Brookhaven National Laboratory

2023 NSLS-II Strategic Plan

September 2022

National Synchrotron Light Source II

managed by Brookhaven Science Associates
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U.S. DEPARTMENT OF ENERGY

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NSLS-II Mission

To develop and operate a premier user facility that embraces diversity to safely and efficiently deliver high-impact and cutting-edge science and technology for the benefit of society.

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Executive Summary

From developing next-generation batteries and microelectronics to designing future pharmaceuticals and quantum computers, scientists tackle the world's greatest challenges by advancing our understanding of materials. However, today's problems are so complex that they require researchers to study materials with highly specialized tools that are not readily available at most institutions. The National Synchrotron Light Source II (NSLS-II) makes such state-of-the-art tools available, together with the expertise to use them, to scientists from all over the world.

NSLS-II

Together, we shine light on the world's most challenging problems

Vision

To be an extraordinary hub for the use of synchrotron light to solve the world's most challenging scientific problems that will improve our lives for decades to come.

Mission

To develop and operate a premier user facility that embraces diversity to safely and efficiently deliver high-impact and cutting-edge science and technology for the benefit of society.

As one of the newest, most advanced synchrotron light sources in the world, NSLS-II strives to be an extraordinary hub for the use of synchrotron light by developing and operating state-of-the-art scientific instrumentation, embracing diversity, and operating safely. The 28 beamlines at NSLS-II offer the widest spectrum—from infrared to hard x-rays—of synchrotron light among all U.S. Department of Energy Office of Science user facilities. As of September 23, 2022, our beamlines hosted 1351 distinct researchers in fiscal year 2022, and 560 papers were published in calendar year 2021 based on work conducted at NSLS-II beamlines. From these papers 48% were in high-impact journals with impact factors IF>7. These demonstrate our important contributions to the research enterprise in the US and abroad.

To ensure the continued high impact of NSLS-II user science, we are committed to deliver on the 5 light sources' data vision as part of our own strategy for easy-access data and multimodal-enabled analysis at the facility. With the ever-growing data rates at facilities such as NSLS-II, we are planning to invest in software tools for data access and analysis, and to accelerating scientific discoveries through technologies such as machine learning and artificial intelligence. Additionally, we will continue to advance our remote experimentation capabilities that were implemented during the pandemic so that a wider, more diverse group of users may benefit from NSLS-II's research infrastructure regardless of where they are based.

We are advancing NSLS-II's mission and vision by developing five new beamlines, planning for additional futures ones, investing in the existing beamlines and implementing a multi-year development plan for the accelerator systems. The plan for the accelerator will allow NSLS-II to reliably operate at 500mA with 8 pm-rad vertical emittance, maturing the accelerator performance from the current 400mA with 30pm-rad vertical emittance and delivering a factor of ~2 increase in brightness to the Users.

On the beamline side, we are constructing a high-energy x-ray scattering and imaging beamline, called HEX, funded by New York State, that will be completed in 2022. Three undulator beamlines, the Coherent Diffraction Imaging (CDI), the ARPES and RIXS Imaging (ARI), and the Soft X-ray Nanoprobe (SXN) are under development with a DOE Major Items of Equipment (MIE) project NEXT-II, which will be completed between 2026 and 2028. Finally, the Infrared Nanospectroscopy (INF) beamline received a funding commitment in 2022 from New York State and will be constructed and be transitioned to operations in 2026. Thus by 2028 NSLS-II will have 33 beamlines in operations, out of its full capacity of ~60 beamlines.

Even though the current portfolio of beamlines offers state-of-the-art, one-of-a-kind instrumentation, we seek funding to further broaden our available tools for users. In collaboration with our user community through a 2019 Strategic Planning Workshop, called "Exploring New Science Frontiers at NSLS-II", we identified 20+ new beamlines that would balance the current portfolio and provide additional capabilities to meet the research needs of the broad scientific community. Over the past two years, we have discussed these with BES and with the NSLS-II SAC to refine the list of new beamlines. As of September 2022, the list of new beamlines included 12 enterprise beamlines based on mature techniques, 9 high-performance beamlines with cutting-edge capabilities, and 2 mission-specific beamlines to meet the needs of targeted research communities. Together with the existing beamlines, this beamline portfolio would further enable our holistic, multimodal research approach, enhance the overall impact and productivity of the facility and deliver on the nation's needs to address its greatest challenges, including clean energy and climate.

In addition to these new beamline developments in the next decade and beyond, we will plan for a facility upgrade to position NSLS-II as the ultimate medium-energy synchrotron, offering a full suite of transformative capabilities run by experts for the scientific community.

In short, our high-level strategy for the next 5 years is to:

- Deliver mature accelerator performance of 500 mA & 8 pm-rad vertical emittance in reliable user operations,
- Recapitalize existing beamlines and keep them competitive with new access modalities in the post-COVID era,
- Achieve our data vision for seamless access to experimental capabilities, compute, storage, and advanced analysis tools,
- Complete the HEX and INF beamlines, and the NEXT-II project,
- To add new beamlines to increase capacity, enhance capability, support multimodal research, and balance our beamline portfolio. This will be achieved by working with DOE-BES to move the NEXT-III project forward and with other funding partners for mission specific beamlines,
- Position the facility for a transformative upgrade in the coming decade that includes a source optimized as the ultimate medium-energy synchrotron, a suite of beamlines with transformative multimodal tools, and a modern data infrastructure that seamlessly integrates experiment, theory, & computation.

The following Chapters describe components of this strategy in more detail and a set of tactical projects that we will pursue in FY23 as the near term as the next steps in these strategies.

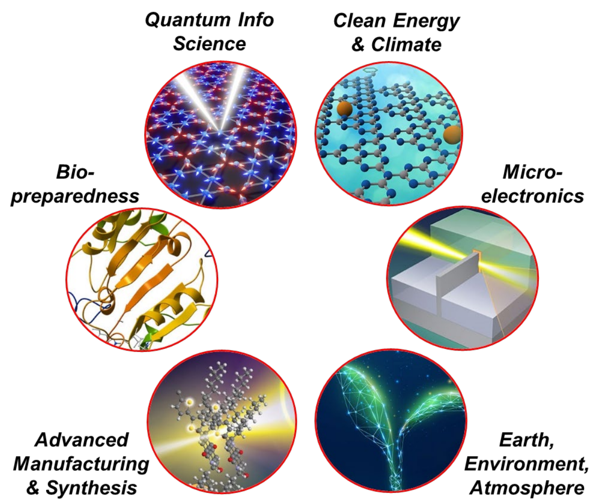
Beamline Portfolio

Note: 33 Beamlines in Operations or under Construction (*)

AMX	*Automated Macromolecular Crystallography*
*ARI**	*ARPES & RIXS nano-Imaging*
BMM	*Beamline for Materials Measurements*
*CDI**	*Coherent Diffraction Imaging*
CHX	*Coherent Hard X-ray Scattering*
CMS	*Complex Materials Scattering*
CSX	*Coherent Soft X-ray Scattering*
IOS	*In situ and Operando Soft X-ray Spectroscopy*
ESM	*Electron Spectro-Microscopy*
FIS	*Frontier Infrared Spectroscopy*
MET	*Magneto-Ellipsometric and Time-resolved IR Spectroscopy*
FMX	*Frontier Macromolecular Crystallography*
FXI	*Full-field X-ray Imaging*
*HEX**	*High-energy Engineering X-ray Scattering and Imaging*
HXN	*Hard X-ray Nanoprobe*
*INF**	*Infrared Nanospectroscopy*
ISR	*In situ and Resonant Scattering*
ISS	*Inner-Shell Spectroscopy*
IXS	*Inelastic X-ray Scattering*
LIX	*X-ray Scattering for Life Science*
NYX	*NYSBC Microdiffraction*
QAS	*Quick X-ray Absorption and Scattering*
SIX	*Soft Inelastic X-ray Scattering*
SMI	*Soft Matter Interface*
SRX	*Sub-um Resolution X-ray Spectroscopy*
SST1	*Spectroscopy Soft and Tender 1*
SST2	*Spectroscopy Soft and Tender 2*
*SXN**	*Soft X-ray Nanoprobe*
TES	*Tender Energy Spectroscopy*

Science Thrust Areas

Scientific research conducted at NSLS-II cover a wide range of scientific disciplines that are crucial to the nation's R&D ecosystem for sustainable energy and environment solutions, technological innovations in quantum and computing, new discoveries of materials and manufacturing processes, and bio-preparedness for future diseases and pandemic.



Recognizing the nation's evolving landscape in science and technology research needs, NSLS-II will develop a number of Science Thrust Areas (STAs) to focus our limited resources in a few scientific initiatives that will lead to the development of additional capabilities at NSLS-II, and to attract new partnerships and new funding to further expand our footprints in the research and development in these STAs.

NSLS-II has been working closely with the scientific community and our sponsors to develop scientific initiatives and technical capabilities to meet the research needs to tackle many of the challenges that our society faces today. Together we have identified the following six Science Thrust Areas (SFAs) to pursue in FY23 and beyond (see figure above) – clean energy and climate, quantum information science, microelectronics, advanced manufacturing, biosciences and bio-preparedness, and earth-environmental and atmospheric sciences. These SFAs are described in more detail below.

Clean Energy and Climate

The U.S. economy is undergoing a clean energy revolution to drastically reduce green-house gas emissions for the pathway to a safer climate future. A 2017 report by Natural Resources Defense Council identified four proven clean energy solutions that the U.S. should pursue in order to reduce green-house gas emissions across the entire U.S. economy by 80% by 2050. This report, and other recent initiatives at DOE point to the following strategies to tackle the climate crisis:

- Implement energy efficiency technologies and system-wide approaches to reduce total U.S. energy demand,
- Expand renewable energy, like wind and solar, to generate more than 70 percent of our electricity supply,
- Employ resulting near-zero-carbon electricity to the greatest practical extent to directly displace fossil fuels,
- Decarbonize the remaining fuel use through *e.g.* synthetic fuels, carbon capture, and hydrogen economy.

As a multidisciplinary and multimodal synchrotron facility, NSLS-II plays an important role in our nation's efforts to conduct foundational research to tackle climate change in each of the above areas. We work with our academic and industrial user communities to develop novel catalysts to improve the energy efficiency of chemical transformations and processes, advance R&D on energy storage systems that are vital to the use of renewables and electric vehicles, and research new material systems for biofuels, carbon capture, and hydrogen technology. In the following paragraphs, we describe our strategies in such areas as energy storage, catalysis, and hydrogen.

***Energy storage**:* Development of rechargeable lithium-ion batteries has paved the way to remarkable advances in transportation, electronics, and grid energy storage. Yet, the challenges of decreasing costs, longer life span, higher energy density, and improved safety remain. To accelerate the progress in the field, new chemical formulations beyond lithium-metal systems have to be developed and the factors responsible for performance and degradation in these novel systems have to be thoroughly rationalized. NSLS-II offers X-ray techniques capable of nondestructive characterization of battery materials on different length and time scales, exceptionally well suited to bring about the fine details of the diverse multiscale chemical and physical phenomena. Coupling hard and soft X-ray spectroscopy with scattering and imaging allows probing the electronic and structural features in a working battery through its full lifecycle.

A collaboration with DSSI will deploy production-ready new queue management and Tiled data access services. The immediate goal is to enable a multi-model, multi-fidelity machine learning algorithms for beamline control and experimental orchestration to accelerate materials discovery in battery science among other fields.

INSPIRE (INelastic Scattering, Photoemission, and InfraRed Endstation) - an upgrade of the IOS beamline - endstation is in development. Endstation will combine existing capabilities (AP-XPS and XAS) with new capabilities (XES/RIXS and IRRAS). The new capabilities are extremely relevant to all aspects of clean energy research (catalysis, energy storage materials) and will allow multi-dimensional, multi-modal probe: surface and bulk, chemical and electronic states.

Catalysis: Catalysis is a core area of current chemical and engineering sciences. While posing fundamental scientific challenges, it is also a corner stone of the chemical and pharmaceutical industries underpinning a vast range of products and processes worldwide. Developments in catalytic technology, including the design and optimization of catalysts and catalytic processes, rely increasingly on the understanding of catalysis at the molecular level.

For developing atomistic models of catalytic processes, NSLS-II offers a diverse array of techniques based upon diffraction, spectroscopy, small angle scattering and tomography that are having a transformative impact on catalytic science. Moreover, NSLS-II continues to be a crucial asset in enabling in situ and operando experimental studies of catalytic processes under realistic operating conditions. This work is impactful on all areas of catalytic science, including heterogeneous, homogeneous, electro- and bio-catalysis.

The QAS beamline staff and their partner user, the Synchrotron Catalysis Consortium (SCC), are commissioning the combined XAFS- diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS) endstation to study in situ chemical transformations in working catalysts. The design allows the identification of surface intermediates using DRIFTS, and the local environment and oxidation state of catalytic species in the bulk by XAFS. Using both techniques simultaneously gives the advantage of linking the structure, surface composition with activity studies.

Operando high-throughput tender XAS endstation funded through a FIP, this new endstation at the TES beamline will enable world-leading operando XAS studies of batteries and catalysts. The XPEEM microscope at the ESM beamline, with its spatially resolved chemical imaging capabilities (µXPS, µXAS) is well suited for surface studies of catalytically relevant and energy storage materials systems. An environmental sample holder for the XPEEM/LEEM is being developed to enable study of surfaces under increased partial pressure, further expanding the potential for catalysis research.

Hydrogen: Hydrogen is a versatile energy carrier with a highest energy content by weight, that offers many advantages that can help reduce or eliminate carbon footprint of energy-intensive industries, such as electrical power generation, and transportation. Hydrogen produced from a hydrogen-containing feedstock (e.g., water, biomass, fossil fuels, or waste materials) can be stored as a liquid, gas, or chemical compound, and is converted to energy via combustion, electrochemical processes, and other technologies. The challenges of building a viable hydrogen economy include low-cost, efficient, and durable materials, devices and systems for hydrogen production, delivery, storage and conversion.

The hydrogen experimental research program will leverage the extensive range of operando/in situ devices that NSLS-II has been developing, e.g., potentiostats for battery and electrochemical research, reactors for catalysis and synthesis, residual gas analysis and gas chromatography and electrochemical cells. We aim to enhance and coordinate inter-department collaborations (CFN, NSLS-II, ISD) to grow competency and leverage BNL's expertise and capabilities to accelerate the discovery of materials related to the stationary storage of Green Hydrogen at large scale. The CS and HXSS programs will contribute capabilities, methodology and workflows for characterizing the key functional properties of H_2 storage materials under in situ and operando conditions.

Quantum Information Science

Th**is** science thrust area at NSLS-II in quantum information science (QIS) focuses on studies of quantum materials in two research themes: (a) studies of novel materials properties that may lead to future QIS applications *e.g.* new types of qubit systems, and (b) studies to characterize materials structures and imperfections in current QIS systems in collaboration *e.g.* with the BNL-led Co-Design Center for Quantum Advantage (C^2QA). NSLS-II strategy is to work with our partners and the QIS community at large to conduct research to advance the current state-of-the-art in QIS, leveraging our beamline capabilities in a wide-range of photon energies.

Soft X-ray capabilities can be used to study electronic and magnetic properties of ultrathin samples of interest to QIS applications. The relevant areas of research include studies of electron spin and spin wave excitations as potential means to transport and process information and investigations of the structural and electronic behavior of transition metal oxides, which are among the best candidates for neuromorphic applications. For all these systems, the combination of best-in-class energy resolution and microfocus of the ESM and SIX beamlines, together with the nano-focus and world-leading coherence of the CSX beamline, promise to have a major impact. The IOS and SST beamlines have already provided depth-dependent electron spectroscopic information on TaO_x/Ta interfaces as well as in situ investigation of the oxidation/reduction chemistry of the oxide interfaces, an area of investigation in support of the materials sub-thrust of C^2QA. Looking ahead, the ARI beamline currently under construction will provide nano-imaging capabilities complementary to ESM and SIX beginning in ~FY27.

Hard X-ray capabilities are well suited for studies of quantum materials and devices in support of QIS goals. The suite of hard X-ray beamlines at NSLS-II provides both bulk and surface structural techniques. Bulk scattering techniques help address large scale QIS device processing/fabrication problems at a variety of length scales, while surface scattering techniques focus on surface order for next generation qubits. The Pair Distribution Function (PDF) beamline provides capabilities for high-throughput screening, in-situ processing, and micro- and nano-structure analyses of qubit materials. It is possible to characterize film orientation and degree of epitaxy with wide reciprocal space coverage at a high-level of sensitivity and data acquisition rates. NSLS-II will help develop fabrication/processing recipes and structure-property-fabrication relationships to improve qubit performance, such as sapphire-based transmon qubits with tantalum resonators. The In-situ and Resonant tender/hard X-ray (ISR) beamline provides the capability for in-situ structural characterization of growing films, and such capability has been used to study the growth of one of the primary materials systems used in fabrication of qubits: tantalum on sapphire, which may provide important indications as to how best to improve the materials quality for qubits.

Infrared beamlines (MET and FIS) provide a capability for probing a variety of quantum phenomena in materials associated with electronic ordering. The spectral range from 1 meV to 1 eV spans the energy scale for many quantum excitations such as the binding energy for electrons in Cooper pairs (e.g. in Nb and Ta, materials being studied for superconducting qubits) or electron-hole pairs in excitons. With an applied magnetic field up to 7T, transitions between quantized Landau levels as well as other quantum states e.g. magnons and polarons can be sensed. The inductive response of paired electrons can be measured in the THz spectral range. The scanning near-field nano-spectroscopy instrument can be used to drive and to study spatially varying quantum phenomena e.g. novel quantum phenomena as well as phase separation and spatial heterogeneity on nanoscales. A new near-field nano-spectroscopy system is developed to provide the cryogenic environment needed to explore certain quantum states. The FIS beamline allows the use of diamond anvil cells to achieve extreme conditions such that much more of material's phase diagram can be explored, including the hydrides that become superconducting at temperatures well above those found in cuprate perovskites.

Microelectronics

This thrust area focuses on studies and characterizations of materials and devices that represent the current state of the art or future microelectronic systems

Scientific problems associated with microelectronics have long attracted significant attention in the synchrotron x-ray communities, which included characterization of novel materials systems and quantification of interfacial structures of heterogeneous thin-film systems and devices. Today, microelectronics problems are more challenging and diverse than ever before, triggered by the explosive demand for high-performance and diverse applications. In 1985, microelectronics devices contained less than a dozen elements. Today, nearly one-half of the periodic table is used. In an effort to extend the performance enhancement trend, better known as Moore's law, the devices are heterogeneously or vertically integrated with decreasing critical dimensions, introducing additional challenges in fabrication and power management. On the other hand, significant dependence on microelectronics chips fabricated in foreign foundries has raised national security concerns regarding the potential tampering of the integrated circuits used for military applications. NSLS-II has a range of cutting-edge capabilities that are highly instrumental in tackling the multi-faceted microelectronics challenges. There are promising opportunities to attract or strengthen external collaboration, leading to impactful scientific impact or strong justifications in developing more advanced capabilities at NSLS-II.

The Basic Energy Science (BES) report on Basic Research Needs for Microelectronics called for new innovative approaches and identified five high-priority research directions (PRD). NSLS-II's capabilities are highly relevant to four of the PRDs by supporting new materials discovery, characterizing novel memory and storage devices, visualizing heterogeneous co-designs, and exploiting new physical phenomena. NSLS-II has a suite of high-throughput diffraction, scattering, and spectroscopy beamlines that are highly effective for characterizing new materials and novel interfacial structures. NSLS-II also has substantial soft x-ray spectroscopy capabilities that play important roles in quantifying oxidations states of thin metal oxides, particularly those used in new types of non-volatile memory material systems. NSLS-II is the current world leader in nanoscale x-ray imaging in the hard x-ray regime. Full-field imaging capability at FXI using transmission x-ray microscopy has the world-leading imaging throughput and is ideally suited for visualizing integrated chips with 3D resolutions in the range of 20 nm to 50 nm. Under a partnership proposal with Defense Microelectronics Activity (DMEA), the FXI's 3D imaging capability is being optimized for visualizing the integrity of integrated chips of a few mm in size. In collaboration with IBM, the scanning imaging capability of HXN has been deployed to map out the strain field in the nanosheets (the latest configuration of gate-all-around structure), and the HXN's 3D XRF and ptychographic imaging are deployed in characterizing non-volatile memory devices.

