National Synchrotron Light Source II
2020 Strategic Plan
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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.
Executive Summary

The National Synchrotron Light Source II (NSLS-II) is a 3 GeV synchrotron delivering bright photons over a wide spectral range from the far infra-red to the hard x-rays. Since its First Light in October 2014, NSLS-II has rapidly ramped up its accelerator performance, beamline operations, and user science programs. As of September 2019, NSLS-II operates at 400 mA in top-off mode and delivers an operations reliability of 97%. At the same time, NSLS-II pursues a substantial accelerator development and spares program to ensure being able to reach mature performance of 500 mA in operating current and 8 pm-rad vertical emittance in the next 3-4 years. On the beamline side, 28 beamlines are in operations and one other beamline under construction. Funded through a diverse range of sponsors, these beamline capabilities enable a strong user science program and are delivering on the promise of this extremely bright source with high-impact papers in fields as diverse as catalysis and energy storage, structural biology, nanoscience and microelectronics, materials physics, and the environment.

Our overall strategy to achieve our mission is to work with the scientific community to identify key scientific challenges in relevant science focus areas, to integrate our strengths and expertise to develop scientific capabilities, and then to carry out relevant science programs to address these scientific challenges. This 2020 strategic plan outlines a number of major development activities we plan to pursue in the next five years in support of the overall strategy. In addition to our ongoing emphasis on in-situ and operando research of multiscale structure and functions in materials and biological sciences, this year’s plan included several new sections on our current initiatives in quantum information science, beyond-Moore microelectronics, as well as artificial intelligence and machine learning.

In our planning process, we take into account the expected funding in the coming years where we plan to dedicate a small percentage of our operating funds to invest in the development of enhanced or new capabilities at NSLS-II. In general, our overall investment strategy is to maximize the science output of the NSLS-II user facility, using a balanced approach with considerations on (a) accelerator reliability, (b) effective operation of existing beamlines, and (c) development of new beamlines.

For fiscal year 2020 (FY20), our specific objectives are:

1. Maintain reliable accelerator operations at 400 mA and pursue developments to ensure delivery of mature performance by FY23;
2. Efficiently operate the suite of 28 beamlines for general users and ramp up and mature user science programs;
3. Implement controls program plans to ensure reliable data acquisition, management, and analysis at beamlines;
4. Upgrade scientific capabilities at select operating beamlines to meet the evolving science needs;
5. Continue to develop additional beamlines in the context of NEXT-II project and pursue new opportunities as they arise;
6. Pursue enabling technologies R&D, and critical strategic partnerships.
This document will serve both as our high-level strategic development plan and as our basis for budgetary priorities for our development activities in FY20 and in the next five years. It will help drive consistency in our decision-making processes, coherence in developments across our complex organization, and alignment with our stakeholders and community’s expectations. We look forward to working with the scientific community and our stakeholders to make our strategic goals a reality.
Introduction
Introduction

The National Synchrotron Light Source II (NSLS-II) is one of the newest and brightest 3 GeV synchrotron facilities in the world, with 30 straight sections and 0.6 nm-rad horizontal emittance when operating with a full complement of insertion devices including damping and superconducting wigglers. The main design parameters of the NSLS-II storage ring and the current operating parameters can be found at [http://www.bnl.gov/ps/](http://www.bnl.gov/ps/).

Since the start of its user operations in July 2015, NSLS-II has rapidly ramped up its science capabilities and user programs. As of September 2019, NSLS-II operates at 400 mA in top-off mode and has 28 beamlines in operations plus one other beamline under construction. In fiscal year (FY) 2019, more than 1600 distinct scientists conducted their experiments at NSLS-II. This number is projected to increase to ~2000 in FY20.

The vision for NSLS-II is to develop world leading scientific capabilities and leverage them to enable and conduct a broad range of high-impact science and technology programs to address the critical scientific grand challenges in energy security, advanced materials synthesis and manufacturing, microelectronics, environment, and human health. Our overall strategy to achieve this vision is to work with the scientific community to identify key scientific challenges in relevant science focus areas, and to integrate our strengths and expertise to develop capabilities and then carry out relevant science programs to address these scientific challenges.

Our overall strategy remains to: (a) create a vibrant and inclusive environment that attracts world-class staff, users, and partners targeting strategic research programs aligned with our science focus directions; (b) develop and operate world-class accelerator and beamline systems with leading capabilities in our strategic research areas; (c) coordinate with other light sources to advance enabling technologies in accelerator systems, optics and detectors, instrumentation and methods, and data acquisition-management-analysis; and (d) leverage BNL strengths and community interests to facilitate university-industry-government partnerships that support the theme from discovery to deployment.

Our strategy has been developed with close engagement with the scientific community and the key stakeholders in development and operations of NSLS-II beamlines and associated science programs. These engagements include a beamline development process with broad input from the scientific community and the Science Advisory Committee (SAC), SAC meetings every six months on accelerator and photon science operations, beamline advisory teams during the beamline construction process, phased science commissioning with input from potential users, partner beamlines and partner users, community working groups to pursue new funding for new instruments and beamlines, and the User Executive Committee (UEC) to provide advice on operations and user programs.

The development of our strategic plan takes into account two current research trends in synchrotron science today – the increasingly multi-modal nature of measurements and the increasing importance of operando phenomena in all scientific fields. These trends are driven by the complexity of the problems that researchers are facing and the needs in understanding the fundamentals of complex, heterogeneous, real-world systems. These problems require multiple techniques to shed light on the problem, understanding for example, atomic and electronic structure, chemical valence, and structural...
morphology while the system is operating in real world conditions. This places new requirements on the experimental capabilities required for a successful scientific program.

NSLS-II is currently operating and developing a suite of 29 cutting-edge beamlines, along with associated science programs (See side box.). This set of current activities is informed by many years of strategic planning and working with the user community and other key stakeholders. These beamlines, with 28 of them already in operations, provide world-class scientific capabilities in such areas as nanoscale to mesoscale structural, chemical, and electronic imaging, coherent scattering on complex materials and dynamics, photoelectron spectroscopy and imaging, advanced x-ray scattering for materials self-assembly and membrane science, inelastic scattering on complex nanoscale disorder and electronic excitations, science-driven high-throughput structural biology, in-situ and in-operando diffraction and spectroscopy. These beamlines collectively support a large, highly-engaged, productive user community to address scientific challenges in many scientific disciplines. See http://www.bnl.gov/ps/beamlines/ for more information.

This 2020 NSLS-II Strategic Plan summarizes our strategic science focus areas and approaches, and our specific plans of developments in key areas for the next five years. All operations-supported projects and activities take into account the current funding levels and assume reasonable funding expectations in the coming years.

Our overall strategic goals for the next five years (FY20-24) will be:

1. Maintain reliable accelerator operations and deliver mature performance of the storage ring;
2. Effectively operate the 29 beamlines and associated general user programs;
3. Mature data acquisition, management, analysis capabilities in support of user operations, including seamless access to data & compute resources during and post experiments, near real-time analysis on all beamlines, and develop AI and machine learning for experiments and analysis;
4. Upgrade select beamline capabilities to meet the evolving science needs, including a 5-nm focused beam size for hard X-rays, and optimized suite of detectors;
5. Complete construction of the three beamlines in the NEXT-II project, and develop additional new beamlines as part of the strategic vision to reach 40 beamlines by year 2030;
6. Pursue enabling technologies R&D and strategic partnerships in support of the facility’s mission.

Accomplishing our goals will not be without challenges. Currently in accelerator operations, lack of several critical redundant systems, including incomplete buildup of RF, presents significant
vulnerabilities to reliable operations and impedes further improvements to storage ring performance. In beamline operations, challenges exist in ramping up staffing with sufficient level of effort and expertise that match the requirements of high-performance beamline operations and productive science programs. In enabling technologies R&D, increased competitions worldwide and constrained effort of our own make it challenging to stay at the cutting-edge in several technology areas that are critical to our success. In support facilities, the recent change in Institutional General Plant Projects (IGPP) funding would substantially delay the buildout of remaining user laboratories and staff offices in the NSLS-II Lab-Office Buildings. In new beamline development, lack of clearly identified funding routes for constructions of new beamlines adds uncertainty in the buildout of the remaining open beamline ports at NSLS-II, leading to loss of opportunities in bringing in new science programs and user communities. This document outlines our strategy to address these challenges and mitigate the associated risks. Our strategy includes: prioritizing all developing projects with clearly defined plans and objectives, providing seed-funding to encourage collaborations that bring resources to NSLS-II, developing mutually beneficial partnerships with external institutions, coordinating technology developments with other DOE-BES facilities, and working with diversified potential funding agencies and private foundations to secure funding for constructions of new beamlines or new endstations.

This 2020 Strategic Plan will serve as our high-level strategic development plan and as our basis for budgetary priorities for our development activities in FY20-24. The scope of this document does not include the vast majority of essential activities that are necessary for routine operations and maintenance of NSLS-II accelerator and beamline systems. The execution of this plan will depend on the actual funding in the coming years and will reflect these priorities.
Science Program Areas

Working with the scientific community, we have organized our science program in the following five program areas at NSLS-II:

- Quantum materials,
- Complex materials and processes,
- Catalysis and materials science in operando,
- Multiscale structure and function, and
- Structural biology and bioimaging.

These five program areas not only cover a broad scientific spectrum ranging from condensed matter and materials physics, catalysis and energy sciences, to biological and environmental research, but also concisely reflect our collective scientific directions that leverage our strengths and expertise, as well as in-house research interests, at the intersections of multiple cutting-edge beamline programs.

Our long-term vision is to become an internationally recognized science hub in each of the five program areas. Our overall science strategy to achieve this vision is (a) to leverage community and sponsors interests to develop enabling capabilities aligned with the nation’s science and technology initiatives, (b) to promote staff research at the forefront of the science focus areas, often in partnerships with key researchers in the fields, and (c) to integrate the capabilities and the R&D to establish and maintain a diversified and compatible user-driven science portfolio at NSLS-II beamlines.

In the most recent fiscal year, there have been significant new science and technology initiatives at the national and international levels that have substantial impact on our science emphasis and strategy. These initiatives include development of materials, devices, and algorithms in quantum information science and quantum computing, research and innovation in beyond-Moore microelectronics and neuromorphic computing, and development and applications of artificial intelligence and machine learning. NSLS-II has been very engaged in the discussions within Brookhaven National Laboratory as well as with the broader scientific community; These discussions have led to new development initiatives to enable NSLS-II to play a substantial role in the research and development activities in these new initiative areas in the next five years.

NSLS-II will continue to pursue all major development activities according to our strategy. It will help drive consistency in decision-making processes over time, coherence in development across our complex organization, and alignment with the community interests and stakeholders expectations. Our approach in support our science strategy will include:

- Outreach to academia, government labs, and industry to attract and pursue high-impact research projects at NSLS-II, particularly in the areas of emerging initiatives of the stakeholders;
- Seed the development of key partnerships with research groups by funding a number of Director’s postdocs and graduate students for joint projects,
• Allocate a small portion of NSLS-II operating budget, working with partners to pursue additional funding, to develop new capabilities and new data-analysis methods to enhance our programs in science program areas,
• Work with the community and potential funding agencies to identify capabilities gaps at NSLS-II and develop new beamlines to meet the evolving R&D needs of the nation.

In the following sections, we describe our strategic approaches and associated development projects currently planned for the next five years in each of the five science areas. A discussion of our capability gaps and possible new beamlines to develop is included in the Chapter on New Beamlines and Initiatives.

Quantum Materials

Quantum Materials

The main research thrusts in this area focus on understanding and ultimately controlling emergent quantum phenomena, which involves the study of the electronic and magnetic properties in condensed matter, for the purpose to inform the design of practical devices for information and energy technologies of the future.

Quantum Information Science. Quantum information science (QIS) has recently grown into a thriving field of research, as the perspective of practical devices achieving quantum speedup is invigorating the imagination of many in the physics community. Yet, while the QIS momentum continues to grow across the government, industry and academia alike, the tipping point at which quantum computing overcomes the limitations imposed by classical computers is still out of reach. Among the challenges facing mainstream quantum computing, the two biggest roadblocks towards the experimental realization of a fault-tolerant quantum computer – the holy grail of quantum computation – are the limited coherence times and gate fidelities of qubits. While improvements in qubit quality have been mostly driven so far by the advent of new architectures, the focus has recently shifted towards understanding the fundamental role of materials.

It is therefore an exciting time for NSLS-II in the short history of QIS, as the field is now ripe for exploring new avenues of device fabrication based on materials innovations, which in turn crucially rely on fine probes of the electronic structure to make an impact. Our strategy in this area draws upon the world-leading coherent photon flux and energy resolutions of the soft X-ray spectroscopy and scattering beamlines to tackle these challenges on two fronts. The first front is the optimization of relevant material properties in existing qubit designs such as superconducting qubits and NV centers, where a portfolio of targeted research projects in collaboration with key players in the field are already underway and taking full advantage of the complementarity of our experimental capabilities. The second front is the development of next-generation systems based on the exotic electronic properties of quantum materials such as topological insulators and high-temperature superconductors, where the combination of best-in-class energy resolution and microfocus of the ESM beamline promises to have a major impact.

Beyond Moore Computing. Besides quantum computing, another initiative which is currently shaping the future of computing is post-Moore’s law computing, whose aim is to revolutionize the traditional computing paradigm relying on CMOS-based logic in order to reach new levels of processing speeds, densities, and energy efficiency, while overcoming the problem of heat dissipation. Recent technological developments have been sparked by the exploration and integration of novel quantum materials, making the NSLS-II soft X-ray and infrared beamlines remarkably well aligned with this area.
A notable example, which is pursued at BNL, led by the CFN, is the development of 2D materials such as graphene and chalcogenides whose remarkable transport properties offer a possible path to beyond-CMOS technologies. The suite of soft X-ray spectroscopy and scattering capabilities at NSLS-II provides a unique platform for in-depth characterization of the electronic and magnetic properties of ultrathin samples, which will accelerate our understanding and optimization of these 2D materials. Another route to circumvent the Moore’s law slowdown exploits the electron spins, instead of the electronic charge, as the digital state. Here, our objective is to gain insight into the controllability of spin excitations to carry and process information without charge motion, which will leverage the exquisite sensitivity of the SIX beamline to spin waves. Another promising alternative is neuromorphic computing, which uses futuristic architectures emulating the operation of a biological brain. Transition metal oxides (TMOx) exhibiting a metal-insulator transition (MIT) are among the best candidates for neuromorphic applications as a well-controlled and reversible MIT can mimic the functionality of neurons. Preliminary studies at CSX, exploiting the superior coherence of the soft X-ray beam to image electrons in materials, their orderings, inhomogeneity and slow dynamics, revealed habituation, plasticity, and memory-like effects in some TMOx model systems. Future studies at NSLS-II will leverage local in-depth knowledge of the physics of these systems and experience with their specialized characterization requiring the cutting-edge soft X-ray and infrared instrumentation available at NSLS-II. These studies will pave the way for the exploitation of the exotic properties of TMOx in neuromorphic devices.

A number of development projects we plan to pursue in FY20-24 to meet the research needs in these and other areas in quantum materials are described below.

- **Coherent Imaging and Ptychography at CSX** (FY20-21): After an initial phase of progress and improvement, it became clear that the current nanopositioning system, the heart of the whole imaging and ptychography techniques, was progressively degenerating and was becoming the limiting bottleneck for resolution enhancement being out of specs. In spite of the publications achieved, an innovative version of the scanning stages has just been ordered. Its installation and commissioning will provide the suitable platform for the desired sub-100 nm performances during FY20. The new setup will allow to test at high resolution the innovative phase retrieval and reconstruction codes developed as part of this collaboration (with MIT and LANL) and benchmark the CAMERA/SHARP effort in the same direction (parallel collaboration). Ptychography and coherent diffraction imaging activities will also be conducted in partnership with the Condensed Matter Physics and Materials Science Division at BNL. Due to the delays with the provision of the required hardware, the ptychography capability is expected to be made available to general users by the end of FY20. In FY20-21, these techniques will be fully integrated into the user program with the CSX team actively working with the user community.

