium

To capture new research opportunities, the first synchrotron scattering facility in the United States dedicated to polymer science and engineering, was established at the NSLS in 1997 on beamline X27C by a Polymer Research Consortium of scientists from academic (Stony Brook University), government (BNL, NIST) and industrial (Allied Signal, General Electric, Hoechst Celanese, Basell USA) laboratories. The facility included state-of-the-art simultaneous SAXS and WAXD techniques to investigate polymer structures, morphologies and dynamics from atomic, nanoscopic, microscopic to mesoscopic scales in real-time and/or in-situ, often also coupled with additional characterization / processing devices, such as gel/melt fiber spinning apparatus, continuous fiber drawing apparatus, tensile stretching apparatus, high pressure X-ray cell using supercritical carbon dioxide, parallel plate strain-controlled shear stage and stress-control rheometer and Raman spectroscopy. Some examples of the studies carried out at this facility include characterizations of complex fluids (micelles, particles, dendrimers, hyperbranched polymers, and biological systems), crystallization, and phase transitions of polymers, polymer chemical reactions, polymer melts and solutions during shear, fiber formation and deformation. The major benefit of this facility to the polymer community was that no extensive synchrotron experience and equipment preparation were required from general users to carry out cutting-edge experiments. Since its inception, X27C became a major workhorse serving the U.S. polymer community for SAXS/WAXD studies. More than 1000 users from over 100 user groups have carried out experiments at this beamline.

With the availability of new scattering beamline facilities at NSLS-II, such as Soft Matter Interfaces (SMI), Complex Materials Scattering (CMS), and Coherent Hard X-ray Scattering (CHX), the Polymer Research Consortium (PRC), with a combination of former and new members, plans to transition as a Partner User to NSLS-II. The consortium will integrate its existing resources and expertise from its NSLS operations to create and enhance cutting edge research programs in polymer science and engineering with an emphasis on in-situ and real-time studies on structures, morphologies and dynamics over wide spatial (nm-μm) and time (μs-s) domains. Scientific topics will cover nanocomposites, solutions, gels, membranes, fibers, and biopolymers in conjunction with polymer surfaces/interfaces. The PRC also plans to foster industrial usage of NSLS-II scattering facilities by assisting industrial users in the design of synchrotron experiments, providing them with support for data analysis and interpretations. Furthermore, the PRC will offer a series of workshops/seminars for participating members to broaden their knowledge about scattering theory, appreciation for the advantages/limits of these scattering experiments, and knowledge of the latest industrial/academic problems. These activities would catalyze mutual interest and enable the PRC team to meet new materials challenges faced in this century. Another important mission of the PRC is to educate graduate/undergraduate students including the possibility of industrial internships that would provide students with a great opportunity to prepare for their professional careers and build a network of collaborators.

5.1.6 Mesoscale Bioscience.

The interaction between plants and their environment is of key importance in the promotion of healthy and robust growth. Underlying the ability of plants to cope with the stress of growth under variable and often suboptimal conditions lie sophisticated mechanisms to establish and maintain cellular homeostasis. However, the interface between the plant and its environment remains a poorly understood, complex, microenvironment where the balance between chemical, structural and biological stimuli governs the well-being of the plant. To develop a full understanding of the interactions between a plant and the nurturing environment under a range of environmental conditions requires a combination of intercalated scientific techniques with experiments performed by Scientists with very different backgrounds, experience and outlooks. To bring together these teams the NSLS-II is ideally placed to integrate tools and people, our key further task is to develop the infrastructure that will allow for sample preparation and non-invasive examination.

The need to understand complex biological systems over many temporal and spatial length scales presents a significant problem for Science. Generating *data* is not the problem it is the *integration* of data arising from different experimental approaches in a consistent and comprehensive fashion that possess a block to the generation of knowledge. *Understanding in such complex biological systems comes about through the integration of experiment techniques and the development of synergies through computer analysis*. In generating a "toolkit" capable of allowing the investigation of the length scales and dynamics important for the relationships that occur between plants and their environment we will also create a multi-dimensional view of the interfaces between systems that will require modeling and sophisticated data-structures to allow for scientific interpretation of these data.

In providing these tools at BNL we exploit the new capacities afforded by the NSLS-II, our ability to create and measure short lived radio isotopes, multi-length scale synchrotron imaging correlating also with electron microscopy, and we will partner with world leading academic researchers to extend the impact of the developments undertaken at BNL.