To achieve a greater impact on supporting microelectronics research in the US, NSLS-II is exploring three high-level strategies. The first and most obvious is further optimizing the nanoscale imaging. For full-field imaging, the immediate challenge is strengthening the data analysis pipeline by eliminating various bottlenecks or barriers for real-time data processing for a large-scale 3D dataset. For scanning imaging, enabling faster scanning and developing more robust methods for performing 3D imaging using sparse datasets are additional challenges. The second is deploying the collective capabilities of NSLS-II for solving the impactful microelectronics problems that can resonate in not only academia but industry. More aggressive outreach to industrial researchers and lowering the barriers to effective collaboration are some of the steps currently being pursued. The third strategy is articulating future NSLS-II beamlines that could provide more effective or optimized capabilities in addressing microelectronics problems.

Advanced Manufacturing

Advanced Manufacturing (AM) methods, such as additive and AI/ML-guided manufacturing, have the potential to enable energy- and material-efficient, cost-effective, environmentally clean, and sustainable manufacturing.

They can impact a wide range of applications with novel materials and architectures, from printed micro-batteries to high-strength aeronautical/aerospace components to flexible bio-sensors and biocompatible scaffolds for organ growth. However, the fundamental science governing the processing and emergence of materials' functionality remains poorly understood. The 2018 National Science and Technology Council report on "*Strategy for American Leadership in Advanced Manufacturing*" highlights the need for developing world-leading materials and processing technologies. Many federal agencies, including DOE, DOC, DOD, and NSF, now invest in basic and early-stage applied research to spur innovation in AM. In particular, the 2020 DOE/BES *Basic Research Needs (BRN) Workshop on Transformative Manufacturing* highlights the critical role of advances in basic science to underpin applied technology research and development. Key scientific challenges in basic AM research include: design and discovery of new functional materials and material synthesis and processing methods; understanding the non-equilibrium spatiotemporal behavior of complex materials during formation processes across multiple length and time scales; precise, adaptive, and multi-scale control and optimization of material architectures and processes towards desired functionality and enhanced performance.

NSLS-II is ideally positioned to contribute to addressing these challenges, thanks to: its high-brightness source; its slew of available diffraction/scattering, spectroscopy, and imaging techniques; and its existing and emerging strengths in experimental control and automation, high-throughput and in-situ/operando characterizations, multimodal capabilities, data infrastructure, and use of AI/ML methods in experimental workflows. In particular, leveraging these advantages will allow NSLS-II to make significant impact on the priority research directions (PRDs) identified in the BES BRN report, including: (1) achieve precise, scalable synthesis and processing of atomic-scale building blocks for components and systems; (2) integrate multiscale models and tools to enable adaptive control of manufacturing processes; and (3) unravel the fundamentals of manufacturing processes through innovations in *operando* characterization.

Our strategy for AM sciences is two-fold: (i) to grow engagement with users and collaborative partners to expand the AM research activities at NSLS-II and explore partnership opportunities to participate in impactful AM research programs, especially those based on multi-institutional funding proposals; (ii) to expand NSLS-II's technical capabilities for studying AM of polymeric and hard materials, as follows.

AM of polymeric materials: Our efforts in this area focus on *in-situ/operando* x-ray scattering characterizations of a wide range of polymeric materials—amorphous and crystalline, thermoset and thermoplastic, nanocomposites (nanoparticles, fibers), elastomers, organo-gels, polymeric pre-ceramics, and hydrogels—under AM-relevant processing conditions and during the property and reliability testing of AM-derived samples. Our strategy is to advance the following ongoing efforts:

- Development and multi-beamline integration of portable AM instrumentation for multimodal, *in-situ/operando* scattering studies. Such instrumentation includes: a newly developed 3D-printing platform that can accommodate commercial printheads and achieve high print rates, *in-situ* laser annealing and spray deposition systems, as well as tensile and shear stages for mechanical testing. Their key features are: full controls integration (*Bluesky*) compatible with AI/ML-guided experiments; incorporation of non-x-ray proxy/ancillary characterization probes; availability for both online and offline user experiments at beamlines and user laboratories.
- Integration of AI/ML methods in experimental and data workflows to provide prompt, adaptive feedback based on automatic sample handling and data acquisition, real-time data analysis, and machine-guided decision-making. This effort will require computational infrastructure for large data-set processing, engagement of experts in modeling and simulations, and development of generic methods to incorporate physical, system-specific, expert knowledge into decision algorithms.
- Refinement of the science case and technical capabilities for a new undulator beamline focused on studying AM processes that will provide state-of-the-art coherent/incoherent SAXS/WAXS capabilities with microbeam, including SAXS-XPCS, in combination with a unique endstation optimized for large equipment (industrial-scale) and capable of *in-situ/operando* studies.

AM of hard materials: During AM of metals, alloys, and ceramics, the material is subjected to extreme processing conditions (e.g., rapid melting and solidification), which in turn introduce microstructural heterogeneity, grain orientation and texture, strain, and various internal defects that impact the material's properties. NSLS-II can contribute to precise characterizations of these structural features and understanding their origin and role in enhancing or deteriorating the desired functional properties. Elucidating the effects of the material composition and microstructure and the processing history is essential for predicting the performance of AM-derived parts. Our strategy for advancing this research area is to strengthen NSLS-II's capabilities for *in-situ/operando* structural characterizations and to leverage its suite of multiscale, multimodal imaging methods. In particular, we aim to:

- Develop new high-energy x-ray imaging and diffraction capabilities at the HEX beamline, to enable direct, time-resolved characterization of microstructural states of metals and ceramics, during and after AM processes and post-AM testing (e.g., mechanical and thermal fatigue analysis). This includes 3D mapping of micro- and atomic structures and defects, even in high-Z materials.
- Apply the existing arsenal of x-ray tools with different imaging modalities to investigate heterogeneities in AM-derived materials across scales, from the dimensions of final built components down to high-resolution features at nanometer scales. The available techniques, such as x-ray tomography, fluorescence microscopy, spectromicroscopy, and nano-diffraction, will enable comprehensive characterizations of chemical, physical and mechanical properties of the materials.
- Explore new beamline concepts. Comprehensive structural/chemical information on AM-derived materials will be extracted *operando* using new, state-of-the-art diffraction/spectroscopy/imaging beamlines, with a tunable spatial resolution from millimeters to nanometers. The analysis of the microstructure (grain size, orientation and strain distributions, defects, precipitates) is commonly achieved through high Q-resolution diffraction. Adding fast imaging capabilities, including high resolution emission spectroscopy, will enable *operando* investigations of evolving morphologies and chemical heterogeneities during AM processes.

Biosciences and Bio-preparedness

In this thrust area on biosciences and bio-preparedness, our goal is to work with the biosciences research community to understand both how macromolecules are structured at the atomic level and how they are organized at the cellular level. We develop instruments to allow new types of measurements to be made, and we create analysis methods to extract the best possible information from these measurements.

The essential biological processes in cells are all carried out by proteins and enzymes and by assemblies of these molecules, or molecular machines. The use of X-ray crystallography and single particle cryo-EM have been phenomenally successful in delineating the atomic structures of many of these molecules and machines. However, the next grand challenge is to understand how these molecules are organized at the cellular level, and how they are reorganized in different physiological states. To address these challenges we need to build sustainable, adaptable, science platforms that incorporate synchrotron and non-synchrotron experiments, data analysis, and encourage collaboration to provide a research environment for examination of complex science problems. It is our assertion that this approach is the best path for growing Bioscience research at the NSLS-II and BNL, and the approach provides a vibrant environment for attracting and retaining the best talent.

Given the diversity of cellular function, the opportunities for break-through knowledge are almost boundless, here are some examples:

- What is special about the structural organization of molecules that function within membrane-bound organelles to enable them to perform specific functions?
- How are molecules organized as they transmit signals from the cell surface to internal components?
- The disease states of cells may be morphologically different; can we devise more sophisticated imaging techniques to allow for an understanding of the impact of disease on the cell function?
- Ultimately, we need a four-dimensional (3D and time) understanding of the structure, function, and dynamics of molecules in a cellular context.

Our strategy to address these questions is to pursue developments along three directions. *First*, we will continue to develop cutting-edge ***integrated structural biology*** methods including tools for measurements at ambient conditions and to establish new methods for studies of dynamic processes in both the solution state and from crystals of macromolecules. *Second*, we will seize the opportunity from advances in ***cell imaging*** and the associated improvements in analysis and partitioning of the images to understand biomolecular structure and function in the cellular context by correlating data available through tomography, light microscopy, and correlative data analysis. *Third*, to make most of the enormous quantities of data that will be generated, we will work with our funders so that needs for ***data processing, analysis, management, and curation*** meet agreed norms. Standardization of data management and analysis will contribute to, and ease the transition from data acquisition, through interpretation, to publication.

Our intention is to enable hypothesis-driven science with technology development on plant and microbial systems relevant to national priorities in energy security and resilience. To enable multidisciplinary study of complex interactions specifying the function of entire biological systems—*from molecules to single cells to multicellular organisms*—rather than "only" the study of individual isolated components. We work with researchers to recognize new trends and will adapt accordingly, evolving the NSLS-II beamlines with emphasis on ease of use and quality of their output.

At part of our integrated strategy in biosciences and bio-preparedness, we are working with our partners in BNL and in the community to develop a *National Virtual Biosecurity for Bioenergy Crops Center (NVBBCC)*. BNL has received an award from DoE-BER in response to a proposal to develop and lead a prototype platform and roadmap towards such a new BER center to address biosecurity needs relevant to bioenergy/bioproduct crops. We will host a series of community workshops and perform experimental work on a known disease of sorghum, make key initial investments in infrastructure, and conduct a design study of future investments needed for a mature NVBBCC to handle work involving Plant Biosafety protocols (BL1-P through BL3-P). The NVBBCC will comprise four modules: 1) Detection and Sampling, 2) Biomolecular Characterization, 3) Assessment, and 4) Mitigation. NSLS-II and the LBMS will be responsible for the structural characterization. To expand our potential for impact on the process, we will install a cryogenic focus ion beam (cryoFIB) milling machine to enable cryo-electron tomographic investigation of invasion processes. In support of the NVBBCC we plan to continue engage key collaborators on sorghum cultivation and genomics at Texas A &M, hyperspectral phenotyping expertise within CABBI, and key disease diagnostic test development and disease mitigation expertise within USDA.

Geo-Environmental & Atmospheric Science

This SFA leverages the cutting-edge capabilities at NSLS-II in elemental and chemical speciation imaging to investigate the various complex chemical processes in our immediate environment and beyond, covering earth, environmental, atmospheric, and planetary sciences.

In ***geo- and environmental science***, research activities focus on chemical speciation, bioavailability, redox behavior and cycling of nutrients and other elements at various spatial and temporal scales in the heterogeneous materials of Earth's Critical Zone, continental crust, oceanic crust, oceans, and atmosphere. The complexity of these molecular interactions poses significant challenges for all branches of Environmental science, as do the broad length scales (from nano- to mega-meters) and enormous temporal range (from pico- to peta-seconds) over which these interactions occur. To further complicate the picture, biology (*i.e.* carbon) has a profound influence on the cycling of critical elements at the Earth's surface, and the pathways of carbon cycling are linked intimately to biogeochemical processes of other life-sustaining elements (*e.g.* Fe, S, P).

Integration of synchrotron approaches (microscopy, microprobe, bulk) that probe a variety of properties (XAS, IR, XRD) is characteristic of Geo- and Environmental science users that study Earth systems (rocks, soils, sediments, water, and atmosphere). There is no single spatial scale or element that can adequately describe Earth surface processes. Integration across spatial scales and elements (eg C, Ca, Fe) is a unique strength of the U.S. synchrotron portfolio and it supports some of the most pressing science questions. Many of these questions relate directly to changing climate, its complex feedbacks, buffers and tipping points, and the geologic record of past climate. These holistic research questions provide a framework for linking the chemical, physical, and structural aspects of both deep and surficial processes to further our understanding of whole-Earth and climate systems, their components and cycles, as systems in motion.

Several community-driven projects are underway to strengthen bio-environmental research at NSLS-II -- sponsored in part by DOE-BER as TR&D (Technology Research and Development) Projects. These include 1) development of cryo-XRF capabilities for micron and submicron resolution, 2) development of user-friendly tools for multi-modal image visualization and quantitative analysis, 3) development of long-working-distance confocal-XRF spectroscopy, and 4) addition of benchtop XRF imaging station with 10-micron resolution and large (0.2 m) field-of-view for routine sample pre-screening, hypothesis testing, and training/education/outreach.

Overall strategy for growth of the Geo- and Environmental science community at NSLS-II is continued expansion of multi-modal capabilities across energy and spatial scales. Some specific examples include: bridging the current spatial resolution gap between XFM, SRX and HXN beamlines (e.g. SRX-II & HXN-II), expanding the soft/tender energy range from the microscale to the nanoscale (i.e. SXN & TXN), developing high throughput imaging modes (eg pink beam at XFM & HXN-II), and delivering new capabilities of interest to the Geo- and Environmental science community (i.e. MCT).

In ***atmospheric and planetary sciences***, a principal challenge facing all Biological, Earth, and Environmental (BEE) Sciences in general is the understanding of fundamental processes on the small scale that manifest in global-scale patterns that drive temperature, water availability, weather extremes, and climate. This is especially true for atmospheric science, and here research on aerosols especially, that underpins some of the greatest uncertainties in mitigating the negative impacts of climate change and air quality. A next-generation scanning transmission X-ray microscope (STXM) using X-rays in the sub- and low keV energy range with a spatial resolution in the sub-50nm range and enabling X-ray fluorescence measurements, paired with novel automatic high throughput sampling and the implementation of machine learning and artificial intelligence algorithms to optimize analysis, with cryogenic sample handling and micro-reactors, would be an ideal instrument to fill knowledge gaps on the small scale.

This STXM would allow for compositional, structural, morphological and interfacial analyses whereby critical elements can be mapped down to trace elemental concentrations levels such that the chemical state of these elements can be determined. Such next-level studies are needed to fill gaps in the foundational understanding of many geochemical processes that are required to advance predictive models of the Earth system necessary for planning a clean energy future and informing policy. Optimized for X-ray fluorescence and spectroscopy, and versatile but with atmospheric science as the main focus, this STXM would serve geomicrobiology, marine chemistry, planetary science, soil science, or waste management as well. The lack of a STXM dedicated to BEE science is a significant gap in the portfolio of instrumentation within the U.S. Without dedicated instrumentation, leading scientists make use of STXM outside the US and the nation is not equipped to address the next-level analytical challenges for BEE science. However, NSLS-II provides the necessary high brightness to meet the needs of such a next-generation STXM for BEE science and is therefore an ideal place for such an instrument.

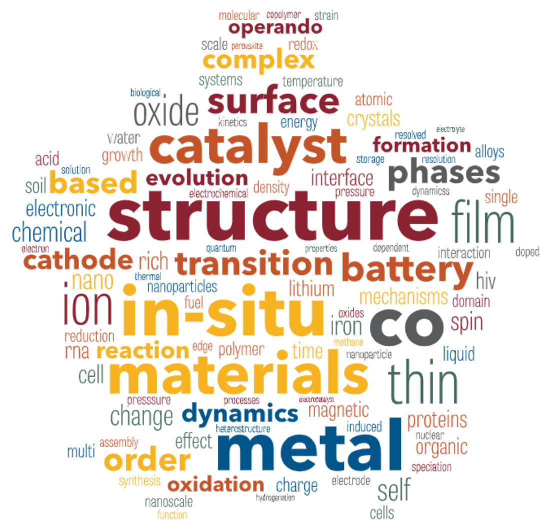
In planetary science, future missions to Mars will yield returned samples sealed in Ti-alloy sample containers. To analyze these samples, complementary, non-destructive, in-situ synchrotron-based techniques that yield full high-resolution, high-sensitivity, structural, mineralogical, morphological and chemical characterization of returned samples without breaking containment would be extremely useful. 3D Computed Tomography (CT) delivers structural and morphological analysis of the samples and fundamental information about the structural integrity of sample container and seal; X-ray diffraction tomography (3D-XRD) yields a spatially resolved mineralogical analysis of the sample; and X-ray Raman spectroscopy (XRS) is an excellent technique for chemical analysis, including organic components. For all three techniques to provide information on samples sealed in 0.50 mm thick Ti-alloy tubes, it is necessary to use a high-brightness, high-energy X-ray source that is only available at modern synchrotron radiation facilities. As one of the most advanced synchrotron radiation facilities in the world, NSLS-II provides world-leading imaging and structural analysis capabilities. Once developed, these techniques could form the core of the first-level of analysis of returned samples in a sample curation and analysis facility associated with an advanced synchrotron facility, such as NSLS-II.

To ensure the preservation of integrity of organic compounds in returned Martian samples, the impact of the proposed synchrotron techniques on such compounds needs to be investigated in detail. In addition to the development of techniques to study samples sealed in Ti-alloy sleeves for first- level analysis, the possibility of transferring samples from Ti-alloy sleeves into sealable X-ray transparent sleeves should be investigated to allow for additional synchrotron-based characterization while preventing exposure to the terrestrial atmosphere. This enables a detailed study of returned samples using additional techniques such as X-ray fluorescence microscopy and XANES spectroscopy.

Samples from Mars will be returned in the beginning of the next decade, but considering the complexity of the analyses and the enormous value of these samples, methods, procedures and potentially new beamlines need to be developed now. Specific geological materials from Earth environments have been identified as Mars analogs and can serve as precursor. Investigating materials from Earth environments not only allows for a more confident interpretation of samples from Mars but, in addition, fills a knowledge gap on terrestrial geological material. Although contemporary sedimentary processes on Mars and Earth are fundamentally different, ancient environments preserved in the Martian rock record illustrate a period in which the two planets may have been more similar. The emphasis is on resolving gaps in the current capabilities of ground-based laboratories for analyses on samples which have been returned from missions to Mars. While focused on missions to Mars, these developments of synchrotron techniques would also be relevant to other missions, such as OSIRIS-Rex and Hayabusa2.

Beamline Science Programs

NSLS-II beamlines are organized into five beamline programs – Soft X-ray Spectroscopy and Scattering, Hard X-ray Scattering and Spectroscopy, Complex Scattering, Imaging and Microscopy, and Structural Biology. Together these programs provide a large suite of experimental capabilities and scientific expertise that enable a diverse and strong user science program at NSLS-II. The word cloud at right, based on word frequencies in user beamtime proposals, shows the diverse range of research being conducted at NSLS-II beamlines. In the previous Chapter, we outlined a set of crosscutting science thrust areas where NSLS-II aims to expand research activities through new capabilities at beamlines and partnerships with the communities. In this Chapter, we provide a more detailed description of the strategies and near-term activities in FY23 in each of the five beamline programs.



Soft X-ray Spectroscopy and Scattering

Mission: The soft X-ray spectroscopy and scattering (SXSS) program's mission is to understand and ultimately control emergent quantum phenomena and novel chemical phenomena by providing a suite of cutting-edge infrared, soft, and tender X-ray capabilities that enable studies of the electronic and magnetic properties in condensed matter and chemical and electronic properties in catalytic and energy storage materials, to inform the design of practical devices for information and energy technologies of the future.