- **Magnetic Fourier Transform Holography at CSX** (FY20-21): After the first difficulties in developing a full new end-station out of the standard operation budget, encouraging results have been achieved. The collaboration with the MIT has brought to the first scientific results (in the publication pipeline at the moment) and some important technical developments. From the data analysis point of view, the competences of the beamline team have been brought to an innovative cross-fertilization between holography and XPCS. From the instrumentation side, a new IR laser pulsed source has just been procured as part of a dedicated FIP, after extensive test performed in-situ with an equivalent source. The idea is to excite magnetic phases (and skyrmion in particular) under in-operando conditions (pulsed electric fields to obtain racetrack memories at room temperature). The resolution is currently limited by some problems at the detector, which we hope to overcome by the end of the calendar year 2019. This should allow to finally achieve the sub-10 nm resolution
needed for harvesting precious magnetic information form small (and mobile) skyrmions in ferrimagnetic materials. We expect this project to be transitioned into operations by the beginning of the calendar year 2020.

- **Enhancing x-ray stability at CSX (FY20-21):** After the directors’ decision of recanting our straight section, the option for a phasing magnet has become obsolete. Then, the beamline staff invested a lot of energies and time in the conceptual design of a dedicated a soft X-ray Beam Position Monitor (XBPM) in order to mitigate the instabilities known to plague our straight section and potentially due to the limited controls available in the electron beam parameters of soft canted straight sections. The project got the interest of the DoE and there is hope to be funded soon. This would spark the development and testing during FY20-21. This project will be crucial in view of the new MIE soft beamlines and potentially for the ALS-U. On the optics side, the fight for noise and instabilities at our monochromator continues. A big leap forward has been achieved by further protecting the optics elements by specific cooling water circuit perturbations. The study on how to further enhance the protection are continuing in strict collaboration with the facility utilities group. We plan to put in place and test the new version of the water circuit decoupling system by the end of the calendar year 2020.

- **Investigation of qubits under in-operando conditions at CSX (FY20-21):** A postdoc has just been hired on LDRD funds. In FY20, the current scattering endstation will be upgraded to host a new sample space dedicated to advanced in-operando investigations of quantum materials, with special attention to the study of next-generation qubits. In FY20-21 these new capabilities will potentially put CSX in a leading position worldwide for the investigation of electronic properties in advanced materials for quantum computing applications in particular.

- **New optical beamline layout and optics schemes for CSX (FY20-22):** Irrespective of the realization of the re-canting of our straight section, a series of improvements of the beamline optics layout should be undertaken. The experimental chambers should be moved downstream in order to finally position some services (selected spectroscopic targets, relative order of fast shutter and horizontal feedback system diagnostic, polarization analyzer, …) in the logical order. The modest beam expansion factor will anyway help the development of new in chamber optics (innovative ZP, part of recent collaboration with ALS, and new fractal pinhole for complex illumination function at the sample, particularly useful in some conditions of reconstructions and potentially for Bragg topography as recently developed on the beamline) accounting for a better overfilling condition to be realized. We plan to extensively test innovative optics by the end of FY20 and open some of them to the users shortly after (depending on the timing of the canting and thus of the end station relocation). A collaboration with CFN has just started in order to produce innovative optics for OAM beams. The new nanopositioner setup (with enhance travel range) should also allow to host different type of optics in parallel into the chamber (thus representing a more efficient solution – no venting require to change setup, and a more flexible configuration for users experiments).

- **Photoelectron Spectroscopy at ESM (FY19):** The Electron Spectro Microscopy beamline (ESM) at NSLS-II has been recently commissioned and is now in operation. It serves two end stations: a high-resolution angle resolved photoemission spectroscopy (µ-ARPES) instrument and a full-field x-ray photoelectron microscope (XPEEM). During its first year of operation, the ESM beamline reached design parameters such as high flux over wide energy range (25-1500eV), high resolution (5meV@100eV), extended x-ray light polarization control, and proved to be competitive at a world level. Technical capability of ESM beamline is further enhanced with:
Elmitec XPEEM/LEEM station has been upgraded with LN2 sample cooling capability and a new CMOS detector with enhanced low contrast imaging and higher read-out speed.

- ML-based polarimeter added to the beamline facilitates the precise definition of the x-ray light polarization and extends chemical imaging to dichroic signal detection to study magnetic and molecular systems.

- New ESM ARPES sample transfer system has been implemented to enhance operational efficiency.

**Photoelectron Spectroscopy at ESM (FY20):** The M4 refocusing ellipsoidal mirror will be upgraded to a new mirror with an improved figure to enhance XPEEM illumination, which should result in a 5x increase of photon flux density. FY19 beamline review defines future ESM development particular focusing on (i) forefront ARPES microscopy capabilities (~µm spot size) as a tool for understanding quantum materials (QM) and (ii) an extended integration of material synthesis stations and spectroscopic probes. To address them, ARPES station will be upgraded with new preparation chamber, integrated optical microscope and new cryo-manipulator with submicron stability and six axis positional control.

**Synthesis of quantum material at ESM (FY20):** Future development of functional compounds and devices depends on our ability to synthesize, characterize, and control quantum materials (QM). Among new material classes particular favoring QM are low dimensional materials, artificial interfaces and quantum states with distinct topological properties. For most of such materials, the measurements performed on small sub-micron sizes specimens are essential, as it becomes extremely difficult to retain quasiparticles wavefunction coherent superposition over large ensemble. Experimental ultra-sensitive microscopies take a priority, and ESM beamline with its micro-ARPES and PEEM stations are particular attractive for QM research. Although, the specimen probing area is approaching micron size, both XPEEM and ARPES currently relay on mm size samples (often crafted by hand). To overcome this limitation, ESM intends to develop a robotic system to handle ultra-small (~100 micron size) specimens. Further, in collaboration with CFN PU, plans to bring an inert environment glove box station at the beamline are underway. This station will be equipped with a survey microscope and ultra-precise piezo translation stages for the synthesis of van der Waals heterostructures. Unlike other conventional synthesis methods (molecular beam epitaxy or crystal growth), the mechanical layer-by-layer exfoliation and stacking technique provides freedom from constraints on chemical compatibility between layers, atomic-scale interdiffusion, or strain, making possible previously inaccessible material architectures with atomically-sharp interfaces between layers and thus with vastly different electronic properties. To foster such technique, DOE has recently awarded a grant to CFN BNL, and ESM vdW station will be a part of this development linking vdW heterostructure synthesis to SR-based spectroscopic and structural measurement techniques. Finally, an in vacuum sample transfer system ("sample railway") will link MBE station for oxide growth, in-house MBE for dichalcogenides, He-lamp ARPES and vdW station in a single sample preparation cluster connected to directly to ESM ARPES and XPEEM stations. MBE system for fabrication of 2-dimensional quantum materials has been built in a partnership with Yale University. After short commissioning in FY20 it will be open to NSLS-II users.

**High and ultra-high energy resolution RIXS at SIX (FY20-21):** In FY19, good progress was made on the commissioning of the ultrahigh line-density grating and associated ultrahigh energy resolution RIXS capabilities. During FY 20-21, this commissioning will continue, and will be extended to the commissioning of the high-line density beamline grating upon its installation.
• **Expanding RIXS capabilities to continuous momentum tunability** (FY20-23): Upon successful completion of commissioning of its optics, one key remaining development of the RIXS spectrometer is a triple-rotation flange connecting the spectrometer to the sample chamber, which will enable RIXS measurements at continuously tunable momentum transfers. In addition, a manipulator with motorized control of the six sample degrees of freedom will be implemented. In late FY20 through FY23, the core RIXS capabilities at SIX will be fully operational and will enable research on investigations of collective electronic excitations in a variety of quantum materials.

• **RIXS under device-operating conditions** (FY20-23): Through the Early Career Project of Valentina Bisogni, RIXS studies of spin dynamics in model materials subjected to device-operating conditions will be enabled at SIX. This 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, will be developed to replicate device-working conditions and implemented at SIX. In FY20, a test version of OPERA will be realized to supply electric field, current, and a temperature gradient to the sample. The equipment will be tested and the first science commissioning experiments will be performed. The design of OPERA will also be completed in FY20, and will incorporate magnetic field capabilities. Testing the full range of functionalities of OPERA will be performed in FY21. During FY21-23, research on collective spin excitations will be explored in quantum materials, in the form of spin waves, topological spin arrangements like skyrmions and spin supercurrents.

• **Commissioning of Infrared and THz spectroscopy at FIS and MET** (FY20): The FIS beamline will be operating for Science Commissioning and then General Users in FY20 for studies of material under extreme conditions of pressure and temperature. The 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. Also 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 will begin technical commissioning early in FY20, with science commissioning to follow. Once fully commissioned, it will enable investigations of novel solid state systems in concert with other tools for tuning material properties. These include temperatures to ~1.8K, magnetic fields up to 10T, and pulsed laser-excitation (e.g. photo-doping). The widest possible spectral range, from 1 meV to 5 eV, will be available for reflectance spectroscopies in combination with Kramers Kronig analysis. Systems of interest include complex oxides displaying competing orders, topologically controlled phases and 2D materials such as graphene, h-BN & metal dichalcogenides, and nanomaterials. Opportunities for testing near-field nanospectroscopy will also be investigated.

• **R&D on zone-plate based RIXS spectrometer for the new ARI beamline** (FY19-20): The ARPES and RIXS nano-imaging (ARI) is a new beamline among the next suite of beamlines to be developed at NSLS-II. It will be a cutting-edge soft X-ray spectroscopy facility with two experimental capabilities - ARPES and RIXS, combined on the same spot on the sample with a spatial resolution of ~100 nm, providing for the first time the ability to measure spatially-resolved near-Fermi-edge single particle and collective electronic excitations. NSLS-II will pursue the R&D to demonstrate a high-collection-angle RIXS spectrometer, based on the novel concept of using zone-plate as its dispersion optic or other equivalent high-collection-angle optical schemes, in collaboration with ALS and CLS. Based on the outcomes of the R&D, the concept for the ARI beamline will be finalized.
Complex Materials and Processes

Simple atomic or molecular systems, colloids, nanocomposites, and polymers exhibit amorphous or self-organized order in orientation or position of varying degree that is often heterogeneous. The structural complexity of these materials along with their kinetics and nonequilibrium dynamics is one of the key themes in materials science studies in the 21st century.

The current NSLS-II scattering beamline capabilities for determination of structure and dynamics include: x-ray photon correlation spectroscopy (XPCS) at CHX (11-ID) that can probe dynamics from amorphous systems to crystalline domains; non-resonant inelastic hard X-ray scattering at IXS (10-ID) that is optimized to study THz phonon dynamics in soft materials; time-resolved, resonant, and microbeam scattering at SMI (12-ID) that can reach the elemental edges of interest in soft and biomaterials, PPLS an instrument on 12-ID for polymer processing and liquid scattering (PPLS); high-throughput complex materials scattering at CMS (11-BM); and in-situ and resonant scattering at ISR (4-ID). NSLS-II also closely coordinates with the NIST-managed capabilities of polarized resonant soft x-ray scattering (RSoXS) extending resonant scattering capabilities to below 200 eV, covering the absorption edges of carbon, nitrogen and oxygen, as well as the near edge x-ray absorption fine structure spectroscopy (NEXAFS) on SST-1 (7-ID-1), which together provide information on bulk and surface ordering of chemistry and orientation.

Our primary areas for strategic development currently include: advanced manufacturing processes, in-situ materials growth, complex fluids, and autonomous experimentation facilitated by AI/ML methods.

Advanced Manufacturing Processes. The studies of out-of-equilibrium structure and dynamics in polymeric materials ranging from polymer nanocomposites, including ceramic precursors, to biological scaffolds for cell growth are energized by the growing industrial importance of Advanced Manufacturing (AM) techniques, such as 3D printing. While these novel manufacturing techniques impact a wide range of applications, from printed micro-batteries to high-strength aeronautical/aerospace components to flexible bio-sensors and biocompatible scaffolds for organ growth, the fundamental science governing the processing and emergence of materials functionality remains poorly understood. Time-resolved structure and dynamics measurements following the temporospatial inhomogeneous processing landscape reveal the nanoscale evolution, solidification and buildup of strain in materials. This experimental basis is crucial for developing models and a fundamental understanding of the processing-property relations which is lacking for a rational design approach in many AM areas.

Our main strategy for polymeric materials AM includes the further development of fully beamline integrable AM instrumentation, compatible with ‘autonomous’ experimental approaches at all of our scattering beamlines. Such instrumentation includes a novel second-generation 3D printing platform covering the typical capabilities of desktop printers, in-situ laser annealing and electro-spray deposition systems, as well as tensile and shear stages for in-situ mechanical testing of materials and fabricated components. A polymer processing and liquids scattering (PPLS) instrument is being added to the SMI beamline to accommodate processing instrumentation as well as extend our measurement capabilities to liquid surfaces. The CMS beamline plans to develop a new ‘open sample’ space to enable proof of principle experiments with large extruders used in Big Area Additive Manufacturing (BAAM). Ultimately, we propose the concept of a scattering beamline that combines CHX/SMI capabilities with
large scale AM instrumentation and other large in-situ sample environments, such as thin film growth chambers.

**In-situ Materials Growth.** Equally exciting developments are the ability to synthesize supercrystals based on nanocrystal or nanoparticle units or layer-by-layer atomic or molecular growth with high-precision. These novel structures exhibit emergent phenomena that are largely optimized using trial and error approaches and there is a lack of fundamental understanding. The scattering beamlines (CMS, SMI, CHX) can accommodate moderate-scale in-situ growth chambers while ISR can accommodate large-scale in-situ growth chambers with gas-handling capabilities. These beamlines are ideally suited to achieve a fundamental understanding, and ultimately control, of the intrinsic and emergent heterogeneities and associated asynchronous and irreversible processes characteristic of materials growth. NSLS-II also offers the opportunity to study the driven dynamics of fabricated complex structures, whether amorphous or exhibiting varying degrees of order, their interfaces, and their behavior under mechanical, chemical, or thermal stress as well as their response to applied electrical or magnetic fields.

**Liquids - Interfacial Synthesis.** Liquid interfaces, both liquid-vapor and liquid-liquid, offer exciting new possibilities for making improved and novel 2D polymers and inorganic materials. Due to the atomically smooth nature of liquid surfaces the possibility exists to synthesize materials to the utmost perfection, such as large graphene sheets fabricated on liquid copper surfaces by CVD processes. Since there are no underlying steps at liquid surfaces, inherent with solids supports, graphene sheets prepared on liquid surfaces are of higher quality - an essential characteristic for the use of graphene in reliable electronic devices. To date, there has been little effort to investigate liquid surface supported film synthesis using x-ray scattering methods, such as those available at the SMI PPLS instrument. In addition to graphene, liquid-liquid interfaces offer the possibility of making well defined metal and semiconductor nanoparticles as well as very thin sheets of crystalline metals, such as silver, some of which are relevant to catalytic processes. Opportunities also exist to explore 2D polymer films. For instance, Reverse Osmosis (RO) membranes provides the most energy efficient means of potable water purification and these membranes are fabricated at oil-water interfaces through an interfacial polymerization process. Of note, efforts are already underway to explore the structure of these interfaces after transfer to a solid phase at NSLS II. In-situ structural studies during polymerization, yet to be carried out, would provide invaluable insight into how to make improved materials. Interfacial polymerization reactions are also used to make may different amorphous and ordered polymer 2D films are these are all well suited to liquid interfaces x-ray studies during processing. The PPLS instrument will be optimized for liquid interface synthesis studies, thus allowing users to identify the best conditions for optimal material’s synthesis. This should allow SMI to attract a new user community.