5.1.7 Protein Factory

With Prof. S Almo, we are investigating the establishment of a collaboration between the New York Structural Genomics research center (NYSGRC) and NSLS-II and Brookhaven National Laboratories. These nascent collaborative interactions provide exciting opportunities for the future in developing programmatic opportunities with the large and enormously productive structural biology community associated with BNL and NSLS-II. To establish this plan we will harness the protein production capabilities (bacterial, anaerobic and eukaryotic) that have been developed at the NYSGRC under the auspices of the NIGMS-supported Protein Structure Initiative.

The relationship will be modeled on, and benefit from, an on-going pilot project at the Australian Synchrotron. The rationale behind this initiative is that structural biologist are among the elite users of protein materials (i.e., protein is viewed as the "only true gift" and there is a near certainty that, once delivered, these valuable reagents will be used). The centralization of these activities at the synchrotron, with a single primary contact person (Dr. Santosh Panjikar) simplifies the logistics, as this large group of individuals can be managed as a single user with a very substantial target list that is fully appropriate for prosecution through the NYSGRC high-throughput infrastructure. To date about 100

purified proteins, from a target list of 600 genes, have been supplied in quantities sufficient for structural and functional analysis.

This same infrastructure and associated strategies are readily applicable at NSLS-II, to a wide range of programs in particular these structures and the proteins will form the basis for a multi-disciplinary systems biology program that also includes proteomics, metabolomics, biochemistry and genetics. We have established as a starting point the protein production for our investigations into the Mesoscale environment for plants (Section 4.1.4) The totality of these data will be critical for confirming existing and predicting new biochemical pathways, and for defining the regulatory circuitry that organize these individual pathways into the complex metabolic networks responsible for responding to environmental ques. The integration of these data will require the state-of-the-art informatics, and petascale and exascale computing capabilities of the DOE Systems Biology Knowledgebase (KBase), which enables the development and testing of hypotheses regarding interactions, at all scales, in microbes, plants, and their complex communities.

5.2 Industry Research

Industry research is an essential and integral part of the research program portfolio at NSLS-II. Establishing a vibrant industry research program is one of the strategic directions at NSLS-II as such a program has the benefits in that (a) it promotes interactions and partnership along the discovery to deployment research pipeline, and (b) it provides the immediate connection and relevance to the general public.

There has been a strong industry research tradition at NSLS, where many researchers from industry have done a variety of experiments and many industrial companies have built highly visible beamline programs throughout the NSLS's 30 year history. This history of collaboration has been productive for both the facility and the industry, and was clearly evident at a recent *Workshop on Industry Research at NSLS-II* with eighty participants, most of whom from industry sectors in polymers, catalysis and petrochemicals, microelectronics, advanced materials, and pharmaceuticals, which captured a broad cross-section of US companies. Workshop participants identified three key areas where NSLS-II can do to enhance industry research: enhanced support for industry users, flexible and timely access to beam time, and common protocols among National Laboratory facilities.

5.2.1 Strategic Directions for Working with Industry

Based on the discussions at the recent Workshop and other industrial engagement and interactions, NSLS-II plans to develop a strong industry research program with the following strategic directions:

- Developing scientific capabilities at NSLS-II beamlines tailored to industrial applications, particularly in the areas of in-situ and in-operando capabilities with automated specimen handling in industry relevant conditions,
- Promoting research partnerships with participations of industry partners, and inclusion of representative scientists from industry in NSLS-II proposal review panels and other advisory committees,
- Developing and implementing flexible and timely access modes to accommodate industry needs within the framework of *NSLS-II User Access Policy*
- Enhancing staff support to industry users when such support is needed, including mechanisms of paid services

- Enhancing communications and outreach to the industry community about NSLS-II capabilities and strategies for industry research
- Coordinating with other DOE facilities on common protocols for industry access to user facilities.

5.2.2 Flexible Access for Industry

NSLS-II User Access Policy allows for a range of flexible access modes for all users including industry users. In addition, NSLS-II can accommodate industry users through proprietary and pay-for-service access. Taken together, the following flexible access modes are envisioned to be useful for industry access:

Partner User Consortium Access: NSLS-II encourages the interested industry partners to establish an Industry Users Consortium at NSLS-II beamline(s) through the Partner User Proposal approach. The intent of the Consortium is to enable members of the Consortium to contribute to beamline operations e.g. by supporting PS staff at the beamline(s), and to gain access to the beamline(s) for their R&D needs in a timely manner and with a guaranteed amount of beam time. This is essentially a model for collaborative research with pooled resources. By making a common investment, members of the consortium can benefit from the joint investment, yet still retain proprietary rights and competitive / economic advantage. This model is well known in the highly competitive microelectronics industry e.g., Sematech.