Strategy: The beamlines in the SXSS program are developed and operated to meet the research needs in three science thrust areas of interest to the Department of Energy: materials, quantum information science (QIS), and chemistry.

Materials: Our efforts in this area are to probe and understand the phenomena that stem from the interactions of electrons through their degrees of freedom (charge, spin, and orbital), especially when those interactions result in novel ordered states. Many such states occur in confined systems such as 2D materials or as edge states in topological materials. The interactions can sometimes be controlled by external means such an applied field or pressure, or intrinsically through the oriented stacking of 2D materials such as graphene, hexagonal boron nitride, and transition metal dichalcogenides ("twistronics"). Measurement techniques are geared toward sensing electronic energies and interactions as a function of wavevector (momentum) using the source coherence at the CSX beamline and the state-of-the-art energy resolution at the ESM and SIX beamlines. High magnetic field (to 7T or 10T) is being implemented at the MET beamline and diamond anvil cells are used for achieving extreme pressures at FIS - both for infrared spectroscopy.

Taking advantage of the brightness of the NSLS-II sources, spectroscopic nanoprobe instruments covering a wide range of photon energies have been and will continue to be developed. These instruments will be used for interrogating confined systems or the spatial variations in electronic properties that can stem from intrinsic inhomogeneity, competing orders, or Moiré effects. Included in this set are three new beamlines, in the design or project development phase, that are dedicated to achieving <10 to ~100 nm spatial resolution. Two of these beamlines, ARI and SXN, are soft X-ray beamlines being constructed as part of the NEXT-II DOE 413.3b project. The ARI (ARPES and RIXS Imaging) beamline will provide ARPES and RIXS measurements with ~100nm spatial resolution, without the flux losses associated with zone-plate focusing. ARI will provide unprecedented capabilities in combining spectroscopic information with spatial resolution at a length scale where quantum confinement becomes important. The SXN (Soft X-ray Nanoprobe) beamline will provide a focused soft X-ray (250 – 2800 eV) beam for scanning and ptychographic imaging with spatial resolution <10nm. SXN will allow spectroscopic imaging covering absorption edges of a wide range of materials of interest to DOE at unprecedented length scales, further expanding the options for materials research at NSLS-II. A third beamline, INF, is expected to be developed starting in FY23, with operations starting in FY24-25. The INF (Infrared Nanospectroscopy Facility) beamline, covering the mid-infrared range from ~10 to 500 meV, will provide low-energy spectroscopic capabilities for sample surfaces with 10 nm spatial resolution. This spatial resolution, which is much smaller than the far-field diffraction limit at mid-IR wavelengths, will be provided by state-of-the-art raster-scanning near-field optical microscopy (SNOM) techniques providing simultaneous topographic and IR spectroscopic information. In addition, INF will provide both ambient and cryogenic (down to 5 K) sample environments and applied magnetic fields up to several Tesla.

Quantum Information Science: The SXSS strategy in the QIS area draws upon the world-leading photon beam coherence and energy resolution of the SXSS beamlines to tackle the two biggest challenges in quantum computation today – limited coherence times and gate fidelities of qubits. We will continue to pursue two fronts: (a) diagnosis and optimization of relevant material properties in existing qubit designs, such as superconducting qubits and nitrogen vacancy centers, in close collaboration with C^2QA partner institutions, and (b) development of next-generation quantum materials systems based on their exotic electronic properties such as topological insulators and high-temperature superconductors.

In addition, we will continue to work with the QIS community to identify and strengthen the science cases for new beamlines in the soft X-ray range. The proposed HTS (High Throughput Soft x-ray scattering and spectroscopy) beamline will provide automated high throughput XAS, XPS, RIXS and X-ray reflectivity measurement capabilities, allowing for fast and effective materials characterization to better inform the design and optimization of quantum devices. The proposed CST (Coherent Soft and Tender x-ray scattering for spectro-nano-imaging) beamline would expand upon the capabilities of the CSX beamline, both in techniques (REXS, fast XPCS, nano-diffraction, and advanced imaging at non-zero momenta) and in energy range (into the tender X-rays for edges of materials relevant for QIS applications).

Chemistry: Our strategy in this area is to provide world-class in situ soft X-ray spectroscopy capabilities for investigations of the chemical and electronic states of energy materials such as catalysts, batteries, and fuel cell electrodes under operating conditions using ambient pressure X-ray photoelectron spectroscopy and X-ray absorption spectroscopy. The aim is to unravel the complex and dynamic changes in the chemical and electronic properties of the materials to understand and control factors that determine their functional properties. This will establish principles for rational design of next-generation energy materials and optimization of operating conditions to achieve the best performance.

The focus for the next few years will be to upgrade the IOS beamline with a new multi-modal endstation known as INSPIRE, which will enable in situ investigations of catalysts, batteries, and fuel cell electrodes to obtain a combined chemical and electronic picture of the material under the same sample preparation and operating conditions. In addition, the SXN beamline will allow for most edges of interest in catalysts, batteries, and fuel cell electrodes to be imaged at the <10nm spatial resolution during operation, providing a new window into the reactions and allowing for a greater understanding of the processes involved. The proposed HTS beamline will also provide the capability of high throughput screening of novel energy materials at high resolution, which in conjunction with results from in situ studies and theoretical calculations will provide invaluable insight into the relationship between the chemical state and the functional performance of energy materials.

FY23 Activities:

Inelastic Scattering, Photoemission, and Infrared Endstation (INSPIRE): Funded through an internal Facilities Improvement Project (FIP), INSPIRE comprises an optics upgrade at the IOS beamline and a new endstation that will offer a unique combination of state-of-the-art ambient pressure XPS, XAS, IR, and XES/RIXS capabilities to study energy and catalytic systems under realistic operating conditions and time scales. It will capitalize on a focused beam spot of 2 µm x 20 µm with spectral brightness enabling very fast RIXS (~1 sec) and AP-XPS (sub-second) data acquisition. New KB mirrors are currently in production with an estimated delivery date in late FY22. Photon delivery system procurement is underway with an expected contract award date in late FY22/early FY23 and delivery/installation timeframe in late FY23/early FY24. Design of the new endstation is in progress and procurement will commence in FY23. The INSPIRE project is designed with modularity to enable a phased construction process to balance the demands of existing user operations with instrument development, with an estimated completion date late in FY24.

Liquid electrochemical cell and gas reaction cell for XAS at IOS: Science commissioning for an in situ electrochemical cell to study liquid-solid interfaces with XAS was started in FY20 and was paused due to Covid-19 and restricted on-site staffing. Commissioning will resume in late FY22/early FY23 as on-site user operations and staffing levels return to closer to normal values. A reaction cell for studying gas-solid interfaces at atmospheric pressures is undergoing testing and optimization at the Advanced Light Source and is expected to be ready for technical commissioning in FY23.

Ambient pressure partial fluorescence yield XAS at IOS: The addition of a Vortex silicon drift detector to the APPES endstation at IOS is planned in FY23. This will enable experiments using partial fluorescence yield XAS under ambient pressure conditions in combination with AP-XPS and partial electron yield XAS for multimodal investigations of the surface and bulk states of materials in the same sample environment. Test experiments using AP-PFY-XAS in FY18 were successful and resulted in two publications.

Coherent imaging and ptychography at CSX: The innovative nano-scanning system installed and commissioned at CSX in FY22 has continued to be optimized to achieve desired performance. During FY23, commissioning with nano-scanners upgraded by Smaract to operate better in relatively noisy mechanical environments is expected to further improve performance. The ptychography capability enabled by the nano-scanning system has produced the first spectacular results, both from the ReconsTeam (collaboration between MIT, LANL, Univ. of Marseille – France, ALS, and led by CSX; work unpublished to date) and the Partner User Group from BNL's CMPMSD (recently published). Reconstruction codes specifically tuned for the resonant soft x-ray regime are expected to be implemented on the beamline servers during FY23.

Fourier transform holography at CSX: This project has been slowed down due to the Covid-19 pandemic, the shift of one staff member to other activities, and the lack of availability of the dedicated fast CCD detector. Despite these limitations, the first manuscript resulting from this project is about to be published. The situation will improve in FY23 if suitable detectors become available for this project.

Enhancing x-ray stability and performance at CSX: The improved water-cooling system for the M1 mirror and PGM monochromator at CSX implemented in FY21 has improved horizontal beam jitter and photon energy stability and continued to be fine-tuned during FY22. Implementation of the associated EPS controls, planned for FY23, will permit implementation of feedback to further improve stability and optimize performance. Commissioning of the phasing magnet inserted between the two EPUs in the 23-ID straight section, delayed by the Covid-19 pandemic, will continue in FY23. In addition, an effort is ongoing to reduce deleterious effects (on electron beam position in the accelerator and thermal load changes on beamline optics) associated with special undulator polarization modes. Assembly, installation, and commissioning of the polarization analyzer to measure the CSX beam polarization, begun in FY21, was completed in FY22 and will be tested during dedicated beamtime (with in-line source configuration) for commissioning of this device in FY23. This analyzer will enable unprecedented control of the polarization for advanced experiments. Finally, a new grating for the CSX monochromator to reduce sensitivity to angular instabilities and improve energy resolution and harmonic rejection (needed to perform advanced coherent scattering experiments), is planned for procurement in FY23.

High resolution ARPES spectroscopy at ESM: The ARPES experiment at ESM operates over a wide photon energy range (20-1500 eV), with full control of the light polarization (two in-line EPUs) and a micro-focused beam (~ 5 microns at the sample). High quality ARPES maps are routinely collected with a DA30 Scienta analyzer with an energy and angle resolution of ~ 6 meV and < 0.1 degree, respectively. The upgrade of the ARPES endstation initiated in FY21 has been completed in FY22. A mu-metal vessel has been installed, hosting the Scienta electron spectrometer as well as a 6-degree-of-freedom cryostat coupled to a low vibration close-cycle LHe refrigerator (lowest temperature ~7K). Additionally, a new preparation chamber for in-situ thin-films growth and characterization has been installed and commissioned.

Synthesis of quantum materials at ESM: Since electron spectroscopies are extremely surface sensitive, ESM pays particular attention to in-situ preparation techniques. Currently, two sample preparation techniques are supported: (i) MBE growth (two existing MBE systems exist: Yale-MBE for oxides and an MBE for chalcogenides) and (ii) exfoliation (provided by a glovebox equipped with piezo motions and an optical microscope). The combination of these two capabilities is expected to be highly effective at ESM, allowing the study of artificial heterostructures prepared under different conditions and forms. Furthermore, the preparation of unique hybrid sample systems, taking advantage of the various growth capabilities, will be possible. For example, the study of proximity effects between chalcogenides and high-Tc superconductors is currently a topic of high interest to be pursued by combining the growth capabilities of the two MBE systems. Similarly, exfoliated materials prepared in the glovebox or in the Quantum Material Press (Q-Press) at CFN can be combined with the other preparation techniques. A postdoc dedicated to preparation of 2d QIS materials at Q-Press and characterization of their properties at ESM and other NSLS-II beamlines was hired during FY22 and will continue to make progress in these areas during FY23. A railway system is under development (conceptual design stage) at ESM, to transfer samples from the growth/preparation facilities to the ARPES and XPEEM endstations under UHV-conditions.

XPEEM/LEEM microscopy at ESM: The XPEEM/LEEM microscope provides direct, full-field imaging of the topographic, chemical, and magnetic properties of surfaces, as well as the electronic band structure with few nm spatial resolution. Use of synchrotron radiation (XPEEM) enables measurements of electronic states (µARPES), magnetic imaging of nanostructures (x-ray magnetic circular dichroism, XMCD), and chemical analysis (µXPS, µXAS) with an energy resolution of ~60 meV and spatial resolution better than ~20 nm. The XPEEM/LEEM microscope is equipped with *in-situ* sample preparation facilities including material deposition, gas dosing, temperature treatment up to 2000 K as well as low-temperature measurement capabilities (down to ~100 K in XPEEM). The instrument is also compatible with CFN's Universal Sample Holder (USH) system, allowing sample transfer via an ultrahigh vacuum (UHV) "suitcase" between the microscopes (including XPEEM/LEEM) and sample fabrication facilities. The microscope is equipped with a state-of-the-art, CMOS-based solid-state detector. This detector has a 4K maximum resolution and a large dynamic range. At the beginning of FY22 the microscope has been upgraded with a new energy analyzer, improving the energy resolution for XPEEM to ~60 meV, which will be a record for such instrument operating at a user facility. For FY23 we are planning to develop new sample cooling capabilities, with a target temperature below ~20K. This is not a trivial task, requiring a redesign of the XPEEM experimental chamber and the sample manipulator that operates at 20,000 V during measurement. Components in the electron optics of the microscope, including an objective lens, are integral parts of the sample environment that also need to be cooled; this portion of the upgrade is undertaken in close collaboration with the microscope's vendor. In parallel, specialized sample holders and methodologies for *operando* measurements will be developed to enable low-temperature spectro-microscopy of 2D and quantum materials-based structures and devices that are fabricated at facilities such as CFN's Quantum Materials Press.

XPEEM catalysis and energy storage materials program at ESM: The XPEEM microscope, with its spatially resolved chemical imaging capabilities (µXPS, µXAS) is well suited for surface studies of catalytically relevant and energy storage materials systems. The XPEEM is routinely used to elucidate morphology and structure, and provide elemental mapping a number of such systems. In FY23 we are planning to develop capabilities for remote control of routine XAS measurements, which will increase further the productivity of the microscope.

High and ultra-high energy resolution RIXS at SIX: Currently, the SIX beamline routinely achieves a total resolving power (beamline plus spectrometer) of 32,000 - 35,000. The goal for FY23 is to reach the resolving power design goal of ~70,000 by resolving mechanical instabilities associated with the water-cooled optics in the SIX photon delivery system. The ultra-high resolution spectrometer grating (2500 l/mm) is planned to be upgraded with a blazed profile to enhance the throughput. In addition, a 1250 l/mm spectrometer grating needed to operate in the medium-high energy resolution mode will be purchased. Similarly, a more efficient high energy resolution monochromator grating (500l/mm) and its improved-design holder will be installed in August 2022.

RIXS with continuous momentum tunability and upgraded sample manipulation & cooling at SIX: The RIXS endstation at SIX was designed using the concept of a triple rotating flange (TRF) connecting the spectrometer to the sample chamber and enabling RIXS measurements at continuously tunable momentum transfers. The TRF was received in February 2020, successfully installed in May-June 2021, and was routinely available for continuous in-vacuum motion of the scattering arm during FY22. Additionally, an R&D project is ongoing to realize a piezo-based sample manipulator offering precise, motorized control of all six degrees of freedom at the sample while achieving cryogenic temperatures at the sample itself. This project represents a major upgrade with respect to the current flow-cryostat manipulator controlled with external XYZ+Theta stages. Design of the new sample manipulator is planned to be completed in FY22-23 and installed in FY23.

RIXS under device-operating conditions: Through the Early Career Award of Valentina Bisogni, RIXS studies of spin dynamics in model materials subjected to device-operating conditions is being developed at SIX. This capability is particularly important as spin dynamics hold promise for high-speed, low-power functional devices. To enable these measurements, a unique sample environment, called OPERA, is being developed to replicate device-working conditions. The test version of OPERA – capable of supplying electric field, current, and a temperature gradient to the sample – is fully functional and commissioned, though changing samples requires venting the sample chamber. A complete version of OPERA will be implemented and commissioned through FY23, together with the development of the new sample manipulator planned for SIX.

Investigation of laser-induced "hidden phases": Funded by an FY21 LDRD, this project will use an ultrafast laser to induce "hidden" phases in materials (*i.e.* those not reachable in thermodynamic equilibrium). Soft RIXS measurements at SIX will then be used to study these phases, uncovering elementary excitations and their evolution from pristine to photo-induced phases. This work is important because these transitions are well known in the ultrafast community, but their mechanism is still not understood, precluding any prediction. These novel metastable phases are promising from the application perspective, as the switching of properties such as resistance or magnetism is useful for novel device concepts. Due to delays in delivery of the ultra-fast laser, this project focused during FY22 on alternative plans based on the use of continuous wave laser. Receipt of the ultra-fast laser is expected in FY23.

Commissioning and Operation of Infrared and THz spectroscopy at FIS and MET: The FIS beamline will continue to operate for General Users in FY23, enabling studies of materials under extreme conditions of pressure and temperature. The FIS program is focused on diamond anvil cell (DAC) techniques for reaching 100s of GPa in combination with temperatures from ~10K (cryo-cooling) to a few thousand K (CO2 laser heating). Studies include vibrational spectroscopy of mineral phases as found deep inside the Earth or other planets and the incorporation of water as complex hydrates. Studies also include electronic spectroscopy to sense the metallization of various hydrogen compounds, including evidence of superconductivity at high temperatures. Capabilities include IR, Raman, and fluorescence spectroscopies. The MET beamline began General User operations late in FY21; the MET user program ramped up during FY22 and will continue to ramp up during FY23 as more experimental capabilities are brought on line. MET enables investigations of novel solid-state systems. The widest possible spectral range of 1 meV to 5 eV will be available for reflectance spectroscopies with Kramers-Kronig analysis. A spectroscopic ellipsometer system being developed by NJIT (but delayed by Covid-19) will be completed in FY23, which consists of a 7T dry magnet allowing for measurements of samples in high magnetic field. Systems of interest include complex oxides displaying competing orders, topologically controlled phases, and 2D materials such as graphene, h-BN & metal dichalcogenides, and nanomaterials. Development of a near-field nano-spectroscopy system (currently on loan from NeaSpec, to be purchased in stages starting in FY23) progressed during FY22 following construction of a fully purged environmental enclosure for this endstation. Development activities will continue in FY23 with implementation of a fast-mirror feedback system for reducing beam motion stemming from mechanical noise and development and commissioning of fast detectors for reaching longer IR wavelengths.

Ultra-fast laser for studies of material dynamics: In FY23, a near-infrared, mode-locked laser system will be received, to be used for transient disruption of ordered phases in materials, initially at the CSX and MET beamlines, enabling studies of photo-excited states of matter and the relaxation processes that control the return to equilibrium order. The pulse structure resulting from electron bunches in NSLS-II will allow for a temporal resolution approaching 15 ps, complementing the capabilities at the X-ray FELs.

Hard X-ray Scattering and Spectroscopy

Mission: The HXSS program mission is to develop and use advanced x-ray scattering and spectroscopy techniques to characterize and explore at the atomic level and mostly under non-ambient and dynamic conditions, the structural and chemical features of functional and naturally occurring materials.

Scope: The program spans a large variety of topics ranging from clean energy solutions and climate change remediation to heterogeneous catalysis, quantum science, and material engineering (*e.g.*, alloys formed by additive manufacturing, new H_2 storage materials, porous materials for nuclear radionuclide separation, or hybrid perovskites nanomaterials for 2D solar cells).

Strategy: The program thrives at delivering world-class x-ray capabilities for studying complex and heterogeneous materials. HXSS focuses on *in-situ*, operando & extreme environments studies, as well as at enabling high throughput and real-time observations. *In situ* and operando approaches are suited for tracking over time transient or metastable states along different synthesis or process pathways. The beamline portfolio of HXSS includes specialized spectroscopy, diffraction and imaging tools, supported by computational resources for high-throughput data analysis and modeling that also integrate Artificial Intelligence algorithms.

Advanced hard x-ray techniques such as high resolution spectroscopy (XAS, XRF, XES) and diffraction (XRD, SAXS, total scattering, reflectivity, pole figures, RIXS) are grouped in a portfolio of six beamlines: Beamline for Materials Measurement (6-BM), Quick X-ray Absorption and Scattering (7-BM), Inner Shell Spectroscopy (8-ID), High-energy Engineering X-ray Scattering (27-ID), Pair Distribution Function (28-ID-1), and X-ray Powder Diffraction (28-ID-2). We recognize that beamline automation is a key element to improve operation reliability and speed: several HXSS beamlines aim to develop robotic sample changers to increase throughput and enable remote data collection.