**Acoustic Metamaterials.** Phononic metamaterials are mesoscale structured systems that control sound propagation through a modulation of their density distribution. Control of phonons in the terahertz frequency window is particularly significant since heat conduction in insulators mainly involves high-frequency phonons as a carrier. The manipulation and control of phonon propagation at terahertz frequency is thus the key to implementing heat manipulation based on the mesoscale structure design. Although terahertz phononics is still in its infancy, it was demonstrated that it can enable the development of a whole class of novel thermal devices such as thermal diodes, thermoelectrics and thermocrystals. Since sound propagation mainly driven by the elastic constants of a material, mesoscale structures composed of materials having large disparate elastic constants with structural variation distances matching terahertz phonons wavelengths effectively interact with terahertz phonons. Hybrid (solid and liquid state) materials organized at nanometer distances, such as superlattices of nanoparticles or complex nanoscale materials as liquid crystals, and block copolymers, are particularly well-suited
candidates to explore terahertz phonon properties. New light on this unexplored field can be achieved through the coordinated use of CFN nano-fabrication tools, the IXS terahertz phonon characterization capability, complementary IR probes, and molecular dynamics simulations.

**AI/ML-Based Autonomous Experimentation.** A key feature of modern complex materials, common to a large majority of industrial materials as well as research-grade functional materials, is that their structure and properties depend on a large number of material composition and processing parameters. In order to generate desired functionality in these materials, it is critical to understand their complex constituent-processing-structure-property relations; this in turn requires an ability to efficiently probe the associated vast, multi-dimensional material and processing parameter spaces, going beyond traditional trial-and-error or exhaustive high-throughput approaches to material exploration. Machine-guided autonomous experimentation (AE) is a promising strategy to address this challenge.

Our strategy in AE includes: application of the prototype AE pipeline, recently developed and deployed successfully at the CMS beamline, to techniques beyond simple SAXS and extension to multiple beamlines, including microbeam SAXS/WAXS at SMI and XPCS studies of advanced manufacturing processes at CHX; incorporation of in-situ material synthesis and processing into the autonomous loop; development of generic methods to incorporate physical, system-specific, expert knowledge into the decision algorithms; ML-accelerated real-time data processing and analysis methods to speed up and/or expand the scope of AE-enabled parameter space exploration and feature/process optimization. The development effort will take advantage of ongoing collaboration with CFN, CSI, and DOE CAMERA. Existing collaboration for scientific application of the AE approaches includes CFN, NIST, AFRL, Columbia U., and U. Warsaw.

As described below we will continue to optimize our scattering beamlines for in-situ determination of complex materials’ structure and dynamics. Our main strategy here is to fully ramp up the user programs at these beamlines and conduct scientific programs in collaboration with a wide range of materials scientists from thin-film growers to physicists and engineers. In addition, we plan to pursue the new development projects discussed below and to establish a wide range of ancillary sample environments to broaden the complex materials research activities at our beamlines.

- **Enhanced beamline optics performance at CHX** (FY20-21): CHX will add the capability of a wide-bandpass multi-layer monochromator, which will increase the coherent flux at CHX by a factor of up to 30 over existing facilities, thereby enabling the measurement of dynamics in the small angle regime on time scales 900 times faster than previously possible. CHX will also incorporate additional diffraction-limited kinoform focusing lenses for XPCS measurements at select energies covering the full 6-16 keV range (currently kinoform lenses are available only for 9.6 keV and 12.8 keV).

- **Addition of a suite of sample environments for in-situ XPCS studies at CHX** (FY20-22): CHX will pursue enhancement options with a full suite of sample environments for in-situ studies including, but not limited to: microfluidic cells for studies of self- of colloidal superlattices and ‘colloidal materials’, and a chamber for high-throughput and high-temperature SAXS-XPCS.

- **Implementation of the VIPIC detector at CHX for XPCS at micro-second scales** (FY21-22): The VIPIC is a prototype pixel array detector, being developed by the NSLS-II detector group, and consisting of a two-level microchip design that provides twice the area per pixel and allows on-detector, real-time, processing to perform auto-correlation for XPCS experiments. Once available (currently expected in FY21), it will be installed at CHX to enable XPCS studies at revolutionary micro-second scales for wide range of dynamic studies. In the meantime, the CHX team will continue
to survey the field for other fast detector options. With the anticipated increase in coherent flux (through e.g. the use of wide-bandpass multilayer optics) it will become possible to access increasingly faster time scales if, and only if, fast – e.g. microseconds or faster – photon counting pixel array detectors become available.

- **Software development to enhance X-ray scattering capabilities** (FY20-21): The CHX team has partnered with the CSX and DAMA groups to join a multi-facility effort involving both the Advanced Light Source and the Advanced Photon Source. The goal of this extended group is to develop a set of tools and libraries for XPCS covering all experimental needs, form data acquisition and data management, to data analysis and visualization. This software package will consist of a library of routines for XPCS including algorithms for multi-tau, two-time, speckle visibility and speckle tracking correlation functions. These modules will be written in C and designed for parallel computation through the OpenMP/MPI platform. These modules will be wrapped into higher-level languages such as Python and be readily available for user data analysis in environments such as XI-CAM, Jupyter Notebooks or other Graphical User Interface platforms.

- **Machine-learning methods for x-ray scattering data analysis** (FY 20-23): The Partner User group from CFN, in collaboration with Computational Science Initiative (CSI), has been developing machine learning (ML) methods to classify x-ray scattering images and extract material structural features from scattering data. These methods will be implemented on a GPU server at CMS to enhance real-time analysis capabilities for SAXS/WAXS data. On another front, in collaboration with CSI, ML methods will be developed to automate and thereby greatly accelerate XPCS data analysis. The scope of this project includes the classification of dynamics and correct choice of analysis model, optimal binning of out-of-equilibrium datasets and ML assisted quantitative analysis of high dimensional XPCS data (out-of-equilibrium, spatially and angular resolved). Successfully implemented, these methods will not only allow users to make timely experimental decisions during beamtime but also will enable autonomous XPCS-based exploration of nonequilibrium material dynamics at CHX.

- **Autonomous experimentation at beamlines** (FY 20-23): To enable intelligent exploration of complex materials in vast parameter spaces, capabilities for autonomous at-beamline experimentation are being developed in collaboration with the Partner User group from the CFN and DOE CAMERA (LBNL). The prototype autonomous pipeline, recently deployed successfully at CMS (11-BM), consists of: automated sample handling and data collection; real-time SAXS/WAXS data analysis; and physics-agnostic, measurement-technique-independent decision algorithms that use the analysis results to select the next experimental point to be measured, providing input for data acquisition to complete the autonomous loop. Application of this pipeline to a select set of user experiments has begun at CMS. The next steps in this effort will explore: generalization to other beamlines and techniques, including microbeam SAXS/WAXS at SMI (12-ID) and XPCS at CHX (11-ID); integration of *in-situ* material generation and processing into the autonomous loop; acceleration and expansion of real-time data analysis capabilities; and continual development of decision algorithms, including generic methods to incorporate physical, system-specific knowledge into the decision process.

- **Enhancing counting efficiency at IXS** (FY20-23): At IXS, the current ~1 meV spectrometer is based on an analyzer scheme combining post-sample collimation and flat asymmetric crystal optics that offers sharp tails in energy resolution function and high Q-resolution – a unique strength for studies of terahertz dynamics in complex soft matter systems. The instrument is currently very photon-flux limited, making all measurements, including diagnostics, difficult and time-consuming. Thus, the
main development direction for IXS in the next five years is to improve this situation. Efforts will include improving the throughput of individual optical elements by identifying and rectifying the sources of losses. An estimated factor of 10 overall gain might be possible. We further plan to implement a new 2 meV upgrade to further increase the counting rate by 4 times by broadening the energy resolution to ~2 meV using a new set of high-resolution monochromator and spectrometer analyzer crystals. Further improvement of the counting efficiency can be made by adding two more analysers to allow parallel data acquisition and/or a new undulator in the straight section (at significantly higher cost). In this plan, we will continue to use the novel analyzer optical scheme thus the upgrade will continue to offer sharp tails in the energy resolution function. Scaling back the energy resolution will allow higher productivity from the beamline. In FY20 timeframe, we will make the decision whether to further improve the IXS energy resolution to ~1 meV or sub-meV based on the lessons learned by that time.

• **Software development to enhance user productivity at IXS (FY20-22):** This effort includes two aspects: (1) implement software packages to enable MD or *ab initio* simulations prior to experiment to identify (E,Q) regions of interest to guide data acquisition, and help subsequent data interpretation. (2) streamline and automate data acquisition, reduction and analysis, including beamline and spectrometer optics alignment and optimization.

• **Ramping-up additional capabilities at SMI (FY20-22):** Several development projects are planned at SMI to advance the core scattering capabilities at both tender and hard x-rays. These include: switching tender x-ray beam polarization from horizontal to vertical to allow probing both s and p scattering to determine molecular orientation in soft and composite materials at S, P, and Cl K-edges; upgrading WAXS detector with a multi-modular 3x400KW detector to improve the throughput in WAXS geometry by >10x; and increasing low-Q resolution for studies of greater range of features in typical materials. Moreover, to more effectively utilize the tender x-ray polarization switching capability, software for data processing and simulation will be developed using the Xi-CAM platform, for use both at the beamline and as a stand-alone software package. A coordinated program will be established with the complementary polarized soft X-ray resonant scattering program at the SST-1 beamline. Finally, in FY20, the WAXS chamber will be equipped with a high energy resolution, wide energy range x-ray fluorescent detector, which, in addition to existing SAXS/WAXS capabilities, will enable simultaneous elemental mapping of samples. This capability will be important for the composites and biominerals communities.

• **Polymer processing and liquid scattering instrument at SMI (FY20):** The Polymer Processing and Liquid Scattering (PPLS) instrument is a versatile x-ray scattering facility sharing the canted straight section at 12-ID (see Page 35). Whereas the long-term vision is for an independent PLS beamline with its own undulator and optics, the interim plan FY20 is to finish commissioning a fully operating Polymer Processing and Liquids Scattering (PPLS) instrument using the 12-ID beam in a time-shared mode. The PPLS instrument utilizes exiting equipment from the former liquid spectrometer at the APS in a unique design with detector stations for XR, (GI)SAXS and (GI)WAXS that will operate at x-ray energies ranging from 8-24 keV. The PPLS endstation would be greatly enhanced by the purchase of dedicated large area detectors for SAXS and WAXS as these were not included in the construction project.

• **Open-platform sample setups for advanced manufacturing studies at CMS and PPLS (FY20-22):** To facilitate in situ SAXS/WAXS studies of materials under processing conditions, open platform setups are being developed at CMS and PPLS. At CMS (11-BM) the first iteration of an open-platform sample staging area is now available - upstream of the main scattering chamber - that
utilizes the CMS SAXS detector and a 300k Pilatus for WAXS. The PPLS instrument, shared optics with SMI, is expected to enter operations in FY20; it will provide a brighter beam, enhanced time resolution compared with CMS, and will share the 300k with CMS. Both instruments are well suited to advanced manufacturing-relevant studies that require medium-scale material processing and testing such as 3D printers, blade coaters, and a shear stage. Taking advantage of these new setups and in collaboration with the CFN Partner Users, instrumentation for in situ materials processing (e.g., photothermal annealing for polymer and nanocomposite thin films) will be developed, integrated into beamline control, and made available to general users. Both the CMS and PPLS efforts will complement ongoing and anticipated future efforts at CHX. At a later stage, it is anticipated that a floor-to-ceiling sample space will be created at CMS and/or PPLS to accommodate industrial-scale processing equipment.

- Additional sample environments and technical capabilities at ISR (FY20-21): Several development projects are planned for the purpose of increasing the breadth of materials physics experiments at ISR. These projects include: extending the x-ray energy range down to 2.4 keV in FY20 to enable 4d transition metal L edge resonant x-ray scattering, with applications to novel order in transition metal oxides and dichalcogenides, magnetic spinels, and superconducting FeS; hazardous gas handling in FY20 to allow in-situ studies of the growth of graphene and nitrides; coherent scattering capability in FY19-20 to investigate dynamics of materials growth and processing, as well as imaging of electronic order domains; addition of a 2.5 Tesla, vertical field magnet in FY20 to enable studies of magnetic-field-induced effects on structure and electronic order; commissioning of polarization control and the addition of a 2.5 Tesla, horizontal field magnet in FY21 for a hard x-ray magnetic circular dichroism (XMCD) capability; and sub-100 µm horizontal focusing for the 6-circle.

Catalysis and Materials Research in Operando

One of the most challenging goals in chemical and materials sciences is to understand how things work in a real functional environment. This is often the key to connect the basic knowledge of materials properties to actual working devices and engineering systems. This is particularly true when materials systems increasingly become more complex – often composed of multiple heterogeneous chemical and phase components and impurities with complex interfaces. There is a clear need for advanced characterization tools to allow investigation of realistic functional materials under working conditions relevant to natural or industrial processes. This section focuses on developing a suite of suitable in-situ and operando capabilities at NSLS-II to meet the research needs in chemical and structural sciences, and address the scientific challenges.

Our scientific objective is to enable better understanding and ultimately control the chemistry and structure of complex and heterogeneous materials and their interfaces, charge transfer and reactivity in catalysis and energy conversion systems, and reaction pathways and products in complex diverse environments. In addition, these in-situ and operando approaches will be supplemented by high-throughput materials genome tactics through which likely materials candidates from a vast number of possible systems are identified for real-time operando experiments and theoretical modelling.

NSLS-II high brightness and flux in a broad spectrum allows highly efficient and effective correlated studies using hard X-ray spectroscopy, diffraction and scattering, and imaging to reveal how things work in a variety of functional systems, including energy storage, catalysis, fuel cells, corrosion protection, and many others. Our development strategy in this area focuses on integrating high-throughput
measurements, database-enabled data mining and analysis, and density functional theory (DFT) modelling with optimally designed in-situ and operando experiments at NSLS-II beamlines. Together this strategy offers a well-balanced portfolio of experimental capabilities that will enhance chemical and materials science research on diverse and heterogeneous materials systems.

Catalytic processes are essential for production of fuels and chemicals. Understanding and optimizing heterogeneous catalysts is critical to many branches of chemical industry. Catalytic performance in terms of activity and selectivity, as well as longevity of the catalyst, are determined by an interplay of interactions between active phase, support, reactants and reaction products. These interactions occur on different length scales from Angstroms (chemical bonds) to microns and millimeters (diffusion in catalyst particles). The timescales for a catalytic reaction vary from seconds (redox chemistry) to femtoseconds (photo-stimulated processes). Intelligent catalyst development and optimization requires detailed knowledge of their structural and electronic properties over the full range of relevant length and time scales. Leveraging its high X-ray flux and broad spectrum, NSLS-II provides a suite of characterization tools, capable of probing the catalysts in operando, i.e., under actual reaction conditions and with the ability to correlate observations with performance.

In-situ, operando & extreme environments, high throughput (large batch of samples, combinatorial studies) and real-time observation (transient states, along different pathways, i.e. away from equilibrium and static conditions) have become essential thrusts of synchrotron research in Materials and Engineering Sciences. As mentioned above, the focus is on the studies of real and complex samples, i.e. away from ideal crystals, in presence of multiple phases and defects or a high degree of disorder and all the way to poorly crystalline or glassy or amorphous state, and over multiple length scale. Combined characterization using in-situ and operando synchrotron X-ray and transmission electron microscopy techniques offers new opportunities for in-depth studies of ion transport, electrochemical reactions, and phase transformations over multiple length and time scales in battery and energy storage science.

The development of Advanced Manufacturing is a shared DOE, DOC, DOD, and NSF agency goal. In this field, NSLS-II can contribute: i) instrumentation for high-throughput ex-situ studies and in-situ growth and processing studies and operando studies that link structural, chemical, electronic properties to material or device performance; ii) high-performance computing for real-time analysis, efficient parameter space exploration, and optimal extraction of information from complex data sets.