Proprietary General User Access: In cases where the access needs to be proprietary, what is preferred is a proprietary access mode with the added flexibility of beamline staff signing a non-disclosure agreement (NDA) with the industrial user. This would ensure the active involvement of the beamline staff in setting up strong collaborative efforts between NSLS-II and industry rather than NSLS-II just becoming a large center of data generation. It was discussed that NSLS-II will have world-class facilities and expertise, and that collaborative work is necessary to fully enable exploitation of these capabilities across the multiple industry sectors.

Rapid General User Access: NSLS-II recognizes that time-to-market and the rapid pace of innovation are vital features of the competitive landscape. Therefore, NSLS-II intends to provide rapid access to a suite of beamline techniques that are highly demanded by industry, with quick turnaround, and to provide the required technical and practical support for meaningful and actionable results. In addition to standard Rapid Access mode, NSLS-II will explore the possibility of extending Rapid Access (RA) to a group of pooled users for a given beamline, allowing block RA group access with greater flexibility in beam time allocations within the group.

Fee-for-Service Access: For smaller companies, especially ones that do not have knowledgeable researchers who can fully interpret data, providing analyzed data for a fee can be an effective alternative. Developing a cost structure and methods to ensure quality of results is crucial. Mail-in sample service is another tier of access to provide rapid turnaround where the beamline staff simply provides the industrial user with raw data under a proprietary access mode.

Automation and Remote Access: Industrial R&D needs require the development of highly automated beamlines with high sample throughput for some key workhorse characterization techniques e.g. XRD, XAFS, micro- and nano-tomography, high energy diffraction, and macromolecular crystallography, that are much sought after for industrial research. Most these beamlines at NSLS-II intend to have the capability for remote access from the home institution where feasible.

5.2.3 Enhancing Staff Support for Industry Users

NSLS-II recognizes that industry researchers are typically non experts in synchrotron or x-ray techniques and the industrial companies typically operate with a mind-set of solutions rather than data. Therefore, providing sufficient staff support with specialized expertise is crucial to the success of a strong industry program.

A number of challenges exist when ramping up staffing for industry program at a new facility, e.g. in the areas of on-demand staff time allocation for timely support to industry users, and timely processing of paperwork for legal nondisclosure agreements, etc.. In this regards, the Industry Consortium model discussed above should help the on-demand staff time allocation issue. NSLS-II will work with the industry community and with BNL to address these and other issues, and will develop a proper plan to enhance staff support for industry users at NSLS-II.

5.2.4 Enhancing Communications and Outreach

Enhanced communications and outreach to industry researchers will be a key to increasing the industry usage of the PS facilities. Given the NSLS-II location at BNL in the Northeast US, with a high concentration of industrial companies and an intellectually rich academia environment surrounding the facility and the Laboratory, and capitalizing on the excitement in the academia and industry community about NSLS-II, the opportunity exists to develop new partnerships and new industry user consortia, thus substantially increase the industry participation and usage at NSLS-II.

NSLS-II plans to pursue the follow steps to enhance the communications and outreach to industry:

- Redesign PS webpages to clearly advocate the cutting-edge scientific capabilities at NSLS-II, the flexible access modes and enhanced support for industry, and our strong interest in forming industry user consortia and partnership at NSLS-II beamlines
- Redouble our efforts on technical outreach to targeted industries to promote the broad usage of NSLS-II capabilities
- Continue to hold community workshops and seminars on specific topics of industrial interests.

5.3 User Access and Communications

5.3.1 Evolution of User Access

The NSLS supported over 57,000 users in its lifetime and was built with a tradition of strong partnerships between universities, industries, government agencies. The success of NSLS-II will depend upon a continued tradition of strong relationships with the user community. While the Participating Research Team (PRT) model for constructing and operating beamlines no longer exists at NSLS-II, Photon Sciences has established a Partner User (PU) Program in order to retain and nurture these important research partnerships. Up to 40% of the available beam time on a beamline may be made available for PU programs. Following the first open call for PU proposals in 2013, 16 Partner User proposals have been approved on NSLS-II beamlines.