Science thrusts:

1. Thrust 1 is related to chemical sciences and relies on *in-situ*/operando characterization to understand the critical electronic and structural properties of the materials during or post chemical reactions on all relevant spatial and temporal scales.
2. Thrust 2 addresses fundamental and applied problems in materials science and engineering and focuses on the study of a variety of treatments and processes (*e.g.*, synthesis from the solid state, from the melt or in gas, doping, coating, high pressure, quenching, annealing, microwave assisted sintering, gas exposure). Atomic structures and microstructures are characterized, and the results are used to inform computational modeling.
3. Thrust 3 is to explore the structural origins of technologically important phenomena in quantum and/or strongly correlated materials, such as superconductivity, charge and spin density waves, frustrated magnetism, and colossal magnetoresistance.

FY23 Activities: To achieve its mission, the HXSS program pursues development in the following directions:

1. Improve beamlines' performance: i) deploy several photon-counting pixelated detectors for improved readout performances at ISS, PDF and XPD and combined operando XAS/XRD at QAS; ii) integrate an energy discriminating silicon drift detector into fly scan data acquisition at QAS; iii) upgrade the PDF side bounce monochromator for fast energy changeover; iv) develop and deploy the XPD analyzer crystal Laue optic for high resolution, high energy x-ray diffraction; v) upgrade the back-scattering analyzer spectrometer to a 5-five crystals array and commission the tender X-ray dispersive spectrometer at ISS.
2. Develop new in-situ/operando capabilities: The HXSS beamlines operate an extensive range of operando/*in situ* devices, *e.g*., potentiostats for battery and electrochemical research, reactors for catalysis and synthesis, residual gas analysis and gas chromatography, electrochemical cells, ALD reactor, furnaces

(resistive, radiative or electromagnetic heating) and cryostats. The high energy diffraction beamlines now include in their user program a 5T superconducting magnet coupled with a liquid He cryostat.

3. Implement multimodal approaches: In FY23 we plan to further develop i*n situ*/operando synchrotron x-ray experimental techniques and data analysis methods to offer new opportunities for in-depth studies of ion transport, electrochemical reactions, and phase transformations over multiple length and time scales. Pairing techniques such as FTIR/DRIFTS and UV-Vis spectroscopy, imaging, XAS, PDF, SAXS and DSC/XRD provides invaluable information on the evolution of complex materials under real-world conditions.
4. Develop and expand high-throughput measurement and analysis capabilities: leveraging their high flux and high-end capabilities, the HXSS beamlines strive at increasing their throughput, serving even more users and facilitating remote operations. Our capacity is often bottlenecked by current collection procedures and on-line analysis capabilities. Advanced automation and AI/ML methods are one major aspect of the solution to realizing effective high throughput operations. Several major efforts are being led by members of the HXSS team in that area, including development of automated analysis pipelines, AI driven optimized data collection, and improved data curation for multimodal measurements (*e.g.*, dealing with heterogeneous data streams from different instruments). This work is being done through a collection of LDRDs, BES funded initiatives, and personal research efforts of staff. Collectively, we are positioning ourselves as leaders in the field of AI-assisted beamline operations for the betterment of both our users and the greater scientific community.
5. Advance HEX construction and community outreach: HEX is meant to be a powerful addition to the HXSS program, augmenting the array of combined *in-situ* & operando studies of the next-generation battery materials for higher storage capacity, efficiency (more cycling and faster rates, lower cost), and sustainability (reducing degradation, extended lifetime, reduced environmental footprint). HEX will provide hard x-ray diffraction and imaging probes in the 30-200 keV range for studies of engineering materials under operating conditions. The central branchline is under construction (first light end of 2022), with affordances for 2 other side branches. In FY23, the HXSS program will continue to work with potential partners in NYS and other funding agencies to fund the HEX branch-lines. Through the partnership with NYSERDA, we aim to attract academic and industrial R&D groups in the fields of battery and advanced materials.
6. Enhance and facilitate external partnerships: HXSS thrives on the additional support from several sponsors and on successful, established collaborations with several consortia and universities:
    - BMM is part of a suite of three beamlines focused on material science applications in energy, health, environment, microelectronics, and national security, and is funded and operated by the National Institute of Standards and Technology (NIST). IBM participates in the operation of BMM through a CRADA with NIST.
    - a large volume, multi-anvil 1,100-ton hydraulic press enables measurements at extreme conditions (20GPa, 2000K), primarily for earth science and material science. This results from a partnership with the COnsortium for Materials Properties Research in Earth Sciences (COMPRES) and the Mineral Research Institute of Stony Brook University.
    - under a partnership with Idaho's Nuclear Science User Facility and Brookhaven's Nuclear Science Department, a combined imaging/diffraction equipment is being integrated into the user program of the XPD beamline. It enables 2D or 3D reconstructions of sample morphology directly from diffraction with 30×20 µm2 spatial resolution and full-field (2×2 mm2) X-ray radiography. This equipment is available for General User Operations in FY23.
    - HEX beamline is nearing the end of construction and is being funded in a large part by New York State Energy Research and Development Association (NYSERDA).
    - PDF beamline's combined program with NOMAD beamline at Oak Ridge's Spallation Neutron Source (SNS) provides complementary neutron and x-ray PDF data to general users. A joint SNS/NSLS-II "Total Scattering Analysis" school is conducted annually.
    - ExxonMobil Research & Engineering and the ISS beamline group lead a collaborative program that focuses on bimetallic catalysis and metal organic frameworks and promotes catalysis research at ISS.
    - The Synchrotron Catalysis Consortium (SCC) and the QAS beamline group lead a joined effort aimed at the development of the catalysis science at QAS, including heterogeneous catalysis and electrochemical catalysis.

- Thanks to the collaboration with the University of Columbia, a vibrant PDF user program and community have been developed at XPD and PDF, making them renowned and leading, total x-ray scattering facilities.

Complex Scattering

Mission: The Complex Scattering (CS) program's mission is to develop cutting-edge x-ray scattering techniques to advance scientific understanding of the spatiotemporal behavior of complex soft, hard, and bio materials to drive transformative discoveries by optimizing material synthesis and processing conditions as well as material behavior under extreme conditions for applications that impact the national health, energy and environmental security.

Strategy: To achieve our mission, the CS program offers advanced x-ray scattering capabilities for elucidating the complex structures and dynamics in modern materials and their evolution during non-equilibrium processes. We aim to contribute to advancing both fundamental and application-driven science, with an emphasis on: advanced manufacturing and synthesis, quantum materials, and energy science. Our high-level strategy consists of the following:

- **Advanced Manufacturing and Synthesis (AM)**. We will continue to strengthen the world-leading status of the CS program in the area of incoherent and coherent scattering methods applied to AM processes of polymeric and nanocomposite materials. Our near-term efforts will focus on: (i) development and multi-beamline integration of portable AM instrumentation for multimodal *in-situ/operando* studies based on X-ray and non-X-ray proxy/ancillary characterizations at the CHX, CMS, and SMI beamlines; (ii) integration of AI/ML methods in experimental and data workflows to provide prompt, adaptive feedback; and (iii) synergistic coordination with the complementary AM efforts on hard materials in the HXSS and IM programs. A long-term strategy is to engage and effectively serve manufacturing-driven research and development communities (*e.g.,* polymer processing/upcycling, film coating, nanomanufacturing) by constructing a new undulator beamline for coherent and incoherent scattering that is optimized for accommodating large industry-relevant set-ups for material processing, synthesis, and growth.
- **Quantum Materials (QM)**. Our near-term strategy is three-fold: (i) increase user engagement and scientific impact by leveraging recent and ongoing technical enhancements, including tender-energy resonant magnetic scattering and microbeam surface diffraction at ISR, inelastic scattering at IXS with enhanced counting efficiency (~13x gain since 2019), and resonant WAXS-XPCS at CHX; (ii) explore opportunities for multimodal studies of QM systems between beamlines in the CS and SXSS programs; and (iii) explore collaboration or partnership opportunities through engagement with C2QA, CMPMSD (*e.g.,* topological materials), CFN (*QPress* effort on 2D materials). A long-term strategy is to construct a 3PW-based diffraction and reflectivity beamline that will facilitate high-throughput and rapid-access experiments on single crystals and thin-film structures. Such a beamline is expected to greatly enhance the utility of more specialized, cutting-edge experiments on QMs at other beamlines in the CS and SXSS programs, as well as address the needs of other research fields such as microelectronics, geoscience, and materials for energy applications.
- **Energy Sciences**. *In-situ* and high-throughput characterization of material structure across scales is essential to underpinning the composition-processing-structure-property-performance relations for novel materials of technological interest. Our strengths in probing nanoscale morphological order in bulk and thin films and atomic- to molecular-scale ordering at interfaces allow users to study a diverse array of material systems for energy applications, including thin films for solar cells (perovskites, OPV), polymeric water-purification and ion-exchange membranes for hydrogen generation, polymer nanocomposite films for selective gas capture (including CO2), electrode and electrolyte materials for next-generation batteries, and interfaces of molten salts for reactor applications. In the short term, we will: (i) enhance the length-scale access from ~200 nm to a few microns by developing the capabilities for USAXS at SMI and submicron-beam SAXS at ISR; (ii) increase contribution to multimodal studies at NSLS-II; and (iii) explore collaboration or partnership opportunities in clean energy through engagement with other beamline programs, BNL/EPSD, SBU, and external institutions. A long-term strategy is to complement the soft and tender resonant scattering programs at the SMI and SST-1 beamlines by constructing a 3PW-based STXM beamline that will facilitate the nanoscale compositional and morphological characterization of soft-matter systems for energy applications.

FY23 Activities

I. Advance Existing Forefront Science and Technology Research

- **Advanced Manufacturing**
  - Establish portable integration and use of the large-format, multiple-printhead, 3D printing platform on CHX, CMS, SMI, and the new Additive Manufacturing Lab, and of the CFN-contributed wide-area CMS WAXS detector on CHX and the SMI-OPLS.
  - Develop simultaneous, multimodal x-ray and non-x-ray *in situ* characterization capabilities for studies of materials under processing and material testing/response conditions (e.g., optical spectroscopy for nanoparticle assembly, tensile/shear stress/strain, differential scanning calorimetry, high-temperature / high-throughput characterizations for polymers and liquid crystals).
  - Procure and start installing a multi-axis robotic arm in the CMS open sample area.
  - Complete the construction and start the operation of the new Additive Manufacturing Lab.
- **Soft Matter (SMI-SWAXS): tender and hard x-rays**
  - Tender: Continue developing *in situ* sample environments for tender x-rays beyond commercially available in-vacuum stages (also used for hard x-rays) with the focus on solution flow scattering capability compatible with SST-1 and in-vacuum humidity environment. Continue modifying and streamlining custom-made data treatment protocols developed in collaboration with a few selected user groups in the prior years to make it routinely available for all tender x-rays user groups as a part of SMI_analysis package.
  - Hard: Finish the installation of the extension of the SMI SAXS pipe to allow measurements into the USAXS region. Streamline the implementation of the existing analysis tools so the users can use it without being Python experts; integrate both in-vacuum WAXS detectors into the WAXS scattering map stitching code.
- **Liquid Surfaces (SMI-OPLS)**
  - Continue to improve operations and instrument alignment efficiency (8-23 keV) with simplified Bluesky macros with smart, auto alignment features. (High throughput essential to accommodate additional users during the APS dark period.) Develop universal, automatic attenuator codes for reflectivity measurements. Commission and implement Bluesky control for a Langmuir Trough with BNL built environmental chamber. Improve, extend and automate Jupyter Notebooks for data crunching for all 3 detectors along with reflectivity analysis support using Refnx. Initiate the first processing measurements. Install Diamond CRLs to improve vertical focusing.
- **AI/ML**
  - Extend autonomous experiments to not only steer characterizations but also control material processing on the fly (e.g., blade coating, 3D printing, rapid thermal annealing) to optimize structural formation kinetics and ordering at the nanoscale. Incorporate expert physical knowledge into decision-making algorithms to enhance autonomous experiments.
  - Use AI/ML approaches to enable real-time analysis of XPCS measurements of nonequilibrium dynamics.
- **Phononics (IXS)**
  - Capitalize the recent 13x improvement in counting efficiency of the IXS to further develop user science on soft matter research and explore expanding the science areas to hard condensed matter systems that benefit from the moderate operation energy of the beamline, especially systems of reduced dimensionality such as surfaces, interfaces and thin films.
  - Implement upgrades to enhance alignment and orientation capabilities of single-crystal samples of quantum materials at ambient and at low temperatures of the meV-IXS spectrometer. Explore the enhanced surface sensitivity of the IXS beamline for studies of topological phonons in quantum materials.
- **Quantum Systems (ISR)**
  - Commission new capabilities for polarization control of the incident beam at ISR for studies of electronic order in quantum materials; add sample environments for hard x-ray scattering experiments: high temperature, variable atmosphere; low temperature, moderate magnetic field, and high-pressure.
- **Materials Growth (ISR)**
  - Enhance capabilities on ISR for in-situ studies of materials growth and processing with the availability of hazardous gases, optimized secondary focusing, and coherent scattering during growth

II. Expand Program into New Forefront Science and Technology Research

- **Quantum Entanglement and Domain Dynamics (CHX)**
  - Continue to develop the DOE-BER funded project on the use of quantum entanglement and other non-local correlations in scattering experiments for reducing the illumination dose on sensitive samples and enabling otherwise impossible coherent scattering experiments on soft and biological materials.
  - Integrate a new *Timepix* detector at the CHX beamline for a 2x enhancement of the optical contrast and a time resolution of 2 ns for studies of phase fluctuations in quantum materials using coherent-WAXS and other fast XPCS approaches.
  - Fabricate kinoform focusing optics for resonant coherent x-ray scattering to study phase fluctuations in quantum materials.
- **Microelectronics**
  - Explore interest in the laser spike annealing technique for local defect healing, which provides dramatic thermal gradient enhancements over the traditional rapid thermal annealing approach.
  - Working with the NSLS-II/APS Diffraction Software User Group and DSSI, develop diffraction software for the *Bluesky* environment necessary for efficient reciprocal lattice mapping using an area detector.
- **2D Van der Waals Materials and Devices (ISR)**
  - Develop experimental methods to study 2D Van-der-Waals materials, such as monolayers of WSe2, graphene and similar materials. An emphasis will be on beamline configurations that will allow users to obtain diffraction patterns from functional electronic devices fabricated from stacked layers and twisted bi-layers of these 2D materials. Beamline configurations to be evaluated will include the choice of beam focusing schemes and the type of diffractometer hardware, sample chamber environment, and window materials.
- **Microbeam SAXS (ISR)**
  - Commission a small, ~200 nm beam, endstation on ISR for hard x-ray scattering in transmission SAXS geometry.
- **Clean Energy**
  - Increase outreach and user recruitment to expand the scattering user base and collaborations in the area of carbon capture (e.g., nanocomposite membranes), hydrogen production (e.g., water purification and ion-exchange membranes) and storage (with HXSS program, CFN, ISD).
  - Actively explore opportunities to join relevant initiatives (e.g., calls expected for DOE hydrogen hubs and Energy Earthshot Research Centers (EERC)).

Imaging and Microscopy

Mission: The imaging and microscopy program is committed to developing cutting-edge x-ray imaging and microscopy techniques and offering them for diverse scientific applications. In recognition of broad scientific needs, emphasis is placed on providing a suite of tools with multiscale and multimodal capabilities, while taking inherent advantages of x-rays for generating imaging contrasts.

Strategy: Three primary thrusts define the strategic directions in the imaging and microscopy program. The *first* is achieving and maintaining worldwide leadership and competitiveness. This goal provides a natural strategic path for FXI, which has world-leading nanoscale imaging throughput (~10X faster than the current competitors), and HXN, which provides multimodal imaging capabilities with a spot size down to ~10 nm. It is critical to ensure that these beamlines retain worldwide leadership. Construction of the CDI and SXN beamlines in NEXT-II also fits into this strategic thrust.

The *second* is attracting targeted scientific communities to establish substantial capabilities at the NSLS-II that will result in continuing growth and competitiveness. One obvious area of growth, well-aligned to NSLS-II as a medium energy storage ring, is bio-environmental imaging. There is a strong growth potential by strengthening the research areas that are aligned with DOE-BER mission science and attracting additional funding for developing new capabilities at NSLS-II, such as a Bio-Environmental STXM (BEST). Another growth area is to enhance in-situ/operando full-field imaging at a micron resolution. While a number of scientific communities are moving aggressively toward in-situ/operando research to examine material structure and properties over wider length scales (nanometers to centimeters), NSLS-II presently lacks a micron-scale full-field imaging capability that can work effectively with the existing imaging capabilities over the comparable energy range. This is a long-term goal of the Imaging and Microscopy program. It is also important to point out that microelectronic research is becoming an important science area for DOE and other US funding agencies, where NSLS-II's current (FXI and HXN) and near-future (CDI) capabilities offer tremendous opportunities. The ultimate goal is to build sufficient interest and justification for the construction of one or more beamlines specialized for microelectronic research.

The *third* thrust is targeted investment in enhancements of the existing capabilities, including beamline instrumentation and further developing end-to-end data analysis workflow. These strategic thrusts and approaches are summarized in Table 1.

Table 1: High-level strategic thrusts and approaches for the Imaging and Microscopy Program

Thrusts	**Approaches**
Achieving & maintaining worldwide leadership	• Continuing development of 5 nm-resolution imaging using MLLs and incorporation of the developed capability into the HXN user instrument. • Enhancement of in-situ 3D imaging at FXI, including diverse in-situ environments, larger probing volumes, and higher resolutions. • Completion of the CDI and SXN beamlines
Attracting targeted scientific communities	• Targeted outreach for biological and environmental science communities to attract substantial investment from DOE-BER or relevant funding agencies, building the case for a Bio-Environmental STXM • Development of a micro-CT beamline operating in 8-30 keV range optimized for in-situ/operando 3D imaging, filling a critically important imaging capability gap. • Development of HXN-II beamline, optimized for strain imaging, ptychography, and projection imaging, complementing the existing imaging capabilities at NSLS-II. • Explore scientific opportunities for tender x-ray imaging and build up a scientific argument for tender x-ray nanoprobe, which effectively exploits the NSLS-II's source property. • Aggressive exploration for growth opportunities for microelectronics research with a goal of building beamlines optimized for microelectronic imaging.
Enhancement of existing capabilities	• Allocation of resources for enhancing data analysis, including the incorporation of the end-to-end data analysis pipeline, machine-learning algorithms, high-speed computation, user-friendly interfaces, and portability of the analyzed data. • Enhancement of nanoscale imaging capability at SRX, bridging the current resolution gap between HXN/FXI and XFM/TES. • Enhancement of the TES capabilities, strengthening in-situ/operando and robust imaging/spectroscopy, and extending the lower energy limit to below 2 keV. • Continuing development of pink-beam based high-throughput imaging at XFM. • Allocation of resources for modernizing fly-scanning capabilities to achieve photo-limited data collection. • Enhancement of nanoscale imaging capabilities at FXI and HXN for higher scientific productivity.

FY23 Activities

Strengthening the microelectronic research capabilities: Here, a two-pronged approach will be used. First, the FXI staff collaborates with DMEA on extending the FXI's IC imaging capability. Significant progress is made in speeding up the data collation and transferring data from NSLS-II to DMEA, supporting near real-time tomography measurements. This project resulted in demonstrating comparing the measured data with the design file, with a goal of detecting the discrepancy of the 3D structure of IC from the design file. Second, the HXN staff continues to collaborate with IBM in performing ultra-high resolution imaging of the gate-all-round (GAA) and non-volatile memory devices. The initial research on strain imaging on nanosheets within the GAA is published (Murray et. al., "Mapping of the mechanical response in Si/SiGe nanosheet device geometries", *Commun Eng, 1 (2022). doi: 10.1038/s44172-022-00011-w*). A postdoc, supported by the BNL Program Development Fund, was hired in FY22 and is spearheading the development of faster and more robust 3D imaging capability for microelectronics research.