Amongst the grand challenges for materials scientists in the 21st century is the discovery of the next-generation materials for energy production, storage and for mitigating the environmental consequences of energy usage. Their development is based not only on the knowledge of their static structure, but more appropriately on an understanding of how the structure changes during operation under real working conditions. Theory and experiment can be integrated in a closed loop in exploratory syntheses, where theory can identify theoretical desired materials that are thermodynamically stable, and in situ diffraction/spectroscopy studies of synthesis could then be used to pinpoint the feasible synthetic routes. In situ tools at NSLS-II are being optimized to track the physical and chemical changes occurring along a set of tentative pathways, provide the critical data required for i) the development of the atomic scale modeling of synthesis, and ii) to rationally steer the reaction through new pathways and toward optimized materials, and generates the raw minable data for machine learning of what manipulations lead to which optimized products.

A pillar of the NSLS-II chemistry and materials research program is to offer a coordinated array of techniques that provides a comprehensive set of spectroscopic and structural data on real and heterogeneous systems over multiple length and time scales. The key beamline facilities at NSLS-II that
focus on operando and high-throughput chemistry and structural research include: Inner-shell spectroscopy (ISS) at 8-ID, quick absorption and scattering (QAS) at 7-BM, in-situ and operando soft x-ray spectroscopy (IOS) at 23-ID-2, X-ray powder diffraction (XPD) at 28-ID-2, pair distribution function (PDF) beamline at 28-ID-1, and NIST partner beamlines soft & tender spectroscopy (SST-1 and SST-2) at 7-ID and materials measurements (BMM) at 6-BM. Planned development projects at these beamlines, including a high-energy X-ray (HEX) beamline under construction, are described below.

- **Commissioning of gas handling systems at ISS, XPD, PDF and ISR (FY20):** Advanced gas handling systems (GHS) are being implemented at ISS, XPD, PDF and ISR beamlines, each with complete gas storage, separation, filtering, control, and exhaust systems to handle a range of hazardous and non-hazardous gases for user experiments. These gas systems will allow in-situ / operando experiments to be conducted involving thin film processing, chemical reactions and materials synthesis with a wider range of gas-phase ingredients and products. Capabilities for rapid switching and the delivery of hazardous gasses will be added to the system in FY20. Additional sample environments will be developed to take full advantage of the GHS offering automatic delivery of multiple-gases, sample heating, and in-line residual gas analysis (RGA) capabilities.

- **Development of sample reactor cells for specific applications at ISS (FY20-21):** We will continue to develop reaction environments for battery, electrochemistry and catalysis research, in support of the high throughput capabilities for the beamline. In catalysis, we will extend the parameter space to cover high pressure relevant to many industrial catalytic processes, through the collaboration with BNL Chemistry supported by an LDRD. Also, we will develop fast switching gas feeding system, which permits modulation excitation spectroscopy and fast kinetic studies. For battery and electrochemistry, we will design and commission experimental infrastructure allowing for parallel experiments with multiple reaction cells, leveraging the measurement speed at ISS. We will also commission the growth chamber for in situ Atomic Layer Deposition at the beamline.

- **Development of sample-tracking and data-analysis tools for operando experiments at ISS (FY20-22):** For many operando high-throughput experiments, one of operational challenges is to be able to identify and track a large batch of samples that may have similar appearance for both experimental measurements and post-experiment analyses. We will work and coordinate with other programs and partners to provide common sample-tracking and data analysis platforms, including the ability to tag datasets with sample identification, as well as the possible incorporation of available materials databases and DFT modelling (in collaboration with CFN) for data analysis. As part of the multimodal science strategy that the NSLS-II is enforcing, these tools will also be implemented at other high throughput beamlines such as XPD and PDF. Tracking and fiducializing the samples across several beamlines and combining different datasets (e.g. spectroscopy and diffraction) in a common analysis framework will considerably leverage the amount of science that can be extracted.

- **Upgraded IO-XAS chamber at IOS (FY20):** In FY19, the IO-XAS endstation was upgraded with a new chamber to enable the operation of liquid flow and gas reactor cells for operando X-ray absorption spectroscopy experiments. This capability will be important for the heterogeneous catalysis, electrocatalysis, and battery communities. This is done in partnership with the Catalysis: Reactivity and Structure group in the BNL Chemistry Division. Technical and science commissioning started in FY19 and will be completed in early FY20.

- **Inelastic Scattering, Photoemission, and Infrared Endstation (INSPIRE) (FY20-24):** INSPIRE will offer a unique combination of state-of-the-art ambient pressure XPS, XAS, IR, and XES/RIXS capabilities for advanced energy and catalysis systems under the same close-to-realistic operating conditions for operando and high-throughput chemistry and structural research.
conditions, at chemically relevant time scales. As described in more detail p. 30, it consists of a new endstation and optics upgrades to the IOS (23-ID-2) beamline.

- **Development of high-throughput spectroscopy experiments at ISS** (FY20-21): High-throughput and data-driven approaches can be crucial for guiding smart operando experiments in catalysis research so that the operando methods can be more effective and impactful. We will work with other partners, including CFN, to pursue these high-throughput spectroscopy experiments. In FY20, we will continue working on the LDRD-funded project to use combinatorial growth and multimodal characterization to optimize silicide synthesis. Such experiments will not only be of scientific interest but also provide real datasets to developing and prototyping data analysis and data mining algorithms for these types of experiments.

- **Developing integrated database- and modelling-enhanced data analysis tools** (FY20-21): In collaboration with NSLS-II data acquisition/management/analysis group, and key interested partners such as CFN, CMPMS, and CSI, we plan to form a working group across multiple beamline programs to work on integrated databases and DFT modelling for experiments and analysis. A new LDRD was funded to start in FY19 for this work. We will initially focus this effort on real-time analysis of near-edge data from x-ray spectroscopy and photo-electron spectroscopy. Further development will also include data from diffraction and scattering. Specific aims of this 2-year LDRD are: (1) to establish a toolbox for structure determination combining a multimodal approach with a data analytics effort which is based on microscopic theory, and (2) to demonstrate tuning of the growth of silicides to discover phases and heterostructures that optimize their quantum functional behavior.

- **Development of low-temperature magnetic field dependent measurement capabilities at PDF** (FY20-21): In collaboration with Condensed Mater Physics and Materials Science department at BNL, the PDF beamline purchased a (0-5) Tesla superconducting magnet that can be coupled with a (0-500) K liquid He cryostat for studies of materials at low temperatures under an external magnetic field. The magnet is currently being commissioned with a 117 keV X-ray beam. Once fully commissioned, it will be used for the studies of magnetic field induced structural phase transitions in strongly correlated materials in a wide temperature range.

- **Commissioning of the small angle scattering (SAXS) setup at PDF** (FY20-21): The PDF beamline end-station is equipped with a movable flight path to provide complementary SAXS data along with PDF and medium resolution XRD data. Once fully commissioned, the PDF beamline will be well suited for *in situ* studies of hierarchical materials, where key structural features exist on atomic to nanoscale to mesoscale length-scales. The fast exchangeability between setups will enable multimodal data acquisition during the same measurement.

- **Building towards a high-throughput mail-in program at PDF** (FY20-22): Thanks to the high-speed gantry available at the end-station, the PDF beamline is well adapted to perform high-throughput measurements on many samples, rapidly measuring PDF, XRD, and SAXS data. We continue to build up capabilities for high-throughput, multi-PI data management, with a goal towards autonomous data delivery. We aim to eventually develop a mail-in program to augment the existing general user program on PDF, which will be modeled after other successful mail-in programs at synchrotron facilities worldwide. Such a program will grow the overall NSLS-II user base, reduce workload on staff, and directly service the greater US Total Scattering community by making synchrotron X-ray total scattering data more readily available.
• **Commissioning of high-resolution configuration at XPD using a multi-analyzer system** (FY20-22): XPD will offer the option of a high-resolution configuration (for structure solving and line profile analysis) by implementing a unique system composed of 8 channels fitted with analyzer Laue crystals. It will use two distinct detector units developed in house, that are angle-scanned simultaneously and collect the sample-diffracted signal with and without the analyzer crystals. One unit is an array of photomultiplier tubes associated with GYSO scintillator crystals, The second unit is an array of $8 \times 8$ CdZnTe chips.

• **Commissioning of the second endstation hutch D at XPD** (FY20): Hutch D is designed to accommodate more elaborate/complex setups for in-situ structural studies, including large pressure cells, large volume press, reaction chambers, combined spectrometry, user-custom devices, etc. In FY19, in partnership with the COnsortium for Materials Properties Research in Earth Sciences (COMPRES), a multi-anvil system (MAXPD) was integrated that consists of a 1,100-ton hydraulic press with DIA, equipped with a unique DT-25 pressure module that can be swapped out for a more standard D-DIA module as desired. MAXPD utilizes monochromatic X-ray beam (usually 52 keV or 67 keV). The experimental setup has provision for imaging the sample during measurements, and for collection of angle-dispersive X-ray diffraction patterns. The MAXPD facility will be developing an on-site fully equipped sample and experiment preparation laboratory, as well as preparation facilities at Stony Brook University that are maintained and operated by the Mineral Physics Institute. MAXPD is ideally suited for high pressure and high temperature experimental deformation /rheological measurements and in situ ultrasonic interferometry experiments at extreme conditions.

• **Development of in-situ synthesis experiments at XPD** (FY20-22): In situ synthesis is one of the major research directions at XPD. It encompasses a large variety of experiments, ranging from high temperature solid state growth, to colloidal nanoparticle growth from solution, flash sintering of ceramics/oxide materials, nucleation & growth of MOFs, and microwave-assisted synthesis. Theory and experiment can be integrated in a closed loop in exploratory syntheses, where theory can identify theoretical desired materials that are thermodynamically stable, and *in situ* XRD synthesis could then be used to pinpoint the feasible synthetic routes. This new approach has great potential to accelerate materials discovery. A pilot project, funded through the NSLS-II joint graduate student program in collaboration with Prof. Jonathan Owen of Chemistry at Columbia University, is meant to build and deploy a flow cell at XPD and to collect Total scattering patterns on PbS, PbSe, CdS, and ZnS nanocrystal nucleation and growth from solution, coupled with high throughput data acquisition and PDF analysis. The project uses a library of sulfur and selenium precursors to unravel the fundamental mechanism of the nanocrystal nucleation and growth process and to identify the best conditions in the material’s synthesis. This pilot project will be extended to a program to develop a growbot for high throughput synthesis of next generation nanomaterials for applications in energy harvesting, lighting and quantum electronics. A large multi-dimensional chemical parameter space will be generated using this growbot through combined time resolved optical & diffraction measurements. These large data set will be used further in AI and ML algorithms to predict targeted nanomaterials.

• **Improved high-temperature sample environment capabilities at PDF and XPD** (FY 20-22): Well controlled, temperature-dependent studies of materials are critical for many inquiries including reaction evolution, synthesis, catalysis, decomposition, and phase-space mapping. By nature of serving such a diverse set of communities, the beamlines must readily adapt to a diverse set of sample conditions, such as small sample quantity, samples that are air sensitive, samples with potentially unbound nanomaterials, and samples with large grain size. To meet these needs, both the XPD and PDF beamlines coordinate and will continue to expand and integrate a large array of sample
environments, integrated in a workflow based on a detection scheme that includes both the near-field and the far-field large-area cameras.

- **Development of simultaneous DRIFTS, PDF and/or XRD measurement capabilities at PDF (FY 20-23):** Paring diffuse reflection infrared Fourier transform spectroscopy (DRIFTS), PDF, and XRD analysis can provide invaluable information on the evolution of surface adsorbates and structural dynamics of materials. The proposed setup will be composed of an FT-IR spectrometer with an external sample compartment, an MCT detector, and a reaction cell that enables measurements in the temperature range (27-600°C). The reaction cell will also be equipped with a mass spectrometer to monitor reaction products. Once fully commissioned, users will be able to simultaneously probe the same sample volume using three different techniques.

- **Development of quasi real-time data processing at XPD and PDF (FY20-22):** This project is meant to develop quasi real-time data processing, pipelining, and visualization that build upon the XpdAcq/Bluesky software in collaboration with Prof. Simon Billinge at Columbia University and in coordination with the NSLS-II data acquisition, management, and analysis group. Throughput and productivity will be augmented by the advent of new theory-and computer-assisted predictive tools: i) database mining engines and search-and-match routines to identify and compare data coming off the detector with experimental and/or calculated data. Tests have started with the open-web based Materials Project; ii) self-similarity or Principal-Component-Analysis (PCA ) algorithms to detect on the fly changes in a flow of diffraction patterns over time that can reveal a genuine structural effect like a phase transition (or an instrument artefact like a beam energy shift); iii) machine-learning techniques taking advantage of the large datasets that the beamlines generate.

We plan to develop optimized hardware and software to allow automated operations and to incorporate machine-learning techniques beyond the current trial-and-error approaches and towards automation. Sample management will be synchronized with both the near-field and the far-field detectors, while using either the low- and/or high-temperature devices (100K – 1,000°C).

- **Development of multiple length scale time resolved measurement capability at XPD (FY20-22):** Often in-situ processes & synthesis of complex materials goes through smaller crystalline length scales (liquids, amorphous, nanocrystalline) to larger length scales crystal phases (10s of microns). To understand the growth processes or reaction pathways one needs time resolved measurements on all the length scales at ones. This project is meant to develop a real-time Total Scattering and High Resolution XRD data collection in sub-sec time scale from the same sample at same condition. As described previously we will be utilizing our experiences and tools for sample environments, 2D detector for Total Scattering measurements and use a high efficiency-fast Striped Germanium Detector (developed at NSLS II) along with multi analyzer system for High Resolution XRD measurements. This capability at XPD beamline will provide a detailed structural evolution information of the sample synthesis & process in both solution synthesis and solid-state synthesis regimes.

- **Development of XRD tomography in hutch-D at XPD (FY20):** Funded by a Scientific Infrastructure Support for Consolidated Innovative Nuclear Research Award from DOE, Nuclear Energy, a new capability for X-ray Diffraction-Computed Tomography (XRD-CT) was designed and installed at the X-ray Powder Diffraction (XPD) beamline. XRD-CT will be used on materials primarily for nuclear energy systems and is intended to provide users 3D reconstructions of sample morphology directly from diffraction patterns and full-field X-ray radiographs. Unlike traditional X-ray computed tomography that is solely based on X-ray absorption, XRD-CT simultaneously supplies
crystallographic structural information with spatial resolution set by the beam size, e.g. \((30\mu m)^2\) at XPD. The structural information available includes; phase identification, phase fraction, grain size and lattice strain in a wide variety of materials (metals, ceramics, composites, concretes and nanocrystalline materials) that have undergone fabrication, mechanical deformation or radiation damage.

Through coordinated scheduling with hutch C, hutch D can also allow long-duration experiments by receiving the x-ray beam intermittently to enable short and repetitive measurements at regular intervals over a long period of time for e.g., corrosion studies, slow growth processes, charging and discharging of batteries, degradation of cathodes and anodes in fuel cells, and environmental effects on solar cell materials.

- **High-energy Engineering X-ray Scattering & Imaging (HEX) Beamline 27-ID** (FY20-22): the HEX beamline is a new beamline under construction, funded by New York State Energy Research & Development Authority (NYSERDA), to provide a suite of most advanced hard X-ray tools required for in-situ studies of engineering-scale material systems using diffraction, scattering, and imaging. The beamline will use a superconducting wiggler as the high-energy high-flux X-ray source. HEX is designed to consist of three independent endstations and a satellite building to provide hard X-ray diffraction and imaging probes in the 20-200 keV range for studies of engineering material systems under operating conditions. Only the central branchline will be fitted out within the construction project, with affordances for the other 2 side branches.

Key science areas at HEX will be in the areas of structural analysis of the chemical reaction fronts and their evolution in real battery systems during charge and discharge cycles, materials microstructural changes under external extreme conditions such as high mechanical stress, high pressure, high temperatures, and corrosive environment, and phase contrast hard X-ray imaging with a large field of view in real space for studies of micro-crack formation and propagations under realistic operating loads, etc. These studies will have significant impact on the economic competitiveness of industries in New York State as well as in the nation. It is expected that the HEX construction will be completed and commissioning will start in early 2022.