At NSLS-II, two principles underlie all user access to beam time. The first is that it is based on proposals that are subjected to peer review that is fair, clear, and expedient, that is sensitive to the needs of users, and that recognizes contributions that improve the overall scientific program. The

second is that all proposals receive a finite amount of beam time for a limited duration that is justified by the need for beam time of the proposed work.

Under this policy, there are three modes of user access to beam time at NSLS-II: General User (GU) access, Partner User (PU) access, and Beamline Discretionary Time (BDT) access. The life cycle for GU and PU access to beam time involves the following steps: proposal submission, proposal review and award of beam time, beam time allocation, beam time scheduling, carrying out the work, and reporting the results. BDT access involves scheduling, carrying out the work, and reporting the results but is reviewed retrospectively.

GU and PU access require peer review of proposals through a central review process managed by Photon Sciences that utilizes Proposal Review Panels (PRPs). Beam time is awarded to GU proposals either by the PRPs or via a Rapid Access process. Beam time is awarded to PU proposals by PS management via a Partner User Agreement based on recommendations from the PRPs and the assessment of PS management. Beamline staff may receive beamtime by being part of a GU proposal or a PU proposal. In addition, beamline staff may also be assigned beam time by beamline management using Beamline Discretionary Time. The award and utilization of all beam time, regardless of access mode, is subject to periodic review by the Science Advisory Committee.

The beam time available for allocation to users does not include time that beamline management requires for commissioning, maintaining, and upgrading the beamlines, and so is typically less than the accelerator operations hours. A minimum of 50% of the available user beam time on every beamline shall be allocated by a Beam Time Allocation Committee (BAC) to GU proposals every run cycle. Up to 40% of the available beam time may be allocated by the BAC to one or more PU proposals in response to their beam time requests for that run cycle. Up to 10% of the available beam time may be allocated at the discretion of beamline management every run cycle for BDT access, typically by beamline staff.

5.3.2 User Portal

In order to facilitate user access to NSLS-II, we are developing an online User Portal where user can have one-stop access to their proposals, safety approval forms, training information, appointment status, publications, and beamline data. Synchrotrons around the world have already instituted such systems, which are coming to be expected by the user community. This system represents a significant upgrade to the previous Proposal Access and Safety System (PASS). A phased role out of the system will begin in September 2014 and is expected to be fully operational within a year.

Initially, the new PASS-II System will accommodate beamtime requests of the standard 8-hour shifts and the proposal process will continue to take 3-4 months. However, future improvements will be necessary to accommodate both rapid-access to beamtime and also allocations of beamtime that may require less than one shift. For example, the short duration and high number of most structural biology experiments require that high efficiency access models to be developed. To be consistent with the expectations of the community, our protocols will be based upon those policies in place at other synchrotron facilities. The NSLS-II access procedures will be extended to make best use of the facilities available. The short duration and high throughput demands of the experiments for both crystallography and solution scattering this will require the possibility of rapid access - typically experiment happens within four weeks of an application, and outside of the normal access schedule.

The high degree of automation available at the MX beamline gives the possibility to develop a sample number based allocation for access where by researchers will have a quota of crystal samples which will be possible to examine during each run. In order for the research teams using the NSLS-II structural biology beamlines to optimize their time usage we will establish protocols to allow for block allocations to research teams where in the overall ambition of the teams research is evaluated but the decision on which project comes at each visit is left to the research team and is not directed by the individual proposals. All of these access mechanisms will be in addition to the normal mode developed in PASS-II and will require additional resources and time to establish smooth operations.

5.3.3 Engaging the NSLS-II User Community

Communications with the NSLS-II stakeholders is paramount to developing a world-class, productive facility. Our stakeholders are very diverse, including the existing user community, potential new users, funding agencies, governing bodies, the media, educators, and the general public. In addition, communications within the Photon Sciences Directorate and Brookhaven National Laboratory is essential for efficient operations and positive morale.

Perhaps the single most important mode of communications is through the NSLS-II website. We are currently in the process of completely overhauling the existing website in order to focus on the rapidly-progressing status of the NSLS-II construction and ramping into operations. Features such as the new User Portal (including the PASS-II system), beamline construction schedules, and accelerator operations schedules will be featured prominently on the homepage. A data content manager will keep information on press releases, science highlights, seminars, and workshop up to date and linked to the BNL website. A SharePoint-based intranet site has become the mechanism of sharing more detailed information from within the Directorate.