Strengthening bioenvironmental research capabilities**:** Several projects are underway to strengthen bio-environmental research at NSLS-II -- sponsored in part by DOE-BER as TR&D (Technology Research and Development) Projects. These include 1) development of cryo-XRF imaging capability, 2) development of user-friendly tools for multimodal image visualization and quantitative analysis, and 3) development of long-working-distance confocal-XRF (cXRF) imaging/spectroscopy. Development of cryo-XRF capabilities remains a core thrust for Bio-imaging and substantial efforts were dedicated to evaluation (i.e. simulations, benchtop testing, beamline testing) of a gas-cooling scheme ("cryostream") as an alternative to the conductive-cooling scheme used now, which is not easily amendable to 3-D imaging like the "cryostream"; a new Oxford cryostream system has been purchased for the program. Significant progress is made for developing the user-friendly data analysis tool (XMIDAS), which is described in the next section. On the other hand, the cXRF development is considerably slowed down due to Covid and a delay by Sigray Inc. in delivering an enhanced capillary optics (from double paraboloid to ellipsoid configuration with ~2 micron resolution). However, a new full-time research scientist/microscopist, Dr. Tiffany Victor, was hired to strengthen the Bio-imaging effort and to facilitate effective collaboration with the Biology and Environmental Division. Following extensive discussions with BNL plant biologists (and others from the Bio-imaging user community) about research needs and aspirations for X-ray imaging at NSLS-II, AttoMap, a laboratory based XRF imaging instrument, will be procured. This instrument will increase sample throughput for Bio-imaging by allowing researchers to perform work offline that would otherwise need performed at the beamline such as: establishing sample preparation and mounting techniques, prescreening samples prior to a synchrotron run, genotype/phenotype screening with replication that would be impractical on beamlines, identification of sample regions of interest to target for high-resolution imaging, hypothesis testing and more. The unique opportunity to leverage inhouse expertise (Plant Science and X-ray Microscopy) and novel instrumentation (XRF system) will lead to new methods for Bio-imaging users, open new doors for BER researchers, and enable cutting-edge "Systems Science" at BNL/NSLS-II.

Development of the CDI beamline: The Coherent Diffractive Imaging (CDI) beamline is a component of the NEXT-II Major Item of Equipment (MIE) project, funded through the DOE Office of Science, and is currently under construction. The beamline will provide a state-of-the-art coherent, lens-less imaging capability to the Program. Operating predominately in the Bragg geometry, the beamline will be used to investigate probe nanoscale structure and deformation in materials. Contracts have been awarded for the photon delivery system and the construction of the satellite building, which will house the experimental end station. In FY23, we will begin procurement of the major components of the endstation and hold the final design review for the photon delivery system. The CDI beamline is on track to meet its projected commissioning in 2025.

Enhancing data visualization and analysis**:** The imaging and microscopy program continues to make excellent progress in enhancing data visualization and analysis. Two different, yet coordinated, approaches are adopted. The resources from the Bio-Imaging Core under the CMBS (Center for BioMolecular Structure) are directed to completing a new data analysis software called NSLS-II XMIDAS (X-ray Multimodal Imaging Data Analysis Software). This project is spearheaded by Ajith Pattammattel in collaboration with DSSI researchers, Xiaogang Yang, and Dmitri Gavrilov. The software's source code is now published in GITHUB (https://github.com/NSLS-II/xmidas). A compiled version distributed through PyPy and conda-forge (https://anaconda.org/conda-forge/xmidas) with comprehensive documentation. A manuscript summarizing its scientific applications, "Multimodal X-ray Nano-Spectromicroscopy Analysis of Chemically Heterogeneous Systems" by Pattammattel *et al.*, is currently under revision for publication at Metallomics. In June 2022, we had a tutorial session with the APS beamline scientists and the software developer, demonstrating the detailed feature and establishing collaboration in widening the user base for XMIDAS. The second approach is to continue developing and deploying Tomviz (https://tomviz.org/), an open-source software for 3D tomography. The efforts aims to enable a workflow including the data processing, tomographic reconstruction and 3D visualization that is integrated with the NSLS-II data infrastructure. The efforts have been coordinated by K. Chen-Wiegart across the imaging and microscopy program to collaborate very closely with beamline scientists at FXI and HXN beamlines (M. Ge, A. Pattammattel, and X. Huang), under a full support of DSSI (led by M. Hanwell in coordination with S. Campbell, D. Allan and D Gavrilov). Part of the efforts have been contracted to Kitware Inc., a service-based small business based in upstate NY. The initial efforts are currently under testing at FXI and HXN beamlines. We expect to fully deploy the software at these two beamlines in early FY23 and to gather feedback from beamline staff and users to keep on developing and further enhancing the functionalities of the software, as well as to discuss the best approach to apply the software to other imaging beamlines.

Nano-imaging capability at SRX: The nano-KB endstation at SRX is commissioned and available for general users. The initial commissioning results is published in JSR, 29 (2022), doi.org/10.1107/S1600577522007056. A hyperspectral tomography project is being pursued in collaboration with DSSI using the tomography capability of this new endstation. Leveraging advanced reconstruction algorithms and AI/ML methods, this project aims to optimize the tomography data collection using on-the-fly reconstructions to inform running scans. The technical developments for this are commissioned with autonomous and AI-guided experiments planned for FY23. Further improving our nanopositioning by integrating laser interferometers and enabling "zero circle of confusion error" is actively in development and is expected to complete in FY23.

Nano-XANES capability at HXN: A new vertical mirror system, funded by the FIP (Facility Improvement Project), is now installed and commissioned at HXN. This new instrument will become the backbone of the HXN's Nano-XANES capability. In addition, Ajith Pattammattel is recruited as the HXN beamline scientist, leading the growth of Nano-XANES user program at HXN and exploring opportunities for growing this technique as a multi-scale tool bridging the nano and micro scale. XMIDAS will become the primary data analysis tool for the Nano-XANES research at HXN.

High-energy extension at FXI**:** Funded through a FIP, high-energy optics will be installed at FXI. This improvement will increase the energy range up to 15 keV (covering absorption edges of important elements such as As, Se, and Br) and increase the probing volume of the sample. The high-energy TXM will provide the nanoscale imaging capability on length scales up to hundreds of micrometers at a spatial resolution ~100 nm. This new capability will have a great impact on investigating complex 3D hierarchical structures under various in-situ conditions, resulting in significant synergy with other imaging and microscopy beamlines at NSLS-II. The FXI team, in collaboration with DSSI, is expecting complete the tasks in FY 23.

Operando high-throughput tender XAS endstation: Funded through a FIP, this new endstation at the TES beamline will enable world-leading *operando* XAS studies of battery, catalyst, and molten salt samples in tender x-ray range. The TES team experienced unexpected delay due to recent issue with the supply chain disruption, which created a significant price increase for the endstation. The team issued a modified tender to mitigate the price increase. A vendor that can work within the allocated budget is selected. The endstation will be delivered in FY23.

Photon delivery system upgrade plan at TES: The TES beamline is experiencing explosive growth in user demand because of the emerging interests in broad scientific areas, including energy storage, catalysis, material science, bio-environmental science, and microelectronics. The oversubscription rate of the TES beamline has been steadily increasing over the past three years, leading to an increased number of high-impact publications. However, a number of outdated components in the photon delivery system makes it extremely challenging to provide robust user operation in a sustainable manner and to achieve its full potential. In addition, the current endstation is inadequate for delivering exciting in-situ capabilities. In FY23, we will develop a facility improvement project to describe an upgrade plan for the TES beamline, with the objective to modernize beamline components and develop robust in-situ capabilities for the user community. This plan will aim to achieve the following scientific goals: (a) enabling micro-spectroscopy from Si K-edge (for microelectronics) to Ni K-edge (important for catalysis and clean energy), (b) enabling higher detection sensitivity and higher throughput by ~10X increase in focused photon flux, (c) enabling in-situ experiments for energy materials and clean energy science, and (d) enabling autonomous experiments with reliable motion controls, and data acquisition and analysis.

Development of Enhanced ptychography imaging at HXN: This development path is based on two FIP projects on an Advanced ptychography instrument by Evgeny Nazaretski and a new Eiger detector by Xiaojing Huang. The new microscope is expected to achieve the state-of-the-art 2 kHz frame rate with multi-modal 3D imaging capability. This instrument provides real-time 3D position monitoring through a novel laser interferometer system, which offers an opportunity to develop a new way of 3D ptychographical tomography by optimizing the data acquisition efficiency using the volumetric overlapping to relax the transverse overlaps on each projection as in the conventional approach. Basic controls for instruments are in on-progress. 2D on-the-fly scans were executed without triggering detectors. The follow-up works on data acquisition with multiple detectors, realizing ~2 kHz frame rate, and X-ray commissioning will be conducted in FY23.

***Exploring funding opportunities for BEST*:** Significant efforts on community outreach have taken place to explore possible external funding for BEST (Bio-Environmental STXM). During a planning meeting at BNL, the bio-environmental science community outlined the necessary specifications of a next-generation STXM. Especially, in the field of atmospheric research, the need for an STXM at NSLS-II became obvious, and key players in the field expressed a strong scientific drive to use an STXM for that research. A workshop at this year's NSLS-II Users Meeting underlined this desire. The current strategy is to secure funding for an endstation microscope, potentially to be installed as the second endstation at the Soft X-ray Nanoprobe (SXN) beamline, currently being constructed as a part of the NEXT-II project. Funding opportunities are being explored in collaboration with the Department for Environmental and Climate Sciences of BNL and Stony Brook University.

Structural Biology

Mission: Our mission is to develop instruments and methods to understand how macromolecules are structured at the atomic level, and how they are organized in biological cells to conduct specific processes.

Strategy: To achieve our mission, we combine macromolecular crystallography, small-angle X-ray scattering, cryo-electron microscopy and tomography, X-ray imaging, and the computing approaches to tackle grand challenge science questions in molecular and cell biology.

The beamline groups within the structural biology program are funded through a number of sources (NIH/NIGMS, DOE-BER, AFRL, Case Western Reserve and NYSBC), enabling an international community of structural biologists' access to, and support for the use of, world-class beamlines for synchrotron x-ray footprinting, macromolecular crystallography, and x-ray scattering.

FY23 Activities

There are two common themes in the strategic activities to be undertaken by the structural biology program in FY23. The themes are designed to strengthen our current position while enabling growth of biological research for the longer term as recorded elsewhere in the document. The FY23 work being the continued enhancement of the capabilities available on the beamlines, and to increase robustness of the automation processes in place. Our expectation is that this combination will allow the program to maintain its service role to a large and active community, while also allowing us to position our beamlines at the forefront of the bio-physical techniques that we have.

Improving reliability of performance with increased levels of automation: In a little more detail, continuing to improve the reliability of performance, add new features and through increased automation of the elements of the processes allowing experiments to be performed: this activity is common to all the beamlines. In a related development we will couple the beamline measurements to the new NSLS-II data infrastructure, allowing for faster and more secure data analysis and distribution to researchers' home institutions.

Macromolecular Crystallography: To improve the performance of the macromolecular crystallography beamlines we have selected several projects that will streamline key processes, including flexible scheduling with mini shifts, overnight fully automated data collection, and automatic energy changes. To improve the science output aiding multi-crystal crystallographic data sets, as are increasingly common, we plan to improve and make available software for data analysis and merging for the creation of optimal data sets. As a further example of the developments, we intend to make links to alphafold2 and RoseTTAFold to further our *de-novo* structure determination portfolio. To enable studies of protein dynamics and data collection at ambient temperature, we will establish room temperature and multi crystal sample handling, along with optimized processing.

Solution Scattering: We are trying to provide solution scattering users with more data analysis options. We will be working on multimodal HPLC data analysis, combining x-ray scattering with multiwavelength UV absorption and Multi-Angle Light Scattering (MALS) data. This is based on preliminary work using iterative Multivariant Component Resolution (MCR) with our collaborators at the CFN. With the help from a LDRD project and the current effort by DSSI to introduce workflow software to beamlines, we will make advanced data analysis such as scattering data-driven molecular dynamics simulations and ensemble modeling, available to beamline staff and users. In the area of scanning mapping and imaging, we will work on automation to better support mail-in and remote measurements.

X-ray Footprinting: For the synchrotron X-ray footprinting effort, we intend to focus on enabling access to the full data acquisition and analysis workflow within NSLS-II, leveraging a nano-LC-MS instrument recently installed and commissioned by the XFP beamline team. We plan to enable seamless access to data from this instrument through the NSLS-II data infrastructure, and stand-up mass spectrometry data analysis resources for the NSLS-II user community. This will provide a complete platform for training and supporting X-ray footprinting users and will also facilitate use of this new resource as a complementary characterization method for other structural biology techniques available at NSLS-II.

Continued development of multimodal imaging and new beamline for soft X-ray cryo-tomography: We will continue to develop advanced methods for biological sample preparations for multi-scale and complimentary imaging techniques that may involve high resolution 4D light microscopy, cryo-X-ray tomography, and cryo-electron tomography (cryo-ET) workflow for multi-scale imaging. We will continue to work with the community and seek funding to develop a new soft X-ray cryo-tomography beamline dedicated to imaging of biological cells.

***Data integration in multiscale and multimodal imaging*:** The challenges we will overcome are manifold: data volume, data standardization, access to these data, provenance and versioning history, repeatability, and the algorithms to create the full picture. The scale of this endeavor is beyond the capacity of an individual PI's laboratory to support. Leveraging the LDRD funding thought BNL, we will develop a framework for multiscale, multimodal imaging data integration to respond to grand challenges.

Data Science

Data generation rates at the U.S. Department of Energy (DOE) Basic Energy Sciences' X-ray light sources are increasing rapidly. At NSLS-II, over 1 petabyte of raw data was produced last year, and that rate is expected to increase as the facility matures. Despite such huge data generation rates, approaches to both experimental control and data analysis have not kept pace. Consequently, data collected in seconds to minutes may take weeks to months of analysis to understand. Due to such limitations, knowledge extraction is often divorced from the measurement process. The lack of real-time feedback forces users into flying blind at the beamline, leading to missed opportunities, mistakes, and inefficient use of beamtime as a resource - as all beamlines are oversubscribed. This is a challenge facing nearly all users of light sources. One promising path forward to solve this challenge both during data collection and post-experiment analysis is the use of artificial intelligence (AI) and machine learning (ML) methods.

Our Vision: NSLS-II has been working closely with the other four DOE-BES light source facilities on data science and data infrastructure. Our vision in this area is to establish a transformative computational fabric that covers the full lifecycle of the data generated at the DOE light sources, including theory, simulation, experiment design, data generation, data analysis, and publication. This will also connect 200+ instruments at light sources with a multi-tiered computing landscape, including edge computing, high-performance computing centers, data repositories, and cloud computing. This will best serve the 10,000+ DOE light source users per year.

In regard to improving the data science and systems integration (DSSI) hardware and software stack at NSLS-II, the DSSI program has defined "tier-1" tasks as those taking 4 FTE-days or less, "tier 2" tasks as those taking up to 12 FTE-months and anything longer as "tier 3." All members of the DSSI program are expected to spend approximately 25% of their time on tier-1 tasks. At the start of FY23 there had been a concerted effort to "burn down" these tasks as tracked by Jira to allow staff to maintain this balance, spending ~50% of their time on tier -2,3 tasks. With the new hires that are underway ultimately on board, this will allow ~ 16 FTE years in the Photon Science Division for tier-2,3 work, corresponding to 2-3 such projects running simultaneously. These will be determined according to the priorities set by the Program Managers, Division Director and NSLS-II Director. Importantly, they will be planned with milestones and completion metrics before they are started and will be tracked to completion, with stakeholders being held accountable for any changes. The first such projects are expected to be underway by November 2022.

In this Section, we outline our recent developments and future directions employing AI/ML methods at the NSLS-II to tackle these data challenges. These activities cover the whole life cycle of an experiment, from improving daily beamline operation, accelerating the pace of data analysis, and even automating experimentation with advanced AI-driven feedback algorithms.

Improving Operations

Advanced data infrastructure: One foundational cornerstone to these developments is the common underlying Bluesky control system that spans NSLS-II beamlines, allowing development and deployment of AI/ML methods for both beamline control and data analysis in a streamlined and extensible fashion. Of note are recent developments of the Bluesky Queueserver and Tiled data access system. These developments are charting a new course for the Bluesky and Data Broker projects, respectively, where client-server architectures are now being developed to enable greater flexibility, extensibility, and reliability at beamlines. These developments offers far greater freedom for researchers to try new things, such as AI/ML agent-directed data acquisition and streaming data analysis.

Automated data guidance: One of the places AI/ML is finding use at the NSLS-II is streamlined operations, where the methods act like digital assistants to the human researchers by automating tedious or repetitive tasks. At NSLS-II's Beamline for Materials Measurement (BMM), a supervised learning model is used to make an initial evaluation of every X-ray Absorption Fine Structure (XAFS) spectrum as it is measured. The purpose of this evaluation is to distinguish measurements that look like XAFS spectra from failed measurements. A failed measurement might be due to network error, failure of a detector, or even something as prosaic as a poorly mounted sample falling from the beam.

Enhanced scanning probe imaging: At the Submicron Resolution X-ray Spectroscopy (SRX) beamline, pre-trained 3D convolutional neural networks (CNN) are being used to improve reconstruction methods and provide autonomous data acquisition for X-ray fluorescence imaging and mapping. XRF is a powerful way to spatially resolve the elemental distributions in materials. The fluorescent X-rays generate a hyper-spectral image, where individual element fluorescent lines can be identified simultaneously. Unlike full-field imaging techniques, in order to build up an image, the sample is rastered through a focused X-ray beam. For tomographic reconstructions, 2D images are collected at many different angles and assembled to form 3D tomographs. Advanced algorithms are being developed to use AI/ML methods to improve the reconstruction quality and data collection efficiency. This includes super-voxel model-based tomographic reconstruction algorithms that require fewer projections. Combining this with AI and adaptive scans will identify future projections that have the greatest impact on improving reconstruction quality, and decrease data collection time for hyperspectral and multi-element volumes.

Streaming Data Analysis

Phase transition detection: ML methods can automate many of the specialized analysis methods, often at speeds on par with the data generation rates. Unsupervised learning approaches are of particular interest, as they can grant model-free insights to researchers regardless of *a priori* knowledge. Non-negative matrix factorization (NMF) is an appealing class of methods for performing unsupervised learning on streaming spectral data. However, canonical NMF methods have no underlying requirement that the reconstruction uses components or weights that are representative of the true physical processes. By constraining a subset of the NMF weights or components as rigid priors, provided as known or assumed values, we can provide significant improvement in revealing true underlying phenomena in a method we refer to as Constrained Matrix Factorization (CMF).

<u>Classifying powder diffraction data</u>: AI package for analysis of crystallography companion agent (XCA) is being developed at NSLS-II. This is an open-source package initially developed for the feed forward classification of diffraction experiments. The classification approach is pseudo-unsupervised, in that it does not require labeled data to be trained. Instead, XCA simulates a realistic dataset that encompasses the perturbations and physics of the measurement. Starting only from proposed crystalline phases, XCA overcomes the challenge of degenerate solutions by training an ensemble of Convolutional Neural Network (CNN) agents that can accurately predict phase existence and uncertainty. The approach has been applied in searching organic porous materials for predicted phases, mapping a ternary alloy's phase diagram, and identifying the subtle phase changes in a ferroelectric material. To accompany the predictive model, XCA can also train a variational autoencoder (VAE), which provides insightful visualization of the experimental measurement . The latent space of a VAE and the reconstruction error can be monitored as proxies for distributional drift, alerting the user when an experiment is beyond the scope of the simulated data used to train an agent. The combination of the Shannon entropy of the output prediction from the CNN ensemble and the reconstruction error of a VAE trained with the same data serves as an explainable AI for identifying outliers and distributional drift.