**Multiscale Structure and Function**

This science focus area covers a broad range of research disciplines, from heterogeneous materials science and engineering, to environmental and energy sciences. A common research theme in all these disciplines is to understand the properties of matter at multiple spatial and temporal scales - from atomic to nano- and micro-scales in length, and from sub-ms to seconds and beyond in time. Here the world-leading brightness, exceptional beam stability, and cutting-edge nano-/micro-focusing at NSLS-II provide unparalleled capabilities to the researchers in the field.

Building upon the enormous atomic-scale scientific knowledge acquired in the past century, it has become apparent that the structural, electronic, and chemical behavior on length and time scales between the atomic and the macroscopic world hold the key to emergent macroscopic behaviors and functions of materials and biological systems. Understanding and controlling the interplay between the multiscale structure, dynamics and functions of materials is central to modern science today. From the processes of materials synthesis that control the crystalline strain quantum microelectronics to the influence of crystalline structure and nanoparticle morphology in electrodes on the lifetime of batteries, NSLS-II
beamlines play an increasingly critical role in the research in these areas. Taking advantages of high brightness and small source size, NSLS-II will continue to develop a suite of advanced structural, electronic, and chemical imaging programs that span multiple length and time scales, enabling cutting-edge correlative and multimodal studies in heterogeneous materials systems.

While all NSLS-II beamlines play some roles in contributing to the knowledge of multiscale structures and functions, the beamlines in the imaging and microscopy beamline program are particularly important to this science focus area. These currently operating beamlines include Hard X-ray Nanoprobe (HXN) at 3-ID, Submicron Resolution X-ray Spectroscopy (SRX) at 5-ID, X-ray Fluorescence Microscopy (XFM) at 4-BM, Tender Energy X-ray Spectroscopy (TES) at 8-BM, Full-field X-ray Imaging (FXI) at 18-ID. Together these beamlines support a diverse and active scientific user community in nanoscience, materials science and engineering, microelectronics, energy storage, geo-environmental sciences, and systems biology.

Given the diversity of the scientific programs, our key strategy in imaging and microscopy is to:

- develop world-leading capabilities in nano-/micro-imaging, leveraging NSLS-II high-brightness and nanofocusing optics R&D;
- develop advanced DAQ capabilities for milli-second scale kinetic studies and fast multi-dimensional imaging of materials systems;
- target leading researchers in their respective fields and develop and perform a number of well-designed, hypothesis-driven projects with high-potential for high-impact results;
- work closely with CSI and NSLS-II data acquisition/management/analysis group to develop high-performance software codes to enable data visualization, analysis, and mining to extract out most relevant scientific information from large numbers of datasets.

Following these strategies, a number of initiatives and development projects will be pursued in the next five years, as described below.

- **Implementing large-aperture sub-10nm wedged MLL nanofocusing at HXN (FY20-23):** Working closely with the X-ray optics group, we are developing large-aperture, wedged multilayer Laue lens (MLL) with a goal to achieve sub-10 nm focusing for hard X-rays (see Page 21). In FY18 we made significant advances in wedged MLL development and demonstrated 7.5 nm line focus with ~30% efficiency at 15 keV. In FY19-21, we will continue to improve the wedging for higher efficiency and pair two wedged MLLs to produce a 2D focus of ~7-8 nm with over 20% overall efficiency. We will implement this new capability and integrate it into general user operations at HXN.

- **Nanospectroscopy capability at HXN (FY20-23):** Nano-spectroscopy provides a unique capability for chemical imaging at the nanoscale with high detection sensitivity. Thus, it is a vital tool in many scientific areas. We have demonstrated nano-XANES with resolution of ~50 nm using current beamline optics, and developed the associated data analysis work flow. To significantly improve the energy tunability and instrument repeatability, we plan to upgrade the existing CRLs with a pair of vertical focusing mirrors. Facility improvement funding has been awarded for this upgrade. Technical specification and statement of work will be completed in early FY20, so that the instrument can be developed through a commercial vendor. The new instrument is expected to be commissioned in FY 22, followed by science commissioning. In FY23, we plan to provide routine nano-spectroscopy capability for general user experiment.

- **Nanoscale strain imaging for microelectronics research (FY20-23):** The HXN beamline, along with the Bragg CDI (CDI) beamline under-development, can provide nanometer-scale mapping of very slight distortions, down to the picometer scale, in the lattice of crystal. The measurement of
coherent scattering data near two or more Bragg reflections can then be used to make a quantitative
determination of the strain within a particular region of the sample. Such strain maps can often be
directly tied to the function of materials, establishing important structure-function relationships that
may be used in QIS materials engineering. The Bragg CDI project will expand the strain-imaging
capabilities of NSLS-II by accommodating larger samples and a wide array of sample environments
to further in situ and operando capabilities, when compared to HXN. When combined with
measurements at CSX, which are more sensitive to electronic structure, the atomic and electronic
structure of materials can be unified to provide a more complete understanding of physical
phenomena. High spatial resolution (~10 nm) of the HXN with high monochromatic photon density
(>10^7 phs/nm^2) is a unique tool for imaging the next-generation microelectronics. The HXN
beamline team, in collaboration with the IBM scientists, has successfully imaged strain from a new
3D gate architecture known as “nanosheet” with the gate thickness down to 7 nm.

- **Feasibility of nano-XRD imaging of phase change mechanisms in neuromorphic devices** (FY20-
  24): Neuromorphic computing is a futuristic computing architecture emulating the operation of a
  biological brain. Transition metal oxides (TMOx) exhibiting a metal-insulator transition (MIT) are
  among the best candidates for neuromorphic applications as a well-controlled and reversible MIT
  can mimic the functionality of neurons. Nano-XRD at HXN provides a novel capability to detect
  structural phase changes during and after an electrical pulse is applied. This research will help the
  researchers in the field to understand and ultimately control how these artificial neurons are fired,
  thus improving their functionality for neuromorphic computing applications. We plan to outreach to
  active research groups working in this exciting research field to conduct test experiments at HXN,
  and will further develop this into an active program if proved feasible.

- **3D multi-modal imaging at HXN** (FY19-21): The goal of this project is to develop and mature an
  efficient multi-channel 3D imaging methodology to provide a comprehensive view of the sample
  system under study. This multimodal imaging approach is critical for understanding functional
  materials. Taking energy storage materials as an example, the structural morphology, elemental
  distribution and strain evolution determine the stability, electrochemical performance and
  reversibility, respectively. At HXN, multimodal imaging using XRF, ptychography, differential
  phase contrast imaging, and Bragg imaging are well developed. The efforts are made on streamlining
  end-to-end process from data collection to 3D reconstruction. Currently, high-speed and user-
  friendly data analysis tools have been developed for DPC, XRF and ptychography. Continuous
  developments will focus on optimizing, accelerating and automatizing each component in the data
  processing pipeline, including XRF spectra fitting, projection reconstruction, image registration and
  alignment, 3D reconstruction and visualization.

- **New sub-micron KB-mirror endstation at SRX** (FY19-21): This facility improvement project aims
  to improve the current endstation at SRX by developing a new set of KB mirrors and precision
  sample positioning stages to achieve spatial resolutions over 0.1 to 1.0 um for multimodal imaging.
  New-generation laser interferometers will be implemented for the sample positioning stage,
  automatically correcting axial run out errors, which will be extremely useful for tomography and
diffraction measurements. Installation, technical commissioning, and science commissioning will
  take place in FY20. The instrument will be used for general user experiments in FY21.

- **Confocal XRF imaging at XFM and SRX** (FY20-24): Certain classes of samples are extremely
difficult to image in 3D using a tomographic approach. Extended sample geometries, such as a single
plant root in a complex root system or a hierarchical sample inside a complex in-situ cell, are good
examples of difficult tomographic measurements. A confocal XRF (C-XRF) approach allows
imaging in 3D of a partial sample volume and is performed without sample rotation or image retrieval (reconstruction) algorithms. A prototype C-XRF development began in FY19 with the assembly of a confocal system at XFM. The first C-XRF imaging experiment using a dual paraboloidal mirror lens was successfully performed by SRX and XFM beamline staff using the SRX endstation. In FY20-24, this project will be funded through CBMS Bioimaging Core. This effort includes development of C-XRF capability at XFM with an aim of achieving 5 um 3D resolution in FY20-22. With an improved capillary resolution down to 1 um, a higher resolution instrument will be developed at the SRX in FY23-24.

- **Dedicated XRF nanoprobe with sub-100 nm resolution at SRX** (FY20-24): Current user operations experience at HXN has shown that there is great demand from the user community to access a reliable XRF nanoprobe optimized at ~50 nm. While HXN can accommodate this community, it may not be the most efficient way to use HXN for this purpose, which should focus on those experiments that require high spatial resolutions sub-10 nm. This project aims to leverage the HXN experience and develop a new, stable, reliable nanoprobe instrument for installation into the SRX side-branch hutch, with sub-100 nm resolution capability in routine user operations. If funded, this instrument will relieve the beam time pressure on HXN, and allow HXN to focus on the most demanding, potentially high-impact experiments, while at the same time enabling SRX to serve part of the XRF imaging community that needs a high-resolution capability beyond sub-micron.

- **Development of high-resolution hard X-ray TXM capability at FXI** (FY20-22): Considerable interests exist from the user community to be able to conduct full-field hard X-ray microscopy experiments beyond the 30 nm resolution that is the current state of the art. We plan to partner with other DOE-BES hard X-ray light source facilities to develop higher resolution zone plates for hard X-rays and implement these high-resolution optics at FXI. Our initial goal is to target 20 nm resolution based on an ongoing collaborative effort with the APS. We will also work with Sigray, Inc., to develop and implement new capillary condensers that is optimized for the FXI beamline to improve incident beam flux and overall performance of the FXI TXM instrument.

- **Development of in-situ and operando capability for catalysis and energy science at TES** (FY20-23): Substantial interests exist in the energy science community to investigate, under in-situ/operando conditions, the chemical states and bonding coordination of light elements in e.g. S, P, Si, and Cl-containing catalysts, electrodes, and electrolyte materials, which requires special sample cells and access to spectroscopy and imaging in the 1.5-5 keV tender-energy range. We plan to develop a second endstation at the TES beamline dedicated for catalysis and battery research. This new capability together with the existing spatially resolved spectroscopy capability will significantly broaden the user community of TES. The new endstation chamber will be located upstream of the exiting micro-imaging endstation, optimized for collecting large solid angle from the bending magnet source without imposing operational complexity with the exiting endstation. Important concepts for this new instrument are high-throughput and “smart” data acquisition taking advantage of advanced real-time data analysis. The instrument concept also includes capability for transferring a large set of samples through a vacuum-load lock and automatic sample loading/exchange to make the air/water sensitive in situ/operando tender x-ray experiment possible. Preliminary design will be completed in FY20, and the implementation of this “smart” spectroscopy endstation may be anticipated in the FY21-22 timeframe.

- **Progressing design of the new CDI beamline** (FY20): Bragg coherent diffraction imaging is a new state-of-the-art beamline that takes full advantage of the world-leading coherent photon flux in the 6-15 keV energy range at NSLS-II. It will enable cutting-edge research on structural evolution in a
wide-range of materials systems under in-situ conditions. NSLS-II plans to develop this capability, at least in part, using a small portion of the operations funds. In FY19, NSLS-II has continued to support the conceptual and engineering design. The new beamline concept was included in a DOE Major Item of Equipment (MIE) proposal in FY19 and work will continue on the CDI beamline design as that project prepares for a CD-1 review. More details on the capabilities of the beamline are discussed below in the New Beamlines section.

- **Developing confocal X-ray fluorescence 3D imaging and spectroscopy capability at XFM & SRX (FY20-24):** Fluorescence tomography using a focused x-ray beam is a powerful method of analyzing 3-D element distribution in hierarchical structures including biological systems. This XRF tomography technique, based on a 2D raster scan plus a sample rotation, has been already successfully implemented for general user experiments at the HXN for both biological and material science research. A serious challenge for XRF tomography is that this method is extremely inefficient in obtaining a local 3D structure from an extended sample, particularly when one desires high resolution. To address this challenge, we plan to develop and implement a new confocal XRF microscope that consists of a direct focused x-ray beam, a capillary lens by Sigray, Inc. as the confocal lens, confocal slits, and XRF detector. This instrument will enable 3D XRF elemental mapping without the need for sample rotation, offering much improved data collection speed and signal to background ratio. Funded through a BER grant as part of the support for the Center for BioMolecular Structure (CBMS, described in the next section), we plan to complete the confocal microscope design in FY20, install and commission the system at XFM in FY21, deploy the instrument for user operations in FY22, procure a higher-resolution capillary and other parts for SRX in FY23, and install and commission the SRX confocal microscope in FY24.

- **Developing comprehensive multi-modal and multi-scale data-analysis workflow for 2D and 3D bioimaging datasets (FY20-24):** Most materials and biological science users have little experience with imaging measurements and image-analysis computations. One of our goals for the imaging and microscopy program (IMP) is to offer user-friendly tools to operate the software. We also aim to offer common or similar tools across the multiple IMP beamlines. Users will seamlessly visualize data from the different IMP beamlines and laboratory instruments (visible-light microscope, SEM, TEM, etc.) with minimal training. One requires considerable computational resources to visualize images or 3-D reconstructions quickly enough (< 10 minutes) to show if the acquired data are sufficient or whether one needs more. Few users can process data without our help, so their productivity depends upon our providing computing pipelines.

With resources provided by the BER supplement to the CBMS grant, we will hire a dedicated data scientist to spearhead a focused effort to develop software, collaborating with the NSLS-II Data Acquisition, Management, and Analysis (DAMA) Group, to enhance productivity for biological and environmental scientists. Such development will benefit all IMP beamline users. Leveraging the common controls hardware and software architectures across IMP beamlines and data processing and analysis workflows that already exist, we plan to develop data analysis workflow in the following five areas:

1. Enabling cross-beamline scientific investigation with minimal user training;
2. Incorporation of advanced imaging methods into the NSLS-II Data-Analysis Library;
3. Visualization and cross-correlation of images of different modalities, and images collected with different beamlines or instruments;
4. Optimization of data suitcases, allowing flexible data packaging for users;
5. Optimized workflow for spectromicroscopy data, and development of GUI-based data-analysis software.
Realizing that the scope of this work is much too large for a single data scientist, we will rely significantly on collaboration from the DAMA Group in developing this data-analysis pipeline and workflow. An external contractor will integrate the tools and workflow, in the form of plug-ins to the existing software.

**Structural Biology and Bioimaging**

Structural Biology stands at an exciting point in its history. The new generations of light source such as NSLS-II are making exquisitely bright, high flux beamlines possible, opening new avenues for structural biology and bioimaging. The advances in biomolecular structure being enabled with structural biology methods are presenting impressive new science on a weekly basis. At NSLS-II the extremely bright source enables the delivery of x-ray beams of unrivalled brilliance, thereby enabling the examination of extremely small crystals of proteins, particularly those difficult-to-crystallize membrane proteins, and other macromolecules.

The current suite of structural biology beamlines at NSLS-II include Frontier Macromolecular Crystallography (FMX) at 17-ID-2, Automated Macromolecular Crystallography (AMX) at 17-ID-1, and X-ray Scattering for Life Sciences (LiX) at 16-ID, all three of which started user operations in 2016 and early 2017. In addition, two additional structural biology beamlines, X-ray Foot-printing (XFP) at 17-BM and New York State Structural Biology (NYX) at 19-ID, are operated by two partner user institutions, Case Western Reserve University (CWRU) and New York State Structural Biology Center (NYSBC), respectively. The FMX, AMX, and LiX beamlines have already enabled MX experiments that were not possible previously, and have led to several impressive high-impact results. The world-leading performance of these beamlines that is being demonstrated represents a leap in the performance hitherto available to the structural biology community.