In addition to the website, NSLS-II relies heavily on the Community, Education, Government, and Public Affairs (CEGPA) office at BNL. We share resources for science writing, graphic design, media relations, and conference management. We also work closely with BNL's Office of Educational Program to recruit and train interns at the high school, undergraduate, graduate, professional, and faculty level. The DOE Office of Workforce Development, NSF, and NIH provide funding for paid internships at many of these levels including the Summer Undergraduate Laboratory Internship (SULI) program and the Visiting Faculty Program (VFP).

With such a diverse user community, NSLS-II seeks advice from many sources. The Photon Sciences Science Advisory Committee (SAC) typically meets 2 times per year in order to provide advice and guidance on all aspects of facility operations and future planning. Importantly, they are involved in the review process for all Beamline Development Proposals (BDPs) and provide guidance on all Partner User (PU) proposals.

The Users' Executive Committee (UEC) is a body of users elected by the user community to represent the users' needs to Photon Sciences management. They meet 3-4 times per year. On the same day as the UEC meetings, we hold a Town Meeting, where the current status and future plans for the facility are presented. The Town Meetings are webcasted for all users. The UEC also organizes the annual Users' Meeting, which is a 3-day event and includes facility updates, vendor displays, social events, and 6-8 scientific workshops. These workshops are a primary way to engage the community in scientific strategic planning.

5.3.4 Education and Outreach

The majority of the users at the NSLS today are relatively inexperienced with synchrotron techniques and unfamiliar with the sophisticated instrumentation at the beamline. This is a direct result of the rapid expansion of synchrotron radiation into new scientific disciplines over the last decade, and will be especially true with the level of sophistication of NSLS-II beamlines. We expect this trend to continue and will enhance our education and training effort to ensure that the new and inexperienced users can make effective use of the allocated beamtime. Specifically, we will enhance our education effort by providing short courses beyond the general introduction of experimental techniques. These courses will target students or researchers who are interested in specific scientific problem, and tailor the training for them. The combination of lecture and hands-on exercises will allow the students or research meet the experts in the field and beamline staff, as well as become familiar with beamline instrumentation.

6. Facility Management and Support

Creating a vibrant research environment includes having the staff, the support, and the infrastructure necessary for researchers to safely and effectively work at the NSLS-II facility.

6.1 Attracting and Sustaining Top Talent

The NSLS-II facility must have programs and processes in place to recruit the best talent, retain our existing experienced and dedicated staff, and to motivate and enable staff to achieve at the highest possible level. Forecasting the needs of future activities and preparing employees for positions of greater or different responsibilities is essential. Our programs and processes must also reinforce our values and instill a culture consistent with those values.

At present, the Photon Sciences Directorate is focusing its efforts on a number of major activities, including the shutdown of the NSLS facility, the completion of the NSLS-II construction project, the start of operations of the NSLS-II facility, and a substantial number of beamline construction activities. This is a very dynamic environment, with significant projects and programs ramping up, others concluding, and still others continuing indefinitely. It is essential that both the workforce and the specific work assignments of people in that workforce change over time to meet the changing demands of these various projects and programs. The workforce and the way it is organized must easily adapt to the different requirements for these evolving endeavors.

The directorate is organized by division with individuals in those division matrixing their support to both operations and projects.

Succession planning is conducted for the senior PS managers and many staff within our divisions work with the BNL training office on development activities that include 360 degree reviews.

HR analytics are used to track the status of current hires, average number of days for acceptance, reasons for chosen candidate turndowns, tracking of age distribution of the current staff and their retirement eligibility, and capturing the types and number of awards received by Photon Sciences staff.

Workforce planning is carried out to forecast and plan the efforts and resources required to support the science program at Photon Sciences. The information collected for that plan is fed back to BNL for inclusion in the lab-wide plans and also becomes part of the internal PS staffing forecast.

6.2 Operational Excellence

In order to accomplish its mission, the Photon Sciences Directorate must have a full range of effective and efficient business operations functions, including both strategic and day-to-day decision support, project performance tracking, risk management, configuration management, document control, records management, financial analysis, financial management, accounting, contracting, and other functions.

Our philosophy of operational excellence is the basis of our efforts to achieve continuous and sustained improvements in the productivity of our research and support functions, our project schedules, and our budget performance.

As we move NSLS-II into operations, we strive to be more formal and rigorous in our processes and have worked significantly over the past few years to develop a conduct of operations culture.