<u>Automating XPCS analysis</u>: X-ray photon correlation spectroscopy (XPCS) performed at the Coherent Soft X-ray Scattering (CSX) beamline is used to quantitatively characterize sample dynamics. This method is based on X-ray speckle intensity correlations within a timeseries of coherent X-ray scattering images, typically using an ensemble approach. Robust, reliable real-time analysis is required to ensure maximal data and beamtime usage in both high-throughput and long duration experiments. Typical XPCS algorithms cannot distinguish sample dynamics and intensity changes induced by instrumental effects, adversely impacting result accuracy. AI/ML methods are ideally suited to aid users in real-time analysis of XPCS data because artifact-induced dynamics have recognizable patterns or signatures. At NSLS-II, we are developing models that are time, sample, and instrument agnostic using derived data and novel normalization schemes to detect artifacts, remove noise, and extract quantitative results with improved resolution for non-equilibrium dynamics.

Adaptive and Autonomous Measurements

<u>Axis of control requirements</u>: A promising application of AI/ML methods at large user research facilities is in enabling autonomous, or "self-driving," experiments. Discovery and optimization of modern materials require an ability to efficiently probe vast, multi-dimensional material and processing parameter spaces, going beyond intuitive or exhaustive high-throughput approaches. Efficient design of adaptive feedback systems can be considered along three axes: coordination motif, source of signal, and required timescale of the loop.

- The coordination motif describes how the experiment and the algorithm interact. In some applications, the algorithm needs to be synchronous "in-the-loop" of the experiment, while in other applications we may need to asynchronously couple the algorithm to the experiment.
- Source of signal describes the nature of the data being used in the feedback system. Often, the information that we want to feedback on can be classified as either engineering values or scientific values. Engineering values are raw machine measurements, such as motor positions or shutter states, and do not require any knowledge of the sample under study to interpret and act upon. Science signals are very tightly coupled to the current experiment and their interpretation is often context dependent.
- The final dimension of adaptive experiments is the required timescale for the feedback. For example, a control loop to maintain hardware alignment may need to run at sub-ms timescales whereas an algorithm to select the next sample to synthesize in a day-long reaction has a much larger time budget.

Each combination of communication motif, signal class, and timescale places considerations and restrictions and constraints on the sort of approaches that can be used for adaptive feedback. Selecting the right tools for a given task can be a critical consideration for successful deployment of such methods. Medium-speed, synchronous "in the loop" feedback on scientific values is the combination of these axes that is of the most interests to beamline operations, and we will now discuss two examples of this type.

Autonomous X-ray scattering experiments: At the Complex Materials Scattering (CMS) and Soft Matter Interfaces (SMI) beamlines at NSLS-II, a collaborative effort to enable intelligent material exploration during autonomous X-ray scattering experiments has been developed. The developed system consists of three key elements: automated sample handling and data acquisition, based on Bluesky; real-time data processing; and decision-making algorithms, which take processed data as input and select the next experimental point to be measured. The algorithms utilize Gaussian process regression in a Bayesian optimization framework, generating surrogate models and uncertainly distributions, using them to define an acquisition function for the given experimental objective, and locating its maximum to make the decision. This approach has been successfully applied to imaging heterogeneous materials and to materials parameter space exploration based on combinatorial sample libraries, combined with a robotic sample exchanger where appropriate to further expand the size of parameter space that can be explored in a given experiment.

Reinforcement learning driven high-throughput PDF measurements: An additional area of AI/ML being explored at the NSLS-II is the use of reinforcement learning (RL) being used to automate and optimize high-throughput data collection. Unlike supervised learning methods, where a very large, labeled set of data is employed to train, RL is trained via a dynamic interaction loop whereby the AI can learn "on-the-fly" as it is interacting with an environment. AI are trained with simulated experiments that recreate raw and processed data streams. It is important that the simulated environment encountered by the AI is sufficiently similar to the real-world data streams encountered at the beamline. In the initial deployment of the agent trained to run high-throughput diffraction experiments on the PDF beamline, a data quality metric is employed, which is calculated independently from the AI. Thus, the decision-making logic learned by the RL agent is more broadly generalized to any scenario, which can output a similar formatted data quality metric. By using this RL agent, the beamline was shown to be 100% more efficient at measuring critical structural information than standard iterative data collection plans.

Enabling Technology and Support Facilities

In addition to the beamline programs discussed in the previous chapter, we plan to pursue development in the following key enabling technology and operations areas in support of our strategy:

- *Accelerator science and technology* that is the foundation for stable and reliable operations and for enhancing the performance of NSLS-II accelerator systems,
- *Experimental development* in x-ray optics and detectors, in nano-positioning and engineering, and in experimental simulations that are required for innovative world-leading programs and to keep NSLS-II beamlines competitive,
- *Data infrastructure and support*, to enable and support new user access modalities and experimentation using advanced simulation, multi-modal experiments, and machine learning driven data analysis,
- *Operations excellence, facility infrastructure, and user services* that are all critically important for the success of the NSLS-II facility.

The development plans in these areas are discussed in this Chapter.

Accelerator Science and Technology

***Mature performance plan*:** NSLS-II was built with affordances such that it can ultimately operate reliably at 500 mA with emittances of 600/8 pm·rad in the horizontal and vertical planes, respectively. In line with these goals, the storage ring design included four RF systems, two third harmonic RF cavities for bunch stretching and a cryo plant of adequate capacity and redundancy. This complement of RF and cryo systems was planned be sufficient with a full build-out of insertion devices (i.e. a total radiated power of about 1 MW), to provide a sufficient electron beam lifetime and to cause only moderate wakefield heating of the ring chambers. Eight years after machine commissioning, the facility operates 5000 hours per year, delivering 400 mA with X/Y beam emittances of 800/30 pm·rad. The NSLS-II storage ring contains three cavities, supplying 0.4 MW of RF power after successful completion of the 3rd RF system in FY21.

Informed by our operating experience, we developed a plan on securing high reliability operations and reaching mature performance. The plan contains several work packages, listed below in priority order:

- Spare 500 MHz RF cryo module – underway and nearing completion
- Spares not in hand (critical priority) – completed in FY20
- 3rd RF system – completed in FY21
- Measures against power interruptions: a new project aiming to decrease impact from frequent power dips on the critical accelerator systems
- Spare cold box - funded in FY21
- Spares not in hand (intermediate priority)
- Injector and dipole power supplies
- Two third harmonic 1.5 GHz RF cavities
- Fourth 500 MHz RF system with RF cryo module and solid-state amplifier.

We note that, depending on the outcome from our ongoing studies of high operating current, we may start operating with 500 mA at the present vertical emittance in FY23. Our cost estimate for this plan is built from vendor quotes and an analysis of the systems that we have built and put into operations in the past several years. The cost profile will follow a tentative 10-year-long schedule as shown below.

version 5/6/2022: Work Packages	FY19	FY20	FY21	FY22	FY23	FY24	FY25	FY26	FY27	FY28	FY29	FY30
Spare 500 MHz RF Cryo Module (SPS)	■	■	■	■								
Spares not in hand (critical)	■	■	■	■								
850 W RF Cryo Plant (AIP)			■	■	■	■						
Measures against Power Interruptions						■						
Spares not in hand (intermediate)					■	■	■	■				float
Injector and Dipole PS (AIP)						■	■					
2 Third Harmonic 1.5 GHz RF Cavities (AIP)						■	■	■	■			
4th 500 MHz RF System with RF Cryo Module and Solid-State Amplifier (AIP)									■	■	■	

The schedule is designed to achieve 500 mA performance at the earliest possible date and is driven by the estimates we received from vendors (Linde, Toshiba, RI, etc.), as well as by the timelines of the manufacturing and assembly sequences developed in-house. To address potential delays with delivery of complex systems by industry and the risks of failures during acceptance testing of cryogenic equipment, we added one year of float to the schedule. This is based on our analysis of risks associated with long lead time items and the discrete nature of the available shutdowns for installation. We are targeting early completion of the entire plan by September 2030, though actual timeline is contingent on yearly funds.

Accelerator R&D: NSLS-II accelerator physicists provide scientific support of facility operations and work on further improvements of machine performance and reliability. A list of major projects and activities related to the NSLS-II operation and developments includes:

- Common tools program on development shared high level applications; online optimization of injector and storage ring performance
- Studies of beam dynamics with three main RF cavities and 3rd harmonic cavities for bunch lengthening
- High current studies: towards routine operations with 500mA, comparison of beam-induced heating with physical models
- Routine lattice characterization and improvement of the nonlinear machine model
- Enabling high-chromaticity operation mode
- Improvement of orbit feedbacks including bandwidth control, long-term drift suppression, development of interface software tools.
- Development of the new operation mode with a high single-bunch current for time-resolved experiments: studies of beam-induced heating and bunch lengthening.

In parallel with the facility support and development, the NSLS-II team will continue actively working on several research and development projects benefitting light source physics and engineering at large and including the following that are essential for the future NSLS-II upgrade.

- Lattice development (TBA, MBA, Complex Bend); optics correction, optimization of nonlinear beam dynamics; lattice and magnet specifications; magnet tolerances.
- Beam-induced heating: radiation; coherent beam energy loss; gap and length limitations for insertion devices.
- Longitudinal beam dynamics and RF specifications: main RF system and harmonic cavities for bunch lengthening under the constraints of low-alpha ring lattices.
- Collective effects: single-bunch and multi-bunch instabilities, intra-beam scattering, ion-driven effects and their impact on the beam lifetime.
- BPM electronics: NSLS-II is developing a new generation of in-house Radio-Frequency Beam Position Monitor (RF BPM) receivers, incorporating the latest technology available in the RF, digital, and software domains.
- Instrumentation front end is being developed to perform R&D in light source engineering and metrology with high power X-ray beams.
- Insertion device (ID) development: our research on IDs is focused on maximizing the brightness and flux of synchrotron radiation in a broad spectral range for user experiments.
- Timing modes: seven NSLS-II beamlines have explored the potential timing-based experiments, which will be enabled by developing and testing flexible bunch patterns in the storage ring current and tight synchronization of these with the beamline detectors.

Work for others (WFO): NSLS-II Accelerator Division (AD) engages in WFO for several reasons. First, it keeps the AD stuff involved in cutting edge instrumentation, of direct benefit to the staff and to the facility. Second, it provides the staff involved a venue to be seen outside of NSLS-II, which is beneficial for career development. Third, the funding it brings in allows us to support a larger staff size than would otherwise be possible, increasing the bench depth and skill set, which is beneficial to the operations of the facility.

AD is supporting upgrade projects at the other DOE light source facilities: APS-U (ANL), ALS-U (LBNL), and LCLS-II (SLAC). This WFO serves the Division well in developing & upgrading NSLS-II instrumentation and positioning us as the provider of choice in the light source business. Under several MOUs, the Accelerator Physics group also makes a significant contribution to the Electron-Ion Collider R&D at BNL.

In engaging in all these activities, work is carefully balanced such that operation of NSLS-II is not compromised.

Exploring NSLS-II upgrade options: NSLS-II is in its eighth year of operations. To keep NSLS-II competitive for the next decade, we have started to explore upgrade options for our facility in the future. After some early discussions, in FY22 we started exploring four possible scenarios to understand the available phase space for an upgrade, with all options using the existing building infrastructure. These four scenarios include (a) medium-scale upgrade that would result in incremental improvements in brightness, (b) high-flux upgrade with 2 Amp current and 100 pm-rad horizontal emittance, (c) low-emittance upgrade with 500 mA current and 20 pm-rad horizontal emittance, and (d) high-energy upgrade with potential 4 GeV, 500 mA, and 35 pm-rad horizontal emittance.

After substantial studies in FY21, we have made the decision not to pursue the 2 Amp high-flux option. This conclusion is based on the heat load challenges on accelerator and beamline components as well as the RF power requirements that would take the valuable straight sections away from the user program. We will continue to evaluate the option to operate the accelerator systems for higher-current (>500 mA) in combination with the other more viable upgrade options. In addition, we have also made the decision not to pursue a medium-scale upgrade as its increase in photon brightness and thus to the overall science program at NSLS-II would only be 2-3x, therefore not worthwhile to pursue.

In FY23, we will continue to assess the remaining upgrade options with a goal to better understand the overall performance gain in 1-12 keV photon energy range with machine parameters in the e-beam phase space defined by higher energy (>3 GeV), low-emittance (improvement of ε_x by >20x), and higher beam current (>500 mA). Our goal is to converge on a firm plan for the future upgrade with the optimal beam emittance and current, and consequently brightness and spectral flux of synchrotron radiation from the optimized IDs. The machine lattice that is being considered is based on the novel concept of Complex Bend Achromat (CBA), developed by the NSLS-II accelerator physicists [G. Wang *et al.*, PRAB **21**, 100703 (2018); G. Wang *et al.*, PRAB **22**, 110703 (2019)]. Furthermore, we plan to continue to study future directions in the Insertion Devices for the upgraded NSLS-II, including IPMU, SCU, and tandem undulator configurations for high-brightness beamlines.

To date, the development of the CBA lattice concept has been supported by two LDRDs from BNL. This funding is not sufficient to develop prototype lattice hardware components for CBA. We plan to work with BES to seek support of the required R&D activities to demonstrate the feasibility of the novel CBA concept. With additional support, R&D for the future of NSLS-II will continue to ramp-up in FY23 and beyond.

Experimental Development

In this Experimental Development section, we discuss facility supported R&D program as integral part of the NSLS-II operations. The role of the R&D program is to support and foster NSLS-II leadership in the field of synchrotron science and technology, and to develop new X-ray technologies that are needed to better serve the broader scientific community. The scope of the R&D program is primarily focused on detectors development, optical metrology, development of advanced x-ray mirrors and nanofocusing optics, precision engineering and nanopositioning, as well as experimental simulations. In addition, the Experimental Development Program works with beamline staff to develop a beamline recapitalization plan to keep the NSLS-II beamlines capabilities up to date. Activities planned in FY23 and beyond include the following.

X-ray Detectors R&D:

HERA, an upgrade of the Maia detector to improve throughput and energy resolution: Maia was a many-element spectroscopy detector based on simple diode sensors and a low-noise ASIC developed by BNL's Instrumentation Division. Hera will adopt SDD sensors, but with the same degree of parallelism and an improved ASIC, to yield better energy resolution and higher throughput. The prototype has 96 SDDs in a monolithic array. Initial testing shows the expected improvement in energy resolution, with 95 of the 96 showing similar performance. In the coming year we will refine the designs and implement a full 384-element detector. We will also use the prototype on select beamlines to validate its performance.

Germanium strip detectors for high-energy spectroscopy and diffraction: We are now able to provide these detectors routinely. We have all the required capability in-house. A detector for energy-dispersive high-energy diffraction to be deployed at the new HEX beamline has been delivered. We have had a request from the Australian Synchrotron for a copy of this detector, bringing up to four the number of copies in the field.

Ge drift detectors: In collaboration with Dr. T. Krings at Forschungszentrum Julich, we are developing the germanium equivalent of the SDD, which will allow large area, very low noise Ge detectors to be built. COVID has significantly slowed down this effort, but we expect to have the first sensor soon. We will read it out using a commercial single-channel ASIC (the Cube) preamplifier.

Imaging detectors with energy-resolution or time-resolution per pixel*:* We have begun two projects to develop imaging detectors in which every pixel in the array is a spectrometer. The two detectors will be very similar, except for the sensor used. One (FFFI) will use silicon sensors, while the other (GALAHAD) will use germanium. The former is funded by DOE-BER, the latter by DOE-BES through separate FWPs. Both will have 100um pixels and high energy resolution. Sensors for both detectors have been produced. We are currently waiting on the completion of an ASIC design for them, which is being done by our Instrumentation Division collaborators.

VIPIC detector for XPCS experiments*:* Based on the most advanced CMOS technology, the VIPIC (Vertically Integrated Photon Imaging Chip) is a unique pixel-array detector for accessing micro-second time regimes in X-ray photon correlation spectroscopy experiments. Funded by DOE-BES and in collaboration with FNAL and ANL, we are currently executing a plan to make a full-scale test version of this detector. In CY22, we expect to receive a test chip of 192 x 192 pixels (65um x 65um each pixel) fabricated from the foundry. Testing of this chip will be a critical step for the VIPIC project. If the chip works, we will be able to make a prototype detector as the next step.

Evaluation of Hi-Z detector materials for X-ray science: The goal of this multi-institutional project is to evaluate promising materials and qualify them for use as sensors for experiments with very hard X-rays (energies >20 keV). Partners in this collaboration include detector groups from Argonne, Brookhaven and SLAC National Labs and Cornell University who propose to perform laboratory and beamline tests. The deliverable is an evaluation of the options to BES, supported by test data and prototype devices built on mature and representative detector readout ASICs for XFELs and storage rings. The mature sensor materials to be evaluated are Ge and CdZnTe. In addition, a new and promising Hi-Z material, CsPbBr3 is being evaluated for use as a sensor when bonded to ASICs.

Amorphous Selenium for hard X-rays: In collaboration with Stony Brook Medicine, we are developing a-Se detector for hard x-rays. The advantage of a-Se is the high spatial resolution it offers at hard x-ray. Furthermore, the low temperature growth process makes it easy to grow the semiconductor directly on the read-out chip. We have fabricated an a-Se layer on an MM-pad ASIC and shown that the layer works as a detector and has good spatial resolution and few defects.

Seven-channel low noise Ge pixel detector for EXAFS: We have fabricated arrays of 7 hexagonal Ge pixels which will be read by low noise CUBE electronics. The readout electronics is under construction. We anticipate the noise to be Fano limited. The detector would be ideal for EXAFS measurement where the silicon-based drift detector has the problem of the silicon escape peak interfering with the EXAFS signal.

Diffraction Limited X-ray Optics R&D:

Development of stitching interferometer and improvements to the Nano Surface Profiler: To fully exploit NSLS-II capabilities, diffraction limited optics with surface figure, slope errors reaching less than 100 nrad rms or surface figure errors close to 1 nm are required. The corresponding mirror inspection needs to be at least at the sub-nm RMS metrology level. Conventional inspection tools at synchrotron facilities are based on one dimensional (1D) scanning deflectometry, with the measurement angular range typically limited to maximum 10 mrad. We have developed and tested two metrology system. Funded recently through an FIP (NSLSII Internal R&D funding), we have improved our metrology capabilities for more challenging, steeply curved mirrors (total slope range reaching 10 to 15 mrad) by upgrading our Nano-Surface Profiler (NSP). Coupled to this development, a prototype interferometry-based two-dimensional (2D) stitching platform has been tested and demonstrated a sub nm measuring precision but with the angular range limited to ~1 mrad. For 1D flat or near-flat mirrors (mainly hard X-ray mirrors), the mirror metrology can be performed with repeatable and reliable results. In FY23, we will continue to refine our process and improve our NSP measurements capabilities. Furthermore R&D are necessary for diffraction limited focusing optics for the ARI and other soft X-ray beamlines at NSLS-II where the total slope range can achieve 20 to 40 mrad.

Development of diffraction limited mirrors: Recently, we demonstrated the ability to produce a diffraction limited elliptical mirror with sub-nm RMS surface height errors using our Ion Beam Figuring instrument. In the next couple of years, we plan to produce a small number of test mirrors for NSLS-II beamlines and other DOE facilities to obtain real beamline measurements. We have secured additional funding to extend our current capabilities. Through this three years FWP grant (FY22-24), we will be able to establish new IBF capabilities for diffraction limited X-ray mirrors beyond our current mirror-length limit of 300 mm.