As of July 2019, NSLS-II has successfully secured a joint 5-year renewal grant by the National Institutes of Health (NIH) and DOE Biological and Environmental Research (BER) office for the continued operations of the three structural biology beamlines (FMX, AMX, LiX) and for the development of bioimaging capabilities at the imaging and microscopy beamlines for the BER community. To support the use of the synchrotron resources for structural biology and bioimaging, we have created the Center for Biomolecular Structure (CBMS). The research CBMS enables will dramatically accelerate our understanding of the fundamental molecular structures and processes underlying biological function, thereby enabling more profound insight and opening the possibility to engineer function and develop medicine. The objectives of the new CBMS are (a) to operate synchrotron beamline resources for individual researchers who have basic research support from a wide range of agencies, especially NIH-funded investigators, and (b) to provide these resources to the BER research community and to improve existing and develop new technologies at NSLS-II that respond to the immediate needs of the community.

Our overall development strategy in structural biology at NSLS-II has been to harness the bright x-ray beams through sophisticated automation and instrument control to allow the elucidation of the structures of the molecular machinery underpinning life in its function and dysfunction. Our principal approach is two-fold: (a) to innovate to create the best experiments that will make optimal use of the NSLS-II source including novel sample delivery methods at room-temperature to allow for the study of transient interactions and enzymatic reactions, and (b) to combine the necessary tools to study complex problems
through correlated research to bring together diverse data to inform scientific deliberation – e.g. transient complexes via scattering or cryo-electron microscopy together with high resolution structures via crystallography.

In bioimaging, NSLS-II is currently the ideal source to provide high resolution, high sensitivity imaging opportunities. Taking advantages of high brightness and small source size, NSLS-II has developed a suite of advanced electronic, chemical, structural, and morphological imaging programs that span multiple length and time scales. Our strategy is to take advantage of these developments and further advance the necessary instrumentation to allow biological imaging in thick 3D samples with a spatial resolution of tens of nanometers, and to provide chemical imaging by x-ray fluorescence microscopy below 100 nm at atto-molar elemental concentrations in biological samples. Multiscale, multimodal, and 3D imaging capabilities at the NSLS-II, together with the Cryo-EM capability will become vital tools for tackling broad range of biological and environmental problems.

Our key development programs structural biology and bioimaging for the next five years are summarized below, in three categories: Macromolecular Crystallography, X-ray Scattering, and Bio-Imaging.

**Macromolecular Crystallography at FMX and AMX:** We aim to keep FMX the benchmark MX beamline for structure solution from the smallest and most challenging macromolecular crystals. We also plan to make use of the beam properties and the flexible design of our endstation to accommodate non-standard MX experiments such as room temperature experiments and experiments, dynamic methods, and samples requiring new sample delivery methods. In the light of competition from international microfocus MX beamlines at upgraded storage rings, this will entail upgrades to the photon delivery system and experimental station, further automation of the photon delivery system, data collection and processing protocols, and the provision of further sample delivery methods. Another focus will be on making these capabilities more accessible to the user community, by outreach and training, as well as making these methods accessible to remote access. In addition, to keep the photon delivery system and endstation at the forefront of beamline performance, we will aim to enhance data collection at the low energy (<7 keV) and high energy (>20 keV) ranges, higher flux density, and a focused beam size of < 1×1 µm² at FMX. For AMX, the main development direction will be on increased level of automation in data collection, in intelligent decision making on spot finding and dataset merging form thousands of small crystals in challenging experiments.

Our plan for next five years includes the following developments and upgrades:

- **Synchrotron based serial microcrystallography at FMX (FY20-21):** In partnership with Arizona State University and other interested groups, we plan to develop serial microcrystallography capability at FMX by installation of a latest generation high viscosity extrusion (HVE) injector to enable high-quality MX data collection on microcrystals of membrane proteins. This technique, originally developed for XFEL application, has shown significant attraction in the synchrotron facilities. The world-leading high photon flux density at FMX will be an ideal place to develop this technology and associated data reduction algorithms such that it can be routinely used for a wide range of microcrystals for structural determination.

- **Fully automated autonomous MX data collection (FY20-21):** Automation depends on the software being able to find diffracting crystals – our low-dose reflection-counting rastering method assures that. One can imagine algorithms to handle complicated situations. Not too difficult is a large crystal with multiple diffracting volumes. More interesting would be a volume where one can see multiple needles in many directions, each of which would benefit from a 3D vector scan. For our crystal-
mounting robot we depend on Spine-Standard caps and the 16-position Uni-Puck cassettes. We know that some in Europe are adopting the denser Mini-SPINE standard where the same form-factor cassette will carry 36 Mini-SPINE caps. Monitoring their progress closely, we will create and commission a robot gripper/end-effector to manage these sample mounts, more than doubling capacity. We will continue to improve these and pursue other workflows to enable optimized MX data collection in a seamless way for our users.

- **Time-resolved serial MX at FMX (FY20-22):** We plan to develop necessary instrumentation and data acquisition methods to allow room-temperature time-resolved serial micro-crystallography at FMX. By mixing and diffusing micro-crystallites with a liquid solution and delivering them onto a moving conveyor belt system, one will be able to measure diffraction patterns at different locations on the belt, and thus at different reaction times between the crystal sample and the solution. This will create a new capability in micro-crystallography for tracking reaction intermediates and processes for studying interactions between proteins and substrates or between viruses and drug targets, at an unprecedented µs-to-seconds time scales.

- **Implement helium flight path for optimal data collection below 7 keV at FMX and AMX (FY20):** We routinely support data collections for sulphur SAD phasing at 6 and 5 keV, which increases the available anomalous signal from 0.7 e- to ~1.0 and 1.3 e- compared to 7 keV operation. To improve the signal to noise ratio in data collections for S-SAD we will implement a helium flight path between the sample and the detector. We have modified an existing SAD data-reduction pipeline, fast_ep_weak, to optimize structure solving under these conditions – weak anomalous signals or low resolution – employing a brute-force approach with many searches.

- **Increasing the level of automation at AMX (FY20-21):** We plan to further increase the level of automation in data collection workflow at AMX, starting with automated vector data collection. We will work on a new spot finder with increased speed and efficiency that will filter ice rings better, and will recognize diffraction from small-molecule crystals. We must explore better ways to find spots for weakly diffracting samples and will seek additional funding/collaboration for this special project. We will implement a hybrid access mode for data collection that will combine automated data collection and users’ feedback, where they will interact with the synchweb front end and not the data collection software. We will improve sample-automation hardware and software to increase achievable sample throughput.

These technical improvements will be a key to enable studies of macromolecule dynamics through data collection from 100’s to 1000’s of crystals from the same specimens, using data-processing programs and algorithm we plan to develop for our NIH R01 application. These will be based on hierarchical cluster analysis based on two passes: similarity of cell parameters, and correlation of intensities. This will untangle many conformations from correlated sets of data, typically either complete data sets from several 100’s of crystals to many 1000’s partial data sets from many 1000’s smaller crystals.

- **Increase flux to 10^{15} ph/s using a multilayer monochromator at FMX (FY20-22):** The serial crystallography experiments at FMX demonstrated that even at full beam these measurements are still flux limited, preventing from using the full diffraction potential of their often very limited amount of crystals. For raster scanning crystallography at the full scanning speed of the piezo goniometer, and the maximal detector frame rate of 750 Hz, the full beam intensity does not deliver the maximum allowable dose to a crystal [Gao 2018]. The same is true for the viscous-injector sample delivery, because the injector flow speed cannot be reduced below 100-300 µm/s. To increase
the flux, we plan to increase the energy bandwidth from 0.01% to 1%, for optimal sample usage and increased throughput, e.g. cutting data collection times with the jet from hours to minutes. A second key application of the increased dose rate is a microsecond time resolution in kinetic experiments.

The addition of a double multilayer monochromator (DMM) to FMX was proposed through a successful NSLS-II Facility Upgrade Proposal in 2018, with an initial planned completion of construction in summer 2020. This DMM will increase the available x-ray flux at FMX by up to two orders of magnitude to $10^{15}$ ph/s, while still allowing the data to be handled using conventional data-handling software and automated pipelines. An important design requirement is to keep the switching time between the two bandpass options under an hour. Funding for this upgrade through the NSLS-II operating funds currently has not been granted, but rather we plan to submit the materials part of this work in a separate proposal to NIH.

- **Replacement of the FMX final focusing mirror** (FY20-22): The FMX horizontal KB mirror, the secondary horizontal focusing stage, is elliptically prefigured to achieve the required short focal distance of 500 mm. This is a bimorph mirror, profile changes for controlling the focus and to correct imperfections are achieved through 16 piezo elements along the mirror profile. Due to a large residual error in the prefigured profile, up to five out of 16 benders are consistently at the limit of their range, thereby greatly limiting the possibility to optimize the mirror figure and limiting the figure error to ~0.5 µrad. With this figure the minimum achievable horizontal beamsize by closing the secondary source aperture is 1.0 µm, whereas a 0.2 µrad figure will allow us to reach 0.5 µm. In addition, the large figure error leads to structure in the expanded beams, beyond the 30% intensity variation initially specified. The mirror upgrade will enable us to obtain smoother beam profiles for a more even dose distribution across crystals and enable data collection from smallest crystals. This upgrade project is to make that replacement; the only barrier is to acquire the funds, and we request these as an ancillary capital expense.

- **FMX detector upgrades** (FY21-22): With a 1% bandwidth, the increased beamline flux will surpass the maximum input count rates of the current Eiger 16M detector. Moreover, the achievable time resolutions in the µs range indicate the need for higher frame rates in the 2-5 kHz range. We will therefore request funding for an advanced pixel array detector of the latest technology available at the time of decision making. First experiments with loaned CdTe based detectors (X-Spectrum LAMBDA and DECTRIS Eiger2 CdTe) have proven the necessity of a non-Si based detector at photon energies above 20 keV. Since the Bragg diffraction pattern at these wavelengths is compressed, a 4M detector will suffice for any conceivable MX application. Such a detector would be dedicated to high-energy experiments aimed at minimizing radiation damage for radiation-sensitive targets (Ueno et al., 2019), as well as for ultra-high resolution structures.

**Solution and Microbeam X-ray Scattering at LiX**: The solution scattering program at LiX has been the main technique delivered to users in the past three years. We have developed world-leading experimental capabilities for automated data collection and processing, with extended reciprocal space coverage. The main challenges are (a) to keep our instrumentation and data acquisition protocols up to date and remain world-leading, and (b) to attract more users to use our beamline and to help our user community turn more good data into high-impact publications.

The microbeam scanning imaging program is still in its development phase. We have achieved impressive results with our collaborators. The current work by our postdoc is expected to attract research activities in areas of interest to our sponsors, both NIH and BER. Outreach is again critical. Scanning
imaging is not a “traditional” scattering method. We need to communicate with more potential users to understand better in what research areas this method will shine.

In the next five years, we plan to pursue the following development activities.

- **Improve automation and implement mail-in access at LiX (FY20-21):** An immediate objective to improve LiX user program is to start supporting mail-in access, which has been well-known in the solution scattering community, mainly due to the service provided by the SYBILS beamline at ALS. This mode of access will help consolidating measurements into longer contiguous runs and therefore more efficient use of beam time. Users then will be able to have multiple virtual “visits” to the beamline within a single cycle. It will also reduce the burden of supporting users at the beamline, allowing staff to concentrate more on helping users interpret their data and therefore boost the scientific productivity of the beamline.

  At this point our instrumentation and software are fully capable of entertaining mail-in access. We have devised a preliminary plan for mail-in operations. We will adopt the same sample container (96-well plate) and description spreadsheet. We have acquired a liquid sample handing robot to translate samples from standard well plates into the beamline sample holders. The current challenge is to implement a web interface for user to upload sample spreadsheet and obtain a bar code to identify the sample plate. We will work with the user office and DAMA group to integrate these features into the PASS system.

- **Broaden the usage of in-line chromatography at LiX (FY20-22):** The in-line chromatography at LiX has been an invaluable tool for X-ray solution scattering from proteins. We plan to branch into the additional modes of operations other than size-exclusion chromatography, for instance ion exchange chromatography, which are commonly used in molecular biology labs. This will require equipment upgrade that includes a gradient mixer. This device would then enable a new mode of high-throughput measurements of protein sample under a wide range of chemical conditions such as ionic strength, pH and ligand concentration.

- **Improve signal to background ratio for flow-mixer-based solution scattering at LiX (FY20):** As the development of flow-mixer-based time-resolved solution scattering continues, we will install a pin-hole immediately upstream of the sample to block off the low-intensity background in the CRL-focused x-ray beam, therefore reducing parasitic scattering from the flow channel sidewalls and improve the signal to background ratio.

- **Installation of XRF detector at LiX (FY20-21):** A multi-element X-ray fluorescence detector will be installed at the LiX beamline. This detector is developed by the NSLS-II detector group and will provide much higher dynamic range compared to the current single-element detector. It will be used in scanning experiments to provide the capability of elemental mapping, as well as for anomalous scattering from solution samples.

- **Improving information contents in solution scattering data files (FY20-22):** We will continue to expand the information contents in the hdf5 data files to include the definition of the data process and analysis pipeline. To do that, py4xs will be expanded to provide a generic method for pipeline definition. This effort will be coordinated with DAMA group. DAMA has also been directed by NSLS-II management to develop a sample manager, to provide functionality similar to ISPyB used in macro-molecular crystallography.
• **Develop double-multilayer monochromator upgrade plan** (FY21-22): The installation of a double-multilayer monochromator (DMM) to increase the x-ray flux by a factor of ~50 is being considered. This upgrade has always been in the long-term plan and the vacuum chambers were installed during beamline construction. It would benefit experiments in which smaller (than the current 5 micron) beam sizes are needed without sacrificing overall beam intensity. We will work on developing a plan how this enhancement may be implemented in the next couple years.

• **LiX solution scattering workbench and outreach activities** (FY20-24): The LiX solution scattering workbench that we run every cycle is intended to address the challenge in developing and broadening our user base. We are also looking into other means to promote the beamline, for instance by visiting universities to publicize the beamline capabilities. At the same time, we are sending our staff to other facilities, to learn about new development in experimental methods, and to speak to software developers to gain deeper understanding of popular data analysis software and become more proficient in using and teaching these tools. We also recognize that it is essential to ensure the reliability of the instrument, to give the users the confidence that they can count on the beamline to collect high-quality data. To do this, we are formalizing the processing of setting up for experiments and supporting user experiments, building into our routine operations periodic measurements on standard samples (empty cell, water, and protein solution) to track the instrument performance.

• **Development of micron-scale scattering-based imaging at LiX** (FY20-24): The LiX beamline is capable of producing micron-sized x-ray beams for scattering measurements with simultaneous small- and wide-angle (SAXS and WAXS) data collection. In the next few years, LiX will be upgrading its WAXS detector for improved azimuthal angle coverage in the WAXS data and install an XRF detector as mentioned above for simultaneous x-ray fluorescence detection. These capabilities will provide new opportunities in the studies of biological tissues with complex hierarchical structures and chemical compositions, for instance in biofuel feedstock development and to help validate new MRI methods for brain imaging. Automation in data collection and processing will make the beamline more accessible, particularly for novice users.

**Bioimaging and Outreach to BER Community:** With the resources primarily supported by DOE-BER, we plan to pursue developments at NSLS-II Imaging and Microscopy beamlines that will enable multi-modal and multi-scale 3D bioimaging and to enhance the productivity of BER user community by providing user-friendly tools for image reconstruction and analysis. The technology development and outreach activities will focus on the following projects:

1. Enabling multi-modal and multi-scale 3D bioimaging and enhancing user productivity by providing user-friendly tools for image reconstruction and analysis.
2. Enhancing user productivity by developing comprehensive multi-modal and multi-scale data-analysis workflow for Bioimaging datasets in 2D and 3D.
3. Outreach to and support the biological and environmental research community to provide expert and non-expert members of the community the means to employ the broad range of state-of-the-art methods in bioimaging.