We routinely plan and conduct organizational assessments to evaluate our performance in implementing management systems that are essential to operational safety and achieving our mission and measure ourselves against standing objectives and measures. Short-term performance objectives and measures are identified and tracked through the Photon Sciences Operational Goals and Performance Management procedure.

Other organizations at BNL are also working to achieve operational excellence and we seek opportunities to improve ourselves by more effectively working with our colleagues elsewhere in the laboratory.

Working closely with our colleagues in the Information Technical Division (ITD), the NSLS Proposal Allocation Safety Scheduling system (PASS) is being upgraded to prepare for NSLS-II operations. That activity includes establishing a system with the ability to:

- Accept research proposals from potential users
- Evaluate those proposals for feasibility
- Review the scientific merit of the proposal
- Review and approve the safety aspects of the proposal
- Schedule the beam time
- Collect end-of-run surveys
- Collect publication information
- Link to data acquisition system
- Provide statistics

The Photon Sciences Directorate uses the services of the BNL Project Management (PM) Center to oversee and manage their projects. The PM Center provides training to the PS Project Managers and Control Account Managers, provides experienced project controls resources, and develops and distributes reports and analyses to assist PS project managers. These resources and tools are key to properly managing the portfolio of beamline projects that are currently under development.

6.3 Excellence in Environment, Safety and Health (ESH)

Every staff member, contractor, user, and guest has the right to go home at the end of the day without suffering injury or illness due to his or her work environment. We must provide a secure environment that protects people, the environment, property, information, and computing systems. Failure to maintain a safe and secure workplace with acceptable environmental impacts can result in the unacceptable consequences of personal injury, illness, or death; property or information loss or damage; and fiscal penalties and criminal enforcement actions. Any of these can quickly and severely erode our ability to pursue and achieve our mission, while meeting these expectations brings a level of trust and support from our stakeholders that cannot be earned otherwise.

Risks of accidents or environmental contamination are proportional to the nature, scale, and complexity of activities, supporting infrastructure, and the condition of physical facilities. Staff in the directorate currently engage in complex activities spread out over our complex. As we ramp up operations of NSLS-II, we will grow to hosting thousands of users each year who will engage in complex and difficult experiments at our facilities, often under time pressure.

Success in ES&H necessitates safety and environmental leadership, whereby all management and staff constantly look out for the well-being of their coworkers. In addition, managers and staff must understand the consequences and cost of failing to perform their work in an acceptable manner. Research and operations personnel must develop, own, and execute work in a manner that fully addresses compliance, safety, security, and environmental protection. Systems, processes, and tools for supporting work accomplishment must be designed to integrate the users' needs with clearly established ES&H expectations.

We will continue to be vigilant in our engagement with our stakeholders and will exhibit demonstrated safety leadership. We will ensure that ESH competence is embedded within our organization and will create and manage an environment that is safe, secure and environmentally friendly.

All beamlines will undergo a standardized and rigorous Instrument Readiness Review prior to the approval to move from construction to operations. This process has been developed and refined over the past year and will be used as we build out the balance of the facility. It is a structured method for comprehensively verifying that the hardware and software, personnel, procedures, and management structures, systems and processes needed for commissioning or operations are ready to permit these activities to be undertaken in a safe, secure and environmentally sound manner.

6.4 Infrastructure

The Photon Sciences Directorate must ensure that the physical infrastructure exists to enable it to carry out its mission. By infrastructure, we mean all of the physical plant that is necessary to support our programs, including: office space; laboratories; high-performance computing and communications services; utilities plants and distribution systems (e.g., electricity, water, sewer, and gas); roads; fire, security, and emergency response services; and waste disposal facilities.

Some of these, such as the construction and operation of the buildings for NSLS-II, are the direct responsibility of the Directorate. Others, such as the provision and maintenance of sufficient and adequate housing for users, guests, and visitors, are the direct responsibility of BNL. Still others, such as utilities, computing, networking, and communications, represent a shared responsibility. We work in partnership with the Laboratory to ensure that our facilities are mission ready and that they are maintained to provide an environment conducive to the most innovative research well into the future.

We must meet the specialized, demanding, and often rapidly changing requirements imposed by our state-of-the-art science programs; accommodate high-technology equipment, computing and networking needs; provide appropriate space for our staff; and provide the Laboratory and support space required to carry out our dynamically changing mix of projects and programs. It is vital that these systems provide the modern capabilities that today's and tomorrow's research programs require, such as adequate cleanliness, fume removal, climate control (i.e. temperature and humidity), vibration control, and others. Our work environments should co-locate equipment, staff, and workflow to the maximum extent possible to enhance organizational efficiency and to promote the exchange of ideas, with resulting improvements in innovation. Use of unsatisfactory space not only reduces productivity and increases costs but can also require reliance on administrative controls to ensure that safety standards and environmental compliance requirements are maintained. We must provide for the safe conduct of our work and protection of the environment while optimizing the functionality and serviceability of our infrastructure throughout its life cycle.