Continuing development and deployment of MLL optics: We plan to continue to lead the development of Multilayer Laue Lens (MLL) optics by advancing the necessary technologies and processes associated with their fabrication - including materials thin-film deposition, sectioning, and polishing techniques - and characterization as well as developing related metrology techniques to fabricate and deploy tilted and wedged MLLs. In the past years, we made significant advances and have demonstrated a clean 7.5 nm line focus at 15 keV. In FY21 and FY22, our efforts focused on the upgrade of several key components of our deposition chamber critical for us to successfully push further the spatial resolution and on the development of a newer version of its control system. The control system upgrade will allow the chamber to be better supported by the NSLS-II IT team and allow compatibility with other IT developments carried out by the facility. This effort is expected to be completed by the end of CY22. These developments will be applied to the fabrication of wedged MLLs to achieve a 5nm focus in the 10-20keV range. In FY23, we will also continue to conduct all post-deposition fabrication and metrology tasks to produce cutting-edge MLLs for routine operations of nanoprobes at NSLS-II as well as at other DOE light sources. The specific areas we will be focusing on are better control of the sectioning and increased working distance for the MLLs.

Bonding of MLL optics using microfabricated templates: The HXN endstation employs state-of-the-art piezo-mechanical components and provides positioning accuracy down to a few nm. The alignment of two 1D MLL optics is a complex procedure that involves eight degrees of motion. Moreover, when approaching a sub-10 nm point focus, conventional alignment approaches may not work due to geometrical constraints and environmental instabilities. We plan to simplify alignment procedures and enable sub-10 nm focusing by bonding two MLLs into a single 2D optic in a well-defined configuration. The Si templates will be used to hold two lenses together in a pre-aligned position, and ML algorithms will be used to quantify the degree of alignment. This work will be carried out through a funded FWP proposal. Once fully developed, such monolithic 2D MLL devices will become standard hard x-ray nanofocusing optics with a potential of being implemented at the existing and future imaging beamlines of NSLS-II (including a sub-10 nm resolution HXN upgrade contingent on available funding) and other DOE facilities.

Next-generation testbed for sub-10 nm nanofocusing and nano-tomography: This project tackles the key issues of global absolute sensing, high stiffness, and minimal heat dissipation that play a critical role in the development of a sub-10 nm tomographic nanoprobe instrument. With an approved facility improvement project, we are in a process of commissioning and testing the developed system. X-ray commissioning is planned to begin in CY22. The developed instrument is equipped with a novel line focusing interferometer-based global sensing system and will enable nanoscale resolution 3D tomographic imaging at existing and future nano-imaging beamlines.

Advanced Simulations of Synchrotron Radiation and Experiments:

Development of magnetic simulation and optimization software: A 3D magnetostatics computer code for insertion devices and accelerator magnets, Radia, and an optimizer code for sorting elements and shimming of such magnets, IDBuilder, will continue to be maintained, developed, and updated. A major on-going development in the Radia code includes its parallelization, to enable fast solving of increasingly complicated and optimized magnet structures, such as combined-function lattice magnets for new ultra-low emittance diffraction limited light sources. One of new developments in the IDBuilder code includes its adaptation for shimming / fine-tuning of the combined-function accelerator magnets. The updated software will be applied to the R&D on "Complex Bend" – the main "candidate" magnet of the future NSLS-II Upgrade lattice, and to fine-tuning of undulators for the new ARI, SXN and Bragg CDI beamlines at the NSLS-II.

Development of simulation software for beamline optics: The electrodynamics / physical optics simulation code "Synchrotron Radiation Workshop" (SRW) for the calculation of synchrotron radiation and the radiation propagation through X-ray beamline optics will continue to be developed and supported within the Experiment Development Program of NSLS-II. A number of extensions and improvements were implemented in this code over the last years, enabling high accuracy and high efficiency simulations of partially coherent synchrotron radiation propagation through X-ray optical elements. One of such developments, considerably increasing the speed of partially coherent calculations, was the implementation of the numerically efficient Coherent Mode Decomposition methods in the SRW code. This and other related developments will greatly help in efficient solving of such complicated problems as independent control of both the spot size and degree of coherence, while preserving the Xray beam waist at the sample position, at the new hard X-ray Bragg CDI beamline, and a large variety of other beamline optimization problems during their design and operation. Among other important on-going developments in the SRW code are the developments of numerical propagators for the efficient simulation of large-aperture optics, such as highly curved KB mirrors and zone plates with very large number of zones, that are planned to be used in the new ARI and SXN soft X-ray beamlines respectively.

Development of experiment simulation capabilities: In FY23, specific plans include: further extending Synchrotron Radiation Workshop to support simulation of coherent X-ray scattering and imaging experiments, including time-dependent experiments (that can be efficiently simulated only by using massively parallel computation methods on CPU-GPU computer clusters), validating the simulations against experimental data, improving the reliability, generality, accuracy and efficiency of the simulations, and implementing optimization algorithms to address solving of inverse problems at experimental data processing.

Beamline Recapitalization Planning

Development of recapitalization plan of the existing beamlines to ensure that they stay at the state-of-the-art was started in FY21. The recapitalization needs were split into four different categories: (1) Replacements of existing equipment due to their finite lifetimes, (2) New equipment and capabilities, (3) New equipment needed to support remote operations and (4) Major beamline upgrades. All DSSI-related items (computation and storage clusters, network, servers and workstations) were omitted since these would be better estimated by DSSI. For each item, the lead beamline scientist (LBS) provided a brief description, an estimated cost and time frame. Follow-up meetings were held with each LBS and their respective program manager, to go over their list. The results of this initial survey were presented to the SAC (March 2022) and at the monthly PSD Division Meeting (April 2022). Focussing on the 1-5 year timeframe, figure X shows the total investments needed by each beamline for the first 3 categories listed above. The total of these investments is $46M, about 45% of which are for detectors. The median amount of investment needed per beamline within the next 5 years is about $1.5M. The amount of investment needed per year is ~ $9M, not including the needs of DSSI. This amount greatly exceeds the typical $1.5-2M per year Facility Improvement Plan budget for the entire NSLS-II (including the Accelerator Division).

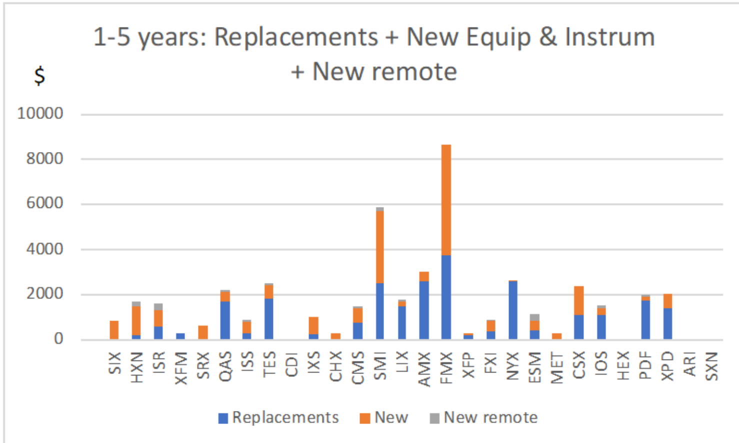


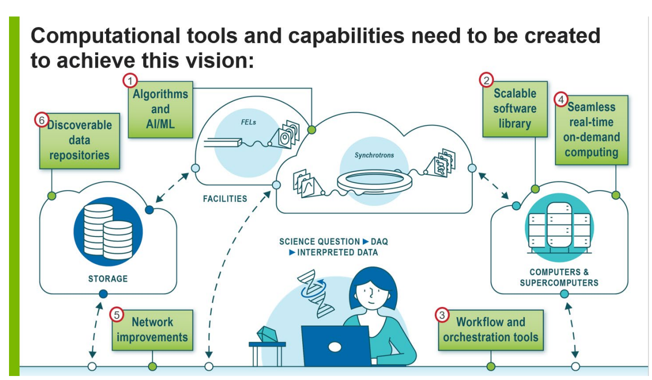
Figure above: Recapitalization needs for the next 5 years for each beamline, based on the three categories (1) replacements of existing equipment, (2) new equipment and (3) new equipment needed to better support remote operations.

Lessons learned: (1) There are significant variance in the level of input obtained from the lead beamline scientists, as can be seen from Figure X. It was clear that some had placed more thought into this exercise than others. (2) There was also a large variance in what LBS perceive the term 'Remote operations' – most were focused on automating sample changes, rather than a broader picture that includes automated beamline alignment, data analysis workflow, and autonomous measurements. (3) Most cost estimates do not include labor and other collateral costs (e.g, need to modify/move other beamline components to accommodate the new equipment) (4) Area detector upgrades are a major driver. More beamlines are requesting them and their unit costs are significant (~$1M each); and, they have a 5-10 year lifetime. As such, a more detailed study, for a facilities-wide detector strategy is warranted.

Based on this initial survey and lessons learned, the next steps are to prioritize the items and update the budget estimates to achieve a more 'budget-realistic' actionable plan. To achieve this, (1) management will provide a budget and schedule envelope to frame a realistic plan, (2) work with PMs and LBS to prioritize the items and seek a more uniform level of response from the beamlines, and (3) obtain realistic budget estimates for the high priority items. Finally, the DSSI-related recapitalization needs will be folded into the plan. The goal is to develop a living, realistic, and actionable Recapitalization plan for the beamlines.

Data Infrastructure and Support

Data infrastructure is an enabling and support technology that allows a wide range of science to be conducted at NSLS-II. It is supported by the Data Science and Systems Integration (DSSI) program of the facility. As a modern light source, NSLS-II data infrastructure consists of advanced data systems ranging from experiment controls, data acquisition, data storage, analysis, and networks, and to the development and maintenance of computational tools such as AI/ML, scalable software libraries, workflow and orchestration tools, seamless real-time on-demand computing, and discoverable data



repositories. In a previous Chapter, we outlined the data science aspect of this program. This section will focus on the support function of the DSSI program.

In general, two basic types of support are provided by DSSI staff – (a) operational support and responding to system failures, which we call Tier 1 support typically handled by the DSSI Assigned Support Team (AST) for a specific program, and (b) development projects in support of the facility's mission, which we classify as Tier 2 and Tier 3 support. The following Table illustrates this tiered support model of DSSI.

Tier Level	How much total effort	How it goes in Jira	Who does the work	Who selects / sets priority
1	up to 4 FTE-days	Task or Bug in the Tier-1 Board for the Program	AST staff for the Program	Program Manager (ACC: Group Leader), with support from AST lead
2	up to 12 FTE-months	Proposed Project issue in the DSSI Board	DSSI and AD / PS Staff	Division Director
3	more than 12 FTE-months	Proposed Project issue in the DSSI Board	DSSI and AD / PS Staff	Facility Director

We have developed a system such that all support and development requests to engage DSSI are captured in Jira (https://jira.nsls2.bnl.gov). In this system,

- the Reporter is the requester of support/development,
- the Assignee is the person tasked by DSSI to do the work, and
- all issues start in the backlog & get selected by Program Managers / Division Director

In FY22, DSSI has focused on addressing many of the Tier-1 issues that had been accumulated over the past year. This enabled DSSI to now concentrate its efforts in FY23 to work on larger scale Tier-2 projects. Such projects should have a clear scientific goal, be strategically important to the facility, be built from teams to do full stack engineering, and have clear objectives, milestones, and definition of completion. Ideally, all these projects will not only have value add, but also deal with technical debt and improvements.

In FY23, DSSI will also work with beamline and accelerator staff to develop a roadmap for the longer-term future. This will be guided by the timeline, the planning, and the executions of the Tier-2 projects that support the facility mission and strategy.

Operations Excellence

NSLS-II strives to create and maintain a vibrant and inclusive research environment for all staff and users. This includes having the staff, the support, and the infrastructure necessary for staff and visiting researchers to work at the NSLS-II facility safely, securely, and effectively. As an integral part of the NSLS-II strategic plan for the next five years, this Section describes the initiatives and development activities we plan to pursue in the areas of workforce development and inclusion and diversity, career development and work-life balance, environmental safety and health, facility infrastructure, user services, and communications.

Workforce Development and Diversity, Equity, and Inclusion (DEI). Workforce skill mix and matrix assignment of staff resources at NSLS-II will continue to evolve to meet our mission needs. NSLS-II recognizes the strength associated with a diverse staff and user population and is working aggressively to create an inclusive environment for people of all backgrounds, gender, and ethnicity. The initiatives that support these goals include: (a) promoting leadership and staff awareness of implicit bias with a goal to reduce unconscious bias during recruitment, performance evaluation, and promotions, and (b) increasing representation and inclusion of women and underrepresented minorities in management, scientific, and engineering job classifications via specific DEI goals for hiring managers. Examples include plans for increasing awareness and outreach to partner with universities with a high number of women or underrepresented minorities in relevant scientific program. Two directorate initiatives include requiring each NSLS-II staff member to have an annual DEI goal and utilizing a hiring process designed to assure a representative candidate pool and promote inclusion for new hires. Aging of the NSLS-II workforce will continue to drive an increased emphasis on succession planning and provisions for knowledge transfer over the next several years.

Career Development and Work-Life Balance. NSLS-II considers its talented and enthusiastic staff with diverse background as the single most important asset of the facility. As a relatively young synchrotron facility, NSLS-II has been able to attract many high-quality and expert staff to join our facility, and the continued career development of our staff as we mature and expand science programs is a critical aspect of NSLS-II facility operations. Recognizing this need of talent management, NSLS-II will continue to implement in FY23 a staff career development and work-life balance plan that includes the following elements.

- *Research & Development Job Classifications*: Following BNL guidelines for scientific staff promotions and recognizing the special situations in balancing scientific and support activities, NSLS-II will continue to work with the Laboratory to develop and implement a more optimized scientific staff career development process; This includes developing a new scientific staff review process for the new R&D classification that had been introduced in CY22.

- *Mentoring*: BNL has a Laboratory-wide mentoring program that allows a non-supervisory mentor to interact closely with an employee outside the person's management chain. The mentor may provide useful advice to the employee's career development from a more neutral point of view. NSLS-II strongly supports this program. The human resources manager for NSLS-II will provide the NSLS-II management team the details on who has participated in the mentor program, as well as plans for others who should participate in the outyears.

- *Work-Life Balance for Staff*: NSLS-II will continue to address the work-life balance issues that were identified in the 2019 lab-wide survey. A Working Group was assembled to review and evaluate NSLS-II employee responses and develop recommendations to senior management to improve staff engagement and morale. These recommendations were detailed in a report dated March 2020 and included a wide range of suggestions ranging from extending flex time beyond a single month so that staff can better utilize excess time accumulated during periods of beam operations, providing opportunities for a bottoms up performance feedback, establish new policies for use of personal and sick time, restoration of onsite services (*e.g.* food, child care and automotive) and improved/more timely staff feedback, Several of these recommendations have been accepted and efforts started to address them. The COVID pandemic has however, been an obstacle to full implementation. Measures will be implemented including a *Beamline Users Guide* to provide clear guidance and expectations on user assistance by beamline staff, remote access and experiments, a beamline policy that allows 'unused' beam time at beamlines, and a more balanced operating schedule for weekends, holidays, and maintenance shutdowns. The new BNL telework policy is also designed to give staff more freedom in balancing their lives. NSLS-II is working with Human Resources to develop a new Flex Time Pilot for NSLS-II staff to be able to extend flex time beyond the pay period. This will be beneficial for our staff who are working on projects and supporting the User Program under periods of tight time constraints.

- *Expanded Postdoc and Graduate Student program*: NSLS-II Director's postdoc and graduate student program is designed to help NSLS-II scientific staff to maintain their research in strategic science areas in partnership with researchers in the scientific community. Starting in FY22, NSLS-II will allocate these postdocs and students as follows:
  - Director's Postdocs: 8 full postdoctoral researchers each year, one in each of the five beamline programs, plus one each in experimental development program, in data science and system integration (DSSI) program, and in the Accelerator Division. In all cases, efforts will be made to solicit candidates from under-represented communities to further enhance diversity, equity, and inclusion at NSLS-II.
  - Graduate Students: 8 graduate students at up to $25,000 (direct cost) annually for each student. The allocations of these students will be the same as Director's Postdocs and will be at the discretions of the managers of the Photon Science beamline programs, experimental development program, DSSI, and the

Accelerator Division. A copy of the graduate student's Ph.D or Master thesis should be submitted to NSLS-II after the student completes thesis work and included in the NSLS-II publication data base.

Environmental Safety, Security, Health & Quality Assurance (ESS&H and QA). ESS&H performance remains a primary objective and strong safety leadership will continue. Other key elements are sustaining a culture where all staff: look out for each other, as well as users, students, and visitors; continuously learn from events and issues; and rigorously plan all scientific and conventional work within a safe, secure and environmentally sound workplace. As we examine our past events and their causes, we are focusing on strengthening our operational discipline in order to raise the rigor of the NSLS-II conduct of operations. QA programs continue to support current operations and will underpin the success of future accelerator and beamline development projects. NSLS-II conducts periodic functional assessments and a broad array of performance measures and metrics are monitored by senior management. Development of a research operations security programs for the NSLS-II continues to evolve to provide general protection for new DOE security initiatives as well as support DOE and user needs to conduct experiments requiring additional security measures. Additionally, enhancements in research screening is underway to ensure compliance with sensitive research requirements.

Buildout of User Laboratories and Offices in LOBs. The primary infrastructure goal for NSLS-II is to provide facilities to attract and retain the scientific and operations workforce, including the user population, and assure safe, secure, reliable facilities to enable the NSLS-II mission. The strategies we deploy to meet this goal are:

- Maintain, renew, and enhance infrastructure and capabilities to enable the mission, and enhance the quality of work life
- Enhance critical infrastructure for mature operations and reliability
- Develop infrastructure to support future beamline build-out, growth of staff and users
- Optimize the footprint of the space

BNL established an IGPP project approach to develop labs for institutional use and make them available to BNL organizations such as NSLS-II under the landlord-tenant model. The first IGPP project using this approach was approved in FY21 for two laboratories followed by another IGPP project in FY22 for two more laboratories. IGPP projects are a subset of CURL projects funded with internal G&A funds, and are prioritized and approved by BNL's Policy Council on an annual basis. Additionally, IGPP projects are reviewed and approved by DOE BHSO and DOE HQ. BNL included in the CURL projects list a phased approach for design-construct IGPP projects for the construction of 12 laboratories in LOB-2, a combination of dry and wet laboratories, over the next 5 years. Construction of the laboratories is the priority at this time to support 5 beamlines, the existing XPD and PDF beamlines and the future HEX and ARI/SXN beamlines. As of August 2022, of the five Laboratory Office Buildings (LOBs), LOBs 1 and 3 are fully built-out with all office/cubicle/conference/laboratory spaces finished and occupied. LOBs 4 and 5 have office, cubicles, conference spaces, and most laboratory spaces finished. LOB 2 remains unfinished.

The IGPP projects are a two-year design-construct projects with design being completed in the first year and construction being completed in the second year. The FY21 IGPP design-construct project was completed to FY22 with the construction of two labs, one lab in LOB 4 and one lab in LOB 5. These labs will support of the Complex Scattering and Structural Biology Programs. The FY22 IGPP project design was completed in FY22 for two dry labs in LOB 2. These labs will support the Hard and Soft X-Ray Scattering and Spectroscopy Programs. The CURL projects are listed below.