**Multimodal and multiscale 3D bioimaging and data workflow:** Specific technology development projects that we plan to pursue in the next five years are described in the “Multiscale Structure and Function” section of this document that cover the imaging and microscopy program operated five beamlines (XFM, SRX, TES, HXN, and FXI). Together this collaboration will provide excellent opportunities for biological imaging, especially of tissues and other biosystems not only related to human-health research needs, but also those related to the needs of the DOE-BER programs (plants, rhizosphere, and soil). These five beamlines offer a variety of techniques, ranging from x-ray-
fluorescence microscopy at micron and nanometer scale, to absorption- and phase-contrast imaging at similar spatial resolutions. With the new development of a confocal XRF microscopy capability, this program will enable optimized studies in biological and environmental research beyond what can be done with the x-ray-imaging capabilities currently available at these beamlines. In addition, BNL is in the process of establishing a cryo-electron microscopy facility next door to NSLS-II structural biology beamlines. With its construction funded by New York State and operations support by DOE-BER, it will offer 3D cryo-electron imaging at sub-Åm resolutions. This new capability, along with protein crystallography and X-ray imaging, will dramatically enhance bio-imaging scientific output and strengthening synergy across x-ray imaging, crystallography, and cryo-EM (see figure at right).

**Outreach to the broader BER research community:** Traditionally BER investigators use a handful of techniques that are readily accessible to them, either at home Laboratory or through service programs available through their Institution or the BER-sponsored Facilities Integrating Collaborations for User Science (FICUS). The research facilities made available through the CBMS, as described in this document, are new and often different from what researchers expect to find at a FICUS facility. Also, even though imaging methods, such as chemical imaging, available at several of the CBMS and NSLS-II beam lines, may be known to several BER funded investigators, it is not clear to most researchers how these methods could complement their conclusions on a specific study. The idea to employ macromolecular crystallography methods and techniques to elucidate structural function relations seems to be even more remote to most BER investigators at this time.

To help solve this issue, we plan to implement a dissemination, education, and training program, aligned to the BER mission, that shows researchers how the investment of their time and effort may contribute to the outcome of their investigation. These activities will include joint workshops by partner facilities, participation in BER sponsored workshops, mutual visits by staff to partner facilities and labs, joint booths with partner facilities at conferences, hosting students and researchers from academia and BER facilities at CBMS, and discussion of multimodal concept by staff at partner institutions to facilitate the propagation of an integrative multimodal research view.

**Establish a partner user program with FICUS facilities:** We recognize that one of the challenges for the dissemination and the education-training program is to develop an integrated program that serves a diverse community of researchers who are not necessarily familiar with synchrotron techniques. To address this challenge, we plan to pursue a partner user program in collaboration with BER facilities, e.g. Joint Genome Institute at LBNL, and Environmental Molecular Sciences Laboratory at PNNL. The partnership will enable existing or new BER researchers to use an existing mechanism that they are familiar with to access the cutting-edge MX, X-ray imaging, cryo-EM facilities at NSLS-II and BNL. We plan to announce a joint proposal call for FY20 with EMSL, JGI, and NSLS-II. This partner user program will simplify and facilitate access to a wide range of complementary methods and techniques that may benefit our understanding of the interaction of micronutrients and the rhizosphere. Other subject areas with potential for partnerships may involve structural biology through the genome-to-structure across BER and BES user facility initiatives.
Enabling Technology and Support Programs

In addition to the science program areas discussed in the previous chapter, we plan to pursue research and development in the following four key crosscutting enabling technology areas in support of the strategic science themes –

- **Accelerator science and technology** that is the foundation for stable and reliable operations and for enhancing the performance of NSLS-II accelerator systems,
- **Advanced X-ray technology** in x-ray optics and detectors, and in nano-precision engineering that is required for the development of innovative world-leading programs,
- **Multimodal capabilities** that plays an increasingly important role in modern science today, from complex materials, operando chemistry, to geo-environmental and biosciences, and
- **Data-driven science** that is crucial to the productivity and the impact of all NSLS-II science programs, and in enabling new modes of experimentation involving advanced simulation, multi-modal experiments, and machine learning driven data analysis.

These four enabling technologies are critical to keep the NSLS-II scientific capabilities at the cutting-edge and for enabling new and high-impact science at NSLS-II.

Furthermore, operations excellence, facility infrastructures, and user services are all important parts of the NSLS-II facility. The development plans in these areas are also discussed in this Chapter.

**Accelerator Improvements and R&D**

The continued evolution of the NSLS-II accelerators is an essential part of the facility strategy. Since the NSLS-II project commissioning in 2014, our facility progressed far in increasing accelerator performance and putting more instruments in routine operations. The next figure illustrates outstanding progress accomplished NSLS-II since the first year of operations.

In particular, in less than 5 years the NSLS-II team was able to bring up performance of the facility in all metrics:

- Increasing and sustaining reliability of operations at 97% level,
- Increasing operating current to 400 mA,
- Extending operations to 5000 hours
- Constructing 21 beamlines

With substantial operating experience from NSLS-II start-up and recent-year operations, we have identified several crucial areas where the accelerator facility is thin in providing sufficient redundancy of critical subsystems or adequate level of spares. Based careful analysis of past
events and trends, it is evident that the under-investments in reliability driven by various constraints in
the prior years present significant risks in major failures of the accelerator system that may lead to
substantial downtimes in the coming years. Given that the aggressive beamline buildout funded through
operations is now complete, NSLS-II plans to pursue a number of accelerator development and renewal
projects to mitigate the risks of major failures to ensure high-reliability operations well into the future.
These projects will proceed in the following priority order:
1) developments that support reliable storage-ring operations including sufficient redundancy of
critical subsystems and adequate level of spares to mitigate major operational risks,
2) developments that are required to ramp up the storage-ring performance to its design values,
3) R&D that will lead to enhanced or upgraded NSLS-II source performance beyond design
specifications.

The first two priority directions are covered by our Mitigating Vulnerabilities to Operations and Mature
Performance Plan that Accelerator Division finalized in 2019 after a year-long planning effort. The Plan
contains seven main packages, targeting areas of NSLS-II accelerator with lowest reliability or required
developments to enable future operations at 500 mA and 8 pm rad.

<table>
<thead>
<tr>
<th>Project</th>
<th>Total Cost, M$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Spare #4 RF Cryo Module $^R$</td>
<td>3.7</td>
</tr>
<tr>
<td>2. Spares not in hand (critical) $^R$</td>
<td>3.0</td>
</tr>
<tr>
<td>3. RF Cryo Plant performance improvements $^R$</td>
<td>5.9</td>
</tr>
<tr>
<td>4. Third Harmonic RF Cavities (THC) $^M$</td>
<td>7.8</td>
</tr>
<tr>
<td>5. 4$^{th}$ RF System $^{R,M}$</td>
<td>11.8</td>
</tr>
<tr>
<td>6. Injector and Dipole PS performance improvements $^R$</td>
<td>3.5</td>
</tr>
<tr>
<td>7. Spares not in hand (intermediate) $^R$</td>
<td>1.9</td>
</tr>
</tbody>
</table>

| Total                                           | 37.6           |

The subscript $R$ marks these packages that are focused on sustaining reliability while the subscript $M$
points to the projects to enable future progress in machine operations.

This Plan has been presented to DOE BES in May 2019 and reviewed by an external committee from 4
US laboratories at the end of July 2019. The review endorsed our Plan and recommended to detail several
scenarios in terms of scope, cost and schedule.

In the following we describe the parts of the Plan in more details.

**3$^{rd}$ Storage-Ring RF System:** A 3$^{rd}$ 500 MHz superconducting RF cavity is being developed since FY17
and is on schedule to be installed in FY20 to serve as a hot spare should either of the two existing RF
cavities fail to supply the needed voltage and RF power. As designed this 3$^{rd}$ RF cavity is also required
to achieve >400 mA operations with a full suite of insertion devices including superconducting wigglers.
This project is currently progressing on schedule, and the new RF system will be commissioned and
integrated into operations at the end of FY20.

Solid-State Amplifiers (SSA) instead of 300 kW RF klystrons: As a part of the 3$^{rd}$ RF system we will
deliver to operations an SSA. Controls test stand for SSA is already funded under an FIP.
4th Storage-Ring RF system: As a part of expansion of the NSLS-II capabilities, both in terms of necessary redundancy of critical subsystems and in terms of extra RF power for supporting the future beamline buildout, we plan to complete construction of the RF system by delivering the 4th system in cell 22 straight section of the ring. This system, as the 3rd one, will be powered by an SSA.

Cryo-plant upgrades: purifier, controls, additional volume of GHe already funded under FIPs. Additional redundant cold box is planned to mitigate possible contaminations and permit to work on the cryoplant while keeping all 4 installed cavities cold.

**Two 3rd harmonic cavities:** NSLS-II storage ring is designed to have two 3rd harmonic 1.5 GHz cavities operated passively. Once the 3rd harmonic RF system is operational, these cavities will increase the beam lifetime by stretching the electron bunch length, thus reducing the levels of beam heating on critical storage-ring components and decreasing the frequency of top-off injections and the interruptions seen by the user experiments. Such system is required to operate NSLS-II at diffraction-limited vertical emittance of 8 pm·rad. The two harmonic cavities and the associated cryogenic system will be located upstream of the two 500 MHz cavities in C24. The current scope includes design and modification of the cryomodule, improved cavity processing, design and fabrication of the tuner, procurement of the HOM damper, and the fabrication of the cryogenic connections. We plan to have these harmonic cavities installed and operational by FY23 to enable the full mature performance of 500 mA and 8 pm-rad of the NSLS-II storage ring.

**Redundant Critical Subsystems:** NSLS-II plans to acquire several critical accelerator subsystems to mitigate the risk of single-point failures that may cause substantial machine downtime. The subsystems under consideration include booster dipole power supplies, storage-ring dipole power supplies in ramp/DC mode to 364A and 1.2kV, and the injector thermionic gun. The redundancy will be developed in the form of hot spares or redundant units.

**4th Storage-Ring RF System:** In addition to the 3rd RF, the 4th RF system will be developed to complete the full buildout of the RF system, with four installed 500 MHz RF systems and a complete spare cryomodule, which can be installed to replace the existing cryomodules when removed for service. This fully buildout RF system will enable full 500 mA operations with full suite of insertion devices as designed, and at the same time, will provide sufficient redundancy to prevent major failures that would cause extended downtime for NSLS-II user operations.

**External Review Follow-up:** Following the July 2019 external committee’s review comments and recommendations, we will put together 3 separate scenarios with different scopes from the Plan summary table, refine workbook with vendor quotes and labor estimates, develop detailed cost and resource-loaded schedule, produce staffing models per every scenario, produce risk assessment matrix and devise mitigation plans, prepare elaborated proposal for the Plan, and submit the review report together with the proposal to DOE in early FY20 for planning the operations funding.

As of September 2019, we have developed the following three packages as our refined plan to move forward, based on the review recommendations:

1. 4th (SPS) cryomodule, category 1 spares, limited scope improvements to cryo plant ($9.6M)
2. 4th RF system (w/o 5th CM), 1 Harmonic cavity, coldbox ($15M)
3. 5th cryo module, 2 harmonic cavity, injector and dipole PS, category-2 spares ($13M).

We will execute according to this plan provided that funding is available.
**Beam Stability Improvements:** Over past several years, staff from both Accelerator and Photon Division has been focusing on increasing positional and angular stability of electron and X-ray beams across the NSLS-II facility. NSLS-II experts worked out a number of impressive improvements to the stability of beams, reduction of drifts and frequency of events perturbing user operations. Notable improvements in this area include:

Optimization of Fast Orbit Feedback System (FOFB) is focused on increasing gain and expanding bandwidth of the feedback loop. In 2019 good deal of progress was achieved in modeling FOFB, measuring and reducing latencies in the loop and testing optimized RF BPM software on the storage ring. As a result, the latency has been reduced by 25% and the feedback bandwidth was expanded from 250 to 350 Hz. This promising work will continue in the next years. As a part of this project, new BPM electronics will replace the currently installed ~250 BPM units, leading to superior performance and higher orbit stability in the source points.

Energy feedback was introduced into operations, substantially reducing magnitude of slow drifts, due to day-night and summer-winter temperature variations. Another useful addition to instrumentation of beamlines were Photon Local Feedbacks that tied up RF BPMs around ID, X-BPM in Front End into a local loop, efficiently correcting slow motion affecting specific beamline. Local orbit bumps, when tuned, were disruptive to the ring orbit stability. Once the algorithm in application of the local bumps was optimized, the operate invisibly to the beamline users.

In 2019 we initiated a new activity, focused on suppression of mechanical noise and vibrations and advancing towards more stable environment, where sources of shaking of accelerator and beamline components are mitigated. NSLS-II facility owns many utility services, including DI and chilled water, air-conditioning, cryocoolers and cryoplant, rotating equipment, etc. These mechanical systems seed vibrations within broad spectrum that propagate across buildings and supports in accelerator tunnel and user floor, being amplified by structural resonances and affecting quality of beams in our facility. The program that has been initiated in the area of facility Mechanical engineering is targeting the sources of noises at NSLS-II, temperature instabilities and, once detected, aims at reducing them at the source and developing feedbacks to further suppress the residuals. We will pursue this new program in the next several years.

**R&D on upgrade options of NSLS-II:** With the rapid development of multi-bend achromat (MBA) based new and upgraded synchrotrons, potential upgrade to NSLS-II accelerator facility will be crucial to keep the NSLS-II source competitive on the world scene. Funded by an LDRD grant and other Lab overhead funding, we plan to conduct R&D to explore potential upgrade options to increase capabilities of the source and maintain competitiveness with rapidly changing community of world’s light sources. At this point we are considering three potential upgrade directions, all within the same NSLS-II facility infrastructure:

- **Limited upgrade** with no perturbation to beamlines: these studies aim towards a split-dipole upgrade to create a 5-bend achromat lattice design that would be a low-cost, effective upgrade option to reduce the NSLS-II horizontal emittance by a factor of 2-3, with no perturbations to beamline locations.
- **Low-emittance upgrade**: We are considering a Complex Bend idea that would push the MBA lattice design to its limit within the NSLS-II infrastructure footprint. This upgrade option would potentially lower the horizontal emittance by a factor of 30x, delivering almost diffraction limited X-rays at 10 keV.
- **High-flux upgrade**: A third option being considered is to raise the operating current by a factor of 4x and at the same time reduce the horizontal emittance by a factor of ~6x. This upgrade option
would potential benefit all beamlines, instead of just those beamlines making use of photon brightness. Significant technical challenges exist with all these upgrade options. These challenges include, for example, nonlinear effects and heat load on accelerator systems, and high-heat-load and low-distortion X-ray optics and other components on the beamline side. We plan to pursue studies of these options in FY20, with a goal to produce a white paper that summarizes the potential performance goals, technical issues and challenges, and possible mitigation plans to address the challenges. This white paper will help select the best option to pursue and develop a science case for the selected option.

**Prototyping and testing a low-energy version of the novel Complex Bend concept at ATF:** We have developed a novel concept using superconducting “complex bend” modules as the ultimate multi-bend achromat lattice for potential future upgrade of NSLS-II and other facilities. We plan to fabricate and instrument a low-energy version of this novel concept and conduct testing at the Accelerator Test Facility (ATF) of BNL. Funded by an NSLS-II facility improvement project, this development project will engage other accelerator expertise onsite and maintain a high level of accelerator skills at the NSLS-II.

**X-ray Optics, Detectors, and Simulations**

Advances in synchrotron beamline technology, particularly in X-ray optics and detectors, play a critical role in enabling new, broad, and high-quality scientific applications at synchrotrons today. Meeting the NSLS-II strategic objectives requires continued research and development in advanced X-ray optics and detector technologies. Leveraging upon the experience gained and infrastructure already established at NSLS-II, we plan to pursue the following X-ray optics and detector R&D projects in the next five years.