These demands, coupled with constantly aging infrastructure, growing operational legacies, expanding regulatory requirements, and escalating costs, combine to make infrastructure management an enormous challenge. We must properly maintain our infrastructure to effectively support our mission, including preventive maintenance, repairs, replacement of parts and structural components, and other activities. Deferring maintenance can lead to an inability to support the mission, safety hazards, and increased costs. Capital investment may be required to expand the capacity of our infrastructure or otherwise upgrade it to serve changing needs or to replace it when it reaches the end of its service life.

A substantial infrastructure for computing will be required to support the needs of the NSLS-II experimental program. We need to develop plans for providing the necessary computing infrastructure and to identify the resources with which to implement them.

At present, there is not a sufficient amount of appropriate housing for the many users and guests that will use NSLS-II. We will partner with BNL to exploit various options to improve housing for our users in coming years.

The seating and laboratory requirements that we will need to provide well into our future have been analyzed and discussed with the central BNL Facility and Operations Directorate. After completion of the thirty beamlines currently under construction, our most likely beamline buildout scenario is one that brings two beamlines per year to operations, starting in FY2018. That level of beamline build out will require office and work space for our staff, visitors, students and users at the level shown in Figure 20(a). Sufficient space to accommodate these individuals is not currently available in the office space in the Laboratory Office Buildings (LOBs) of the existing NSLS-II facility complex and will require work with BNL to have an office build out plan that matches the black line in the Figure.