- Bldg 744, Lab 5: The dry lab has with the controls, services and laboratory casework to support high-performance research.
- Bldg. 745 Lab 10: The wet lab is a double lab and has controls, services, laboratory casework, a biological safety cabinet, chemical fume hood, shaker, floor mounted centrifuge, refrigerator, minus 80 freezer, autoclave/sterilizer, ice maker, and glass washer..
- Bldg. 742, Lab 4: The dry lab was designed with controls, services, laboratory casework, and a lifting area with an overhead bridge crane and two mobile cart stations.
- Bldg. 742, Lab 5: The dry lab was designed with controls, services, laboratory casework, a portable hood, mobile toolbox, mobile work benches, incubator, and space for a future battery tester.

Although this IGPP approach allows for larger scale projects needed for non-shelled spaces in LOB-2, the time horizon is still long due to the limited internal G&A funds for IGPP projects and the total cost will rise substantially. Under the current IGPP rules, BNL is also exploring an approach for the buildout of LOB 2 office space for future growth of staff to support the future beamlines as part of the landlord-tenant model.

As a result of the COVID-19 Pandemic, we made temporary and permanent facility modifications. Temporary wellness screens were installed at receptions desks and beamlines, and office space cubicle walls were permanently raised to provide a barrier where staff sit facing each other in open areas and shared offices. Space planning considers future use in a pandemic and post-pandemic environment. Impacts may include reduced occupancy levels, the need for flexible space, the design of high-wall cubicle spaces; incorporation of wellness barriers, and ventilation considerations. Additionally, a hybrid environment of telework, remote, and on-site staff is being considered including designs of equipment in conference rooms that can accommodate both.

The schedule for the remaining LOB buildouts is critical. With the previous aggressive IGPP project buildout plans, the available labs and offices were keeping just slightly ahead of projected staff and user growth. A stretch-out program which delivers at most 1-2 labs per year could cause a disruption to the NSLS-II mission within the next 5 years.

Discovery Park. Discovery Park is a new vision for the gateway to BNL. The concept for Discovery Park at BNL's entryway includes creation of more than 600,000 gross square feet on approximately 60 acres of previously developed, publicly accessible land. Developers, collaborators, and entrepreneurs may propose, build, and operate facilities that complement the DOE and Brookhaven Lab's missions. Discovery Park is envisioned to include a welcome center, housing accommodations for visiting researchers, a privately funded public science education center, and a technology park where collaborators and entrepreneurs can leverage privately funded research and development with close proximity to BNL.

Science User Support Center. The laboratory is constructing a new welcome center building , called the Science User Support Center (SUSC), located in Discovery Park. This new building will replace the old badging office at the main entrance to the Laboratory, and accommodate much of the functions of the guest, user, and visitors (GUV) center currently located in Bldg.400, for BNL's thousands of guest researchers and facility users. With approximately 75,000 gross square feet, this federally funded building will also offer workspace for approximately 250 Brookhaven employees as well as meeting space for collaborations and conferences. The construction of the SUSC building started in early 2022 and is expected to be completed in 2024.

New User Proposal Administration System. At NSLS-II, the Proposal, Allocation, Safety, and Scheduling (PASS) system is currently the electronic mechanism by which users request beam time. The system also includes the feasibility review by the beamline staff, scientific review by the Proposal Review Panel, and a fully functional Safety Approval Form system. However, the evolving user science needs require substantial improvements to the PASS system. In FY19-20, we conducted two external reviews of the PASS system to determine its strengths and limitations both at present, but more importantly, in the future. In FY20, the decision was made to replace PASS. In FY21, in collaboration with APS and LCLS, development of the new "Universal Proposal System (UPS)" began. The initial phase of the project will include proposal submission, feasibility review, scientific peer review, and allocation. This phase is expected to be delivered in the summer of FY23.

New Beam Time Scheduling System. In FY21, NSLS-II decided to retire the PASS Scheduling system and adopt the ALS Scheduling System. In FY22, the ALS Scheduler code was obtained from LBNL and is being significantly modified to accommodate NSLS-II allocation information. It is now fully integrated into PASS and we expect to launch the new NSLS-II Scheduler in early FY23.

NSLS-II Communication Strategy. For a facility such as NSLS-II to strive, communicating the expertise, capabilities, and success of the facility is vital. Due to the continuously changing landscape of scientific research and modern communication tools, the overall communication strategy needs to be adaptable on a yearly basis, while still pursuing the overall essential goals. Therefore, we are setting five-year long-term goals, while pursuing specific goals each year that support the long-term goals.

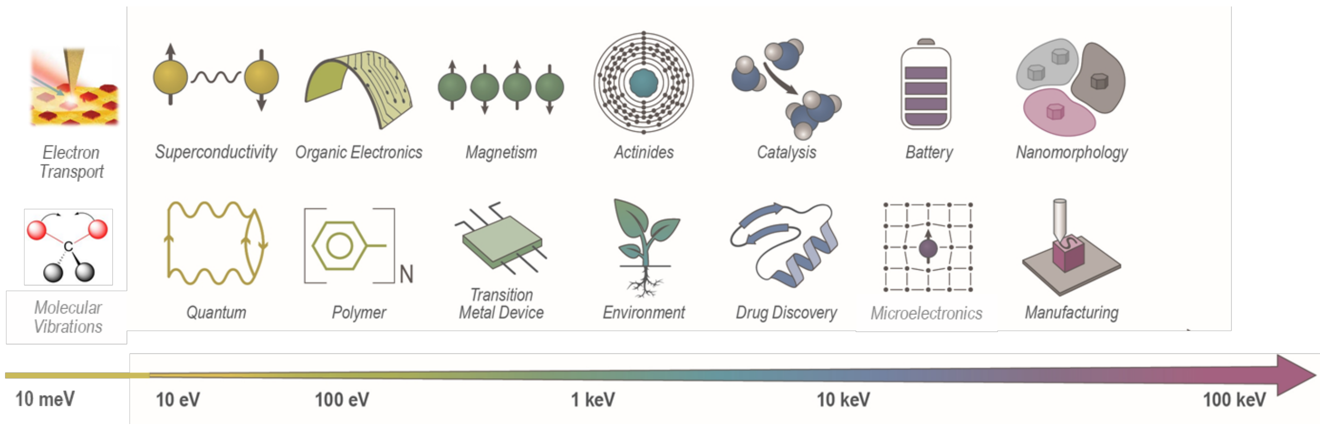
Our long-term goals are:

1. Showcase NSLS-II's position as a hub for the use of synchrotron light to solve the world's most challenging scientific problems to attract world-class researchers and partnerships
2. Raise NSLS-II's profile as a leader in data, computation, remote access, and autonomous/AI-powered experimentation
3. Highlight NSLS-II staff's expertise in beamline development, beamline-related R&D, accelerator R&D, and general mission support
4. Grow positive relations with all stakeholders, including DOE, BNL, and partners

To support these long-term goals in FY23, we will focus our efforts on writing engaging overview stories covering impactful scientific topics, profiling our staff members to showcase their expertise, creating communication materials for our staff and users to support their outreach efforts, and working on a new video for the facility.

Future Outlook

NSLS-II's mission is to tackle the science and technology challenges facing society today by providing world-leading capabilities to researchers. Today's challenges are complex and multi-scaled in both time and space. To make substantive progress require a multimodal approach enabled by analytical tools with different resolutions, sensitivities, modalities, and advanced data science capabilities.



To achieve its mission, NSLS-II will continue to assemble an optimized portfolio of world-leading capabilities together with the scientific expertise to use them. The facility is well positioned to do so. First, as a medium energy, high-brightness storage ring, it can deliver exceptional performance from the far-IR to the hard x-ray region of the spectrum. As shown in the figure above, this is what is required to tackle the broad range of problems that society is facing today. Second, NSLS-II is designed to house ~60 beamlines and as of now is nearly half built out, thus offering the scientific potential to build out the rest of the beamline program with new and needed capabilities in a cost-effective way.

As part of our 10+ year strategy, we will pursue two large-scale development initiatives to help achieve our mission – (a) to develop of a suite of additional new beamlines to fill the capabilities gaps, and (b) to prepare for a future accelerator upgrade in the next decade. Together the two initiatives, as described in more detail below, will retain NSLS-II leadership in the field of medium-energy storage rings and allow NSLS-II to continue to meet its mission of delivering world-leading science through the mid-21st Century.

New Beamlines

Based on discussions through engagement with our user community, input from the broad scientific community at the 2019 NSLS-II Strategic Planning Workshop, and the advice from NSLS-II Science Advisory Committee (SAC), we are pursuing a new beamlines development strategy that include the considerations of the following factors:

- capability gaps and capacity needs in the current beamlines portfolio,
- potential scientific, programmatic, and societal impact,
- critical role in enabling and supporting multimodal research,
- alignment with NSLS-II and BNL strengths,
- the national light sources landscape, and
- maturity and readiness of the new beamline concept.

In the national synchrotron landscape, NSLS-II is the only high-brightness medium-energy facility. As such NSLS-II has unique strength in the photon energy range of tender and soft X-rays through infrared, and a competitive strength in the traditional hard X-ray range around 8-15 keV. These strengths in high-brightness are supplemented by the high-flux capabilities in the high-energy X-ray range that have attracted a regional scientific community to conduct in-situ and operando materials research including under extreme conditions. We have been working with our SAC and our community to take into account these national and regional contexts in the development of our new beamlines concepts.

These extensive discussions have led to our conceptualization of 23 new beamlines that will be required to meet the research needs and fill the capability gaps in the current NSLS-II portfolio, particularly in such key technology areas as:

- High-resolution X-ray spectroscopic chemical mapping,
- Full-field imaging of structure and dynamics in materials and biosystems, and
- High-throughput, high-resolution structural analysis.

Compared to the 22 beamlines list described in last year's Strategic Plan, we added two additional beamlines in the tender energy X-ray range based on strong recommendations from SAC – one Tender X-ray Nanoprobe (TXN), and the other a high-throughput BM-based Advanced Tender X-ray Microspectroscopy (ATM). The TXN beamline will supplement the nanoprobes in soft and hard X-ray ranges, SXN and HXN, to provide unique capabilities in nano-imaging in the tender energy range at NSLS-II. The ATM will supplement the existing TES beamline for routine spectroscopy experiments, and enable a tailored endstation dedicated for energy science applications. We also added a new soft X-ray beamline concept that will bring new and improved coherent scattering and imaging capabilities in the soft and tender X-ray range (CST) to our user community, complementing the existing CSX beamline. Finally, we removed the Materials in Radiation Environment beamline (MRE) from the list due to the fact that much of the interests from the original community has shifted to using existing beamlines (e.g. XPD) to meet their evolving research needs. We also removed INF from this new beamlines list since the INF beamline is now funded as part of the New York State contribution to the DOE-funded C2QA QIS research center at BNL.

Together these 23 new beamlines will provide the needed capabilities and capacity to support a wide range of multimodal, multiscale, operando research at NSLS-II. As discussed in this report last year, we categorize these 23 new beamlines in following three groups:

- 12 enterprise beamlines with mature techniques to balance our beamlines portfolio and support broad range of science, typically high-throughput and remote friendly, with a large mature scientific user base;
- 9 performance beamlines that provide cutting-edge high-resolution capabilities, enabling high-impact research beyond what can be done using mature techniques;
- 2 mission-specific beamlines to meet targeted mission needs of other specific federal agencies.

The following table shows the list of these 23 beamlines in enterprise, performance, and mission-specific categories and how they map to the capabilities development needs in high-resolution chemical imaging, multiscale full-field imaging and dynamics, and high-resolution structural analysis at NSLS-II:

	High-resolution X-ray spectroscopic chemical imaging (9)	Full-field imaging and dynamics of materials and biosystems (6)	High-throughput high-resolution structural science (8)
Enterprise beamlines (12)	• Micron resolution X-ray spectroscopy (MRX) • Scanning transmission X-ray microscope (STX) • Advanced Tender x-ray Micro-spectroscopy for energy sciences (ATM)	• Micro-CT and instrumentation (MCT) • Microelectronics imaging (MCT-II) • Soft X-ray tomography for cell imaging (SXT) • Full-field nano-CT for microelectronics (FXI-II)	• Rapid access X-ray diffraction (RAX) • Processing and liquid surfaces (PLS) • Massively automated MX – 3PW-based (MAX) • High-reso pair-distribution function (HEX-II)

			• Energy dispersive X-ray diffraction (HEX-III)
Performance beamlines (9)	• X-ray Raman spectroscopy (XRS) • High-resolution emission spectroscopy (HRS) • Tender X-ray Nanoprode (TXN) • Tender and hard X-ray RIXS nanoprobe (TIN) • In-situ spectroscopy for hazardous chemicals (DTR)	• Coherent soft and tender X-ray imaging and dynamics (CST)	• Advanced manufacturing and processing (AMP) • High-resolution X-ray powder diffraction (HRD) • Massively automated MX – IVU-based (MAX-U)
Mission-specific beamlines (2)	• X-ray investigation of extraterrestrial sample return (MAR)	• Hard X-ray nanoprobe & projection microscopy (HXN-II) for microelectronics	

It presently appears likely that the NEXT-III project will be granted CD-0 ("Mission Need") status early in FY23. Therefore, in FY23, we will work with DOE-BES to define and select the beamlines to be included in the NEXT-III project. In particular, we will continue to work with the User community and our SAC to further develop and refine the concept and scope for each of the beamlines and capture the conclusions in updated 1-pagers, with updated cost estimates. Factors in the prioritization will include impact on the nation's scientific priorities including especially clean energy and climate, biopreparedness and quantum information science. We will develop a white paper to summarize the science case for each of the high-priority new beamlines, and refine the scientific and technical scope leading towards the conceptual design of these selected beamlines. We will work with BES to understand the overall scope of the project and funding profile in order to finalize the selection of a number of high priority beamlines to be built first in the new construction project.

Future Facility Upgrade

As described in the previous section and shown in the figure below, NSLS-II has a vision to develop and operate a balanced portfolio of 56 high-performance, enterprise, and mission-specific beamlines in the coming decade. To fully meet the science needs of the community and to remain competitive in the evolving synchrotron world, an upgrade of the NSLS-II facility is needed in the next 10+ years.

In our vision, an upgraded NSLS-II (NSLS-IIU) will be a transformative scientific user facility in the 21st century, consisting of three integral parts:

- Upgraded source with photon flux & coherence optimized as the ultimate medium-energy storage ring,
- Optimized beamlines and detectors to take full advantage of the upgraded source across,
- Automated data flow integrated with artificial intelligence, discoverable repository, theory and modelling, and on-demand experiment feedback and data analysis.

In FY23 and beyond, we will continue to explore the available parameter space for an upgraded source, as described on p.32. In addition, we will work with the scientific community to identify key science areas and refine science case examples that will take full advantage of an upgraded NSLS-II source.

In addition to accelerator systems, there is also the need to improve NSLS-II existing beamlines so that all beamlines would benefit from such a future upgrade. In FY20-21, two taskforces were formed to look into the two critical technology areas – optics and detectors. Initial reports from these taskforces have been developed. These reports will help to optimize future X-ray optical system designs, X-ray detector strategies, and integrated schemes for photon detection and data acquisition, when constructing the suite of new beamlines at NSLS-II.

Finally, further development of the conventional facilities complex will be critical to meet the science needs of the growing NSLS-II facility. In particular, as discussed on p.39, there is already an unmet demand in user science laboratories and office spaces with the current set of 33 beamlines. To fully meet the future science needs of a substantial built-out portfolio of 56 beamlines, additional laboratories and offices are clearly required. In FY23, we will continue to discuss within BNL to develop an NSLS-II Conventional Facilities Master Plan. This plan will take into account the staff and user needs in the post-COVID era and will serve as our master guide for conventional space development at NSLS-II in the next decade and beyond.

Summary

It is an exciting time at NSLS-II. Entering the 8^{th} year since its start of user operations, NSLS-II is delivering on its promise to be a premier synchrotron facility.

Looking to the future, in the next five years, we will:

- deliver reliable accelerator performance of 500 mA & 8 pm-rad vertical emittance, nearly doubling the present brightness of the source
- invest in existing beamlines to keep them competitive, with new access modalities post-COVID,
- provide data infrastructure for seamless access to experimental capabilities, compute and storage
- complete the NEXT-II project,
- develop new beamlines to increase capacity, enhance capability, support multimodal approaches, and balance beamline portfolio, and
- develop an upgrade plan for a transformative NSLS-IIU facility.

We look forward to working with our stakeholders and the scientific community to make our vision a reality.

List of Acronyms

3PW	Three-Pole Wiggler
AI	Artificial Intelligence
ALS	Advanced Light Source
AM	Additive Manufacturing
ANL	Argonne National Laboratory
AP-PES	Ambient Pressure Photo-Electron Spectroscopy
APS	Advanced Photon Source
AP-XPS	Ambient Pressure X-ray Photo-emission Spectroscopy
ARPES	Angle-Resolved Photo-Electron Spectroscopy
ASCR	Advanced Scientific Computing Research
ASIC	Application-Specific Integrated Circuit
BER	Biological and Environmental Research
BES	Basic Energy Science
BL	Beamline
BM	Bending Magnet
BNL	Brookhaven National Laboratory
CBA	Complex Bend Achromat
CDI	Coherent Diffractive Imaging
CFN	Center for Functional Nanomaterials
CMOS	Complementary Metal–Oxide–Semiconductor
COMPRES	COnsortium for Materials Properties Research in Earth Sciences
COVID	Coronavirus Disease
Cryo-EM	Cryogenic Electron Microscopy
CY	Calendar Year
DAC	Diamond Anvil Cell
DSSI	Data Science and System Integration
DOE	Department of Energy
DTRA	Defense Threat Reduction Agency
ESS&H	Environment, Safety, Security & Health
FIP	Facility Improvement Project
FWP	Field Work Proposal
FY	Fiscal Year
GU	General User
HXSS	Hard x-ray Scattering and Spectroscopy
I&D	Inclusion and Diversity
ID	Insertion Device
IGPP	Institutional General Plant Projects
INSPIRE	Inelastic Scattering, Photoemission, and Infrared Endstation
IR	Infrared
KB	Kirkpatrick Baez
LBNL	Lawrence Berkeley National Laboratory
LCLS	Linac Coherent Light Source
LDRD	Laboratory Directed Research and Development
LOB	Laboratory Office Building
MBA	Multi-Bend Achromat
MBE	Molecular Beam Epitaxy
MID	Metrology and Instrumentation Development
ML	Machine Learning
MLL	Multilayer Laue Lens
MOU	Memorandum of Understanding
MX	Macromolecular Crystallography
NE	Nuclear Energy
NEXT-II	NSLS-II Experimental Tools II
NIST	National Institute of Standard and Technology
NREL	National Renewable Energy Laboratory
NSLS-II	National Synchrotron Light Source II
NYSERDA	New York State Energy Research & Development Authority
NV	Nitrogen vacancy
OPLS	Open Platform and Liquids Scattering endstation
PASS	Proposal Administration, Safety, and Scheduling
QA	Quality Assurance
QIS	Quantum Information Science
R&D	Research and Development
RF	Radio Frequency
RIXS	Resonant Inelastic X-ray Scattering
SAC	Science Advisory Committee
SAXS	Small Angle X-ray Scattering
SBIR	Small Business Innovation Research
SCC	Synchrotron Catalysis Consortium
SDD	Silicon Drift Diode
SRW	Synchrotron Radiation Workshop
STXM	Scanning Transmission X-ray Microscope
SXSS	Soft X-ray Spectroscopy and Scattering
TEM	Transmission Electron Microscopy
TXM	Transmission X-ray Microscope
WAXS	Wide Angle X-ray Scattering
WFO	Work for Others
XAS	X-ray Absorption Spectroscopy
XES	X-ray Emission Spectroscopy
XPCS	X-ray Photon Correlation Spectroscopy
XPEEM	X-ray Photo-emission Electron Microscopy
XPS	X-ray Photon-emission Spectroscopy
XRD	X-ray Diffraction
XRF	X-ray Fluorescence