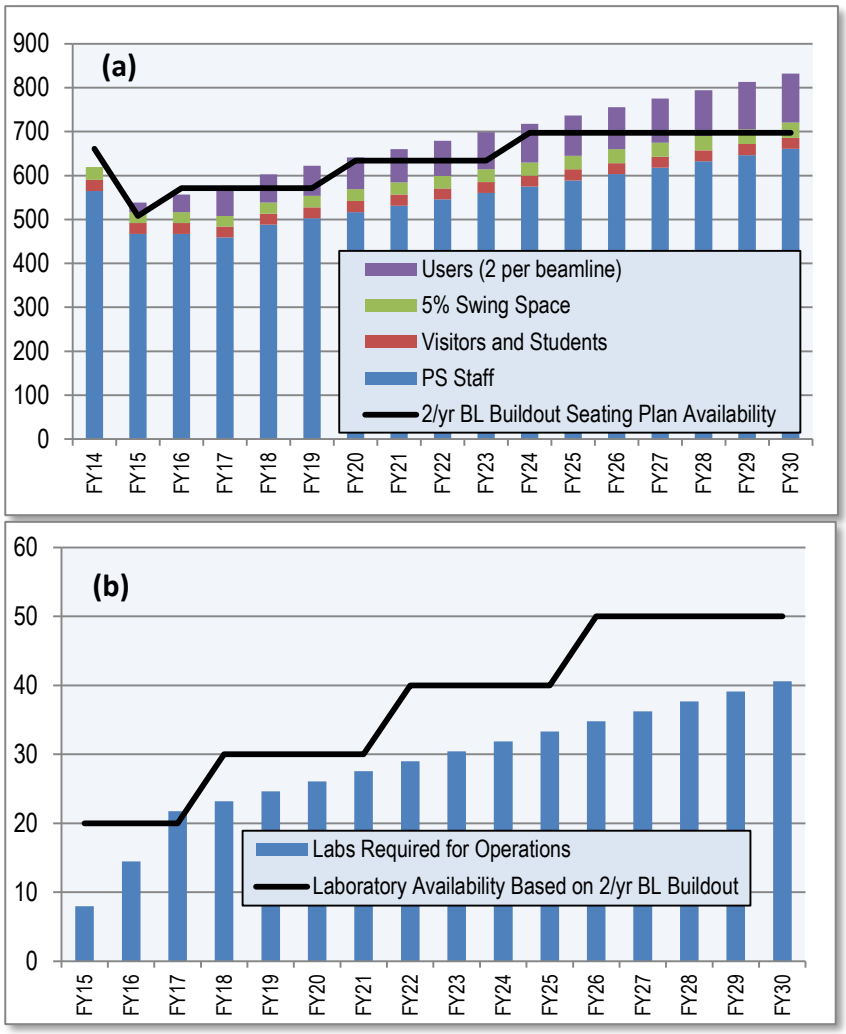


Figure 20: (a) Estimated office and seating needs for PS staff and users (columns) and seating availability based on our current plan (black line). (b) Estimated growth in laboratory needs as more beamlines enter user operation (columns) and the current BNL plan to bring up the LOB laboratories to operations. Note that the requirements presented in (b) take into account *only* the user and staff needs directly related to beamline operations. Additional laboratories are needed for longer-term research as well as for accelerator engineering and instrumentation developments, which are not included.

Also, laboratory space will be required to adequately provide for the research needs of the facility staff and users, based again on the assumed beamline build out shown in Figure 20(b). Our ability to provide that support means that additional lab space needs to be added to the existing laboratory office buildings. Figure 20(b) assumes that the number of NSLS-II facility laboratories that are available for beamlines needs to increase as beamlines become operational. All laboratories for beamlines at the NSLS-II facility are currently assumed to be shared and laboratory allocations for operations are currently underway. It is assumed that beamlines at or near to the laboratory office buildings will have laboratory availability close to their beamline. As with the office space, PS management has been working the BNL Facility and Operations Directorate on planning for the infrastructure needs of the facility and both organizations have agreed on an initial laboratory and office construction plan that would meet the needs of the NSLS-II community. This initial plan is shown in Table below.

BNL IGPP NSLS-II Buildout assuming 2/y BL buildout

	FY13	FY14	FY15	FY16	FY17	FY18	FY19	FY20	FY21	FY22	FY23	FY24	FY25	FY26
1/2 Offices in LOB4		Design & Construct		Occupy										
Labs in LOB5				Design & Construct		Occupy								
1/2 offices in LOB2						Design & Construct		Occupy						
Labs in LOB4								Design & Construct		Occupy				
1/2 Offices in LOB2										Design & Construct		Occupy		
Labs in LOB2												Design & Construct		Occupy

Additional laboratory space for R&D and research activities currently exists with the Photon Sciences R&D office spaces located on the BNL site, but not contiguous to the NSLS-II facility.

The availability of machine shop capability is also important to NSLS-II community and plans for shop space have been taken into account in the design of the NSLS-II facility. Each laboratory office building (LOB) has space allocated for a machine shop. The fully constructed machine areas in LOB3 and LOB1 are being outfitted to support beamline installation and subsequent user operations. It is anticipated that a tiered level of qualification will exist for use of the shops ranging from the ability of staff and users to have work done for them, to limited shop use, and finally a more advanced shop use. Additionally, medium-size machining work will be handled in a dedicated machine shop close to the NSLS-II facility and larger machining work can be sent to BNL's Central Shops.

While there is much yet to be done, we are in the midst of a very exciting period that is literally transforming much of our infrastructure into world-class, mission ready facilities. This will enable us to develop new and unique capabilities that are ready to support our science mission. Furthermore, by working closely with the other organizations in the laboratory, we can help to develop and implement plans to achieve mission ready status for the overall laboratory complex.

7. Summary Outlook

The next decade will be truly exciting for NSLS-II and its community. It will be a crucial time period for NSLS-II to achieve its vision, to accomplish its characteristic capabilities goals, to develop and mature its strategic science programs and communities, to demonstrate its high scientific and societal impact, and position NSLS-II as the leader in internationally recognized areas in the synchrotron community worldwide.

This Strategic Plan consolidates much of the many interactions in the past decade between NSLS-II and the scientific community at large, and summarizes our strategy and approach, our science priority programs, our beamline facilities and development programs to meet the science needs, and our initiatives to enhance the impact of NSLS-II.

For the next 5 years, our strategic goals are:

(a) to ramp-up NSLS-II accelerator to its full design capabilities and mature its steady-state operations;
(b) to complete the constructions of the 30 beamlines currently under development, and ramp-up science programs at these beamlines;
(c) to develop and mature beamline science programs and community partnerships, including programs and partnerships with industry, in areas strategic to NSLS-II mission;
(d) to advance R&D in areas critical to meeting the research needs and NSLS-II capability goals; and
(e) to begin development of additional beamlines along the NSLS-II strategic directions.

We look forward to working with our community and stakeholders to make these goals a reality.

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