**Development of large-aperture wedged multilayer Laue lenses (MLL):** Leveraging several critical advances in the multilayer Laue lens (MLL) optics development made in the past few years, we plan to continue to lead the development of MLL optics by advancing the necessary technology and processing including materials thin-film deposition, sectioning and polishing techniques, and characterization as well as developing related metrology techniques to fabricate and implement tilted and wedged MLLs and their associated mechanical systems to achieve 5 nm focus in the 10-20 keV range. In the past two years, we have made significant advances and have demonstrated 7.5 nm line focus at 15 keV, which is a significant achievement towards our five-year 5 nm goal. In FY20, we will continue to refine the processes that will lead to interfacial boundary sharpness and manageable film stress for thick multilayers. We will 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 such as APS.

**Bonding of the 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. Alignment of the two 1D MLL optics is a complex procedure which involves eight degrees of motion and requires a complex instrument with nm-scale resolution and nm-scale stability. We plan to simplify such an instrument by bonding two MLLs together using microfabricated templates. Initial experiments carried out in FY19 demonstrated sub-15 nm point focus. In FY20, we are fabricating improved Si templates to hold two lenses together in a pre-aligned configuration. Once fully developed, such monolithic 2D MLL devices will become standard nanofocusing optics which will be adopted and easily installed at the existing and future imaging beamlines of the NSLS-II.
Developing of robust MLL optic assembly to broaden MLL applications: Working together with Sigray Inc., we will develop a robust, easy to use mechanical system to allow MLL nanofocusing optics be broadly applied to synchrotron beamlines and lab-based instruments. Funded by a BES SBIR grant, we will attempt to develop a prototype MLL-based endstation with a wide-aperture collection optic from Sigray. We plan to implement and test this device at one of the imaging beamlines at NSLS-II during FY20-FY21 timeframe. This new technology will benefit other NSLS-II imaging beamlines such as the new sub-100 nm nanoprobe at SRX.

Next-generation testbed for sub-10 nm nanofocusing and nano-tomography: This project will attempt to tackle 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 plan to design, fabricate and commission a next generation test-bed suitable for sub-10 nm diffractive optics characterization and nano-tomography. It will be 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.

Development of 2D stitching interferometry for high-accuracy metrology of highly curved X-ray mirrors: This is essential to enable measurements of figure errors at sub 100-nrad levels. This targeted R&D strategic plan will be done by upgrading instrumentation in the existing NSLS-II optical metrology laboratory and efforts on the development of new instruments for slope error measurements to reach 50 nrad slope error accuracy and stitching interferometry capabilities for sub nm rms accuracy, both on highly curved surfaces. These efforts will be combined towards the construction of new instruments with stitching capabilities using interferometer and Shack Hartmann and software configurable optical test stations to perform 2D mapping of the optical surfaces in order to feed a deterministic polishing process based on ion beam figuring. We started this R&D in late FY18 and expect to complete by end of FY20.

VIPIC for X-ray Correlation Spectroscopy: A detector optimized for X-ray photon correlation spectroscopy (XPCS) experiments is essential for accessing micro-second time regimes and is ideally suited for a high-coherence X-ray scattering beamline such as the CHX at NSLS-II. The VIPIC (Vertically Integrated Photon Imaging Chip) is a unique design for this purpose, based on the most advanced CMOS technology, and proving the viability of this technology for x-ray and HEP detectors. We are currently developing a plan to make a full-scale (i.e. 1 megapixel) version of this detector. This project is funded by DOE-BES scientific user facilities. At the same time we are working on prototyping the next generation of such a detector. It would improve the time resolution by a factor of at least 100 compared with the first detectors, i.e. from 10 µs to 100 ns. That requires testing some circuit ideas. This project is a three-way collaboration between BNL, FNAL and ANL, and we anticipate that the project will be completed by end of FY20.

Cryo-cooled Ge-based Pixel Array X-ray Imaging Detector: This is a prototype detector which provides full spectral information for every pixel, i.e. a true "color" x-ray camera that is essential for spectroscopic hard X-ray imaging. This project will leverage two key technological capabilities developed at BNL –
Ge pixel array sensor fabrication in the NSLS-II detector group and cryo-cooled ASICs in the Instrumentation Division of BNL. This project received DOE-BES Accelerator and Detector Research funding and will start in FY19 for five years. Once developed, the prototype will potentially revolutionize full-field x-ray fluorescence imaging and Laue diffraction as well as other hard x-ray spectroscopic applications.

**Full-field fluorescence imager:** The current method of obtaining elemental maps involves forming a small x-ray spot on the sample, and rastering the sample through this beam. This data is used to form an image based on the fluorescence detected by an energy-resolving point detector or small array. The mechanical motions required make this essentially a slow process. An imaging detector with per-pixel energy-resolving capabilities would enable a full-field instrument, which should in principle be faster and involve less sample radiation damage. Funded through a BER grant as part of our bio-imaging initiative, this project aims to develop, not only the spectroscopic imaging detector, but also the optical system to magnify the fluorescent image. We are investigating several approaches to the optics: Wolter reflection optics, coded aperture masks and polycapillary arrays. The detector development is being done in collaboration with BNL’s Instrumentation Division.

**Maia-II, an SDD-based version of the Maia system:** An updated version of the well-known Maia x-ray fluorescence microprobe system, replacing the current silicon diode sensor array with an array of silicon drift detectors (SDDs) designed and fabricated at BNL. It will also be equipped with a new readout system based on a new lower-noise integrated circuit and an advanced digital section based on an FGPA with embedded processors. It should provide better energy resolution and higher count-rate than the existing system.

**Low-gain avalanche photodiode array:** A new class of sensors with moderate charge gain (x5 to x10) has been developed and fabricated at BNL. We will explore the performance of these devices as fast detectors (~ns) and as soft x-ray detectors for the 500-2000 eV range.

**New capabilities for simulations of coherent X-ray propagation from source to experiments:** Recent progress in accelerator physics has driven a very substantial reduction of electron beam emittances in storage ring based light sources. Efficient usage of these low-emittance, high-brightness coherent X-ray sources requires better modelling tools to allow ordinary non-expert synchrotron users to properly plan, execute, and analyze coherence based experiments. Currently no such tools are available for non-experts, and lacking such capability has led to inefficiencies in using the cutting-edge tools. Funded by the SBIR and the most recent accelerator R&D by BES, we will develop new capabilities to enable realistic simulations of coherent X-ray scattering and imaging experiments on user-defined prototypical samples, based on an upgraded Synchrotron Radiation Workshop (SRW) software package. It will leverage and build upon the recent improvements in the high-accuracy SRW package with a friendly user interface and high-accuracy simulation capabilities of the partially-coherent synchrotron radiation, advance beyond the processes of wave generation and propagation through beamline optics to allow simulations of interactions directly with experimental samples as well as modelling of the experimental detection systems. High accuracy wave optics simulations will be extensively used for the development of new NSLS-II beamlines and for bench-marking existing beamlines. Successful execution of this new project will make possible detailed simulations of user experiments before their actual execution, and will help to use the light sources most efficiently and increase the scientific productivity and impact of the BES light source facilities.
Multimodal Capabilities

NSLS-II recognizes the opportunities in utilizing complementary techniques across multiple NSLS-II beamlines, and in combining synchrotron techniques with other techniques, such as the electron-based imaging methods at CFN. Such holistic approach will bring higher impact and deeper understanding in complex, heterogeneous systems, critical for many research fields in the 21st century. In response to such needs, NSLS-II established a multimodal issues taskforce to identify issues associated with such multimodal approach and to make strategic recommendations. Based on such recommendations, NSLS-II will continue to pursue multimodality capabilities in technical needs including both hardware and software at beamlines, and in the logistics that support such activities including logistics on user access. A number of specific planned activities are described below.

**Multi-beamline data acquisition and analysis.** Across beamlines and programs, the opportunities and needs have been identified regarding the data acquisition, management and analysis. To ensure a successful data strategy, NSLS-II has identified, and will address, the urgent basic IT needs in data sharing across beamlines for multi-modal data acquisition, management and analysis. In FY19, NSLS-II started to develop a centralized sample registration and management database, integrated with the data acquisition and analysis, to effectively track samples and tag associated datasets, and thus allow multimodal experiments successfully performed at multiple beamlines. This development activity will continue in FY20. This sample management system will also be needed for high throughput techniques and for complex data analysis as the conventional approaches on sample tracking became very inefficient and unsustainable.

**Sample manager and sample environment.** On beamline hardware and software, we plan to continue coordinating the development of multimodal capabilities at NSLS-II for two types of scientific needs – measuring the same sample across multiple beamlines (*static measurement*) and measuring the same system in-situ/in-operando using multiple probes (*in-situ/operando measurement*).

For static measurements, simple and fast sample registration between beamlines and laboratory techniques is critical. We plan to meet these needs by developing common fiducial markers, common sample mounts, data acquisition with automated sample position registration, and data analysis tools for data merging, analysis, and integration. Radiation dose may need to be tracked and addressed to ensure samples truly remain unchanged across beamlines. In the near term, our overall goal is to first establish sample mounting, measurements and analysis across a small number of beamlines within the Imaging and Microscopy Program, with an aim that the efforts will be expandable to other beamlines/programs.

Operando/in-situ experiments require measuring samples that are evolving under various conditions, and in some systems, it may not be feasible to measure the same samples across different beamlines because the samples may have evolved after one measurement and cannot be reused. To address this challenge, we plan to develop and implement *in-situ* sample cells that are compatible across different beamlines in order to create the same *operando* conditions for correlative measurements using multiple techniques, and to develop data handling software that provides the ability to align, analyze, correlate, and integrate the *operando* data measured from different beamlines and techniques. In the near term, the facility has efforts in developing and implementing high temperature cells that are designed to be compatible multiple beamlines. To ensure coordination across beamlines, we will continue the efforts in developing a facility-wide searchable database for sample mounting and sample environment for effectively facilitating multi-modality research at NSLS-II.
Multi-beamline user proposals. On multi-beamline user access, a plan has been developed based on lessons learned from the trial proposals in FY18 with multi-beamline requests. Implementation of multi-beamline user proposals started in the 2019-3 run-cycle and this new proposal mechanism has been well received by the user community. In FY20, we will continue the implementation of the new multi-beamline proposal mode and work closely with ITD to make a number of necessary changes in the NSLS-II proposal administration, safety, and scheduling (PASS) system to ensure its success.

Controls and Data Acquisition, Management, Analysis

Experimental controls and Data Acquisition, Management, and Analysis (DAMA) forms a critical part of the NSLS-II user facility. They serve as the actual physical interface between an experimenter and the experimental capability that the user is using at NSLS-II for his/her experiment. A properly designed and implemented experimental control infrastructure and data acquisition interface will enable the user to take full advantage of the NSLS-II beamline capabilities and allow the user to focus on the science questions he or she is seeking answers for. It is therefore fair to state that without a working and reliable controls and DAMA system, no synchrotron light source would be viewed as a successful facility, no matter how advanced its accelerator and beamline capabilities are.

Controls Improvement Plan. NSLS-II recognizes the very importance of experimental controls and plans to address the problems and issues that have emerged as more beamlines transitioned into full user operations. In FY19, considerable efforts by the Controls Program went into discussing various issues on controls with beamline staff and identifying the prime causes of the various operational problems and issues they were experiencing. This led to a better understanding why the various data acquisition symptoms occur and how one may be able to solve the root of these problems. A detailed controls program peer review was conducted in July 2019, and a set of high-priority controls issues were generated and prioritized with input from beamlines and controls staff. The emphasis was on user experience and user confidence. Out of these discussions, a set of thirteen controls improvement projects have been created and are being executed to address the identified high-priority controls issues. Below we describe in some detail the highest priority six improvement projects that we plan to pursue immediately.

- **Improving the performance of network core and peripheral switches** (FY20-21): The network serves as the backbone of experimental controls and data acquisition and management, and thus must provide both reliability and performance for the beamlines. The network core switch was purchased in 2017 and has proved to be problematic primarily due to failure of vendor software support for the hardware. The lack of support has meant that there are random slowdowns caused by network routes being improperly formed and/or the cores not evenly spreading the load, leading to the possibility of network failure if redundancy does not work properly. Our plan to tackle this issue includes the following:
  - Outsource network maintenance and upgrade responsibilities to the Network Engineering group in the BNL Information Technologies Division (ITD). This has been done in FY19.
  - ITD network engineering has recommended replacement and reconfiguration of the network core via two purchases. The network core routers will be replaced in December 2019.
  - Many of the outer, peripheral switches are nearing “end of life and unsupported” status beginning in October 2019 and need to be replaced. This includes 180 devices on the accelerator which already out of date, and on average three devices per beamline which are not yet at end of life.
An ongoing, long-term replacement strategy for all these switches will be developed in FY20, and will be implemented in the coming years depending on available budget. The success metrics for this project are to ensure that beamline users will see no random slowdowns caused by the network. We plan to monitor the network very closely, and our objective is to eliminate the bulk of the network slowdowns, and to ensure that the core network uptime exceeds 99.9%.

- **Implementing standard naming conventions for servers, workstations, and devices** (FY20-21): Keeping the beamlines software and hardware environments uniform greatly helps with staff efficiency and allows for better working software tools. Naming standards are required to do this. Currently the naming standards are not uniformly enforced across NSLS-II beamlines, causing considerable issues in troubleshooting and diagnoses. We plan to develop and enforce the naming standards and require that the various standards must be well defined and uniformly applied. We have identified the following eight naming areas that impact everyday life in experimental controls across NSLS-II beamlines:
  1. DNS and machine naming - domain name server IOC, servers, workstations
  2. Component naming standards - including Process Variables (PVs)
  3. Directory naming standards - NFS, GPFS etc.
  4. Fixed device names e.g. Moxas, FPGA’s
  5. Computational services and gateways naming
  6. GIT and collaboration product names and locations
  7. Hardware standards – computing

The first three areas are a priority as these are a prerequisite to enable effective generic tools for data acquisition, management, and processing. Our immediate goal in FY20-21 is to have 100% compliance for anything new including new machine names, new PVs, new GPFS installs, and new NFS users, 85% or greater compliance for existing items (there are approximately 3.5 Million PV’s in total) including machine names, PV names, GPFS installations, and NFS users, and 100% identification of all non-compliant items and development of long term plans for retrofitting them. We will also publish an updated set of standards in all above-mentioned areas.

- **Upgrade GPFS performance on beamlines** (FY20-21): GPFS stands for General Parallel File System (GPFS) as developed by IBM. This system has been adopted by NSLS-II to provide a fast disk access system for data collection, and thus is critical for effective and reliable data acquisition at NSLS-II beamlines. It has been known that the GPFS is not performing well in some cases, with “pausing” or “lockups” and general speed issues impacting performance. Each beamline has different requirements with respect to data collection and processing, and as a result the deployment and tuning of GPFS may need to be different at each beamline. GPFS tuning is very complicated and requires experienced staff. There is currently one “standard solution” for Structural Biology beamlines; and there exist widely variable evolved “solutions” at other beamlines.

We have identified two major tasks to improve performance as part of our plan to improve the GPFS performance. First, all existing GPFS installations will be converted to supported operating systems. Second, every beamline using GPFS will be individually tuned for maximum possible performance defined by the technology. We will measure the improvement on performance after these tasks are completed and devise additional improvements if required.

- **Upgrade NFS performance on beamlines** (FY20-21): Network File System or NFS is a distributed file system protocol (from 1984), allowing a client computer to access files over a computer network much like local storage is accessed. Being an open and common protocol NFS is widely used by
Linux systems. At NSLS-II, every beamline relies on NFS for basic users services, e.g. home directory, self-consistency, small files. It is a critical part of the user experience at NSLS-II. While not a high-performance solution, NFS should perform better than we have experienced so far at NSLS-II. NFS at other facilities (Argonne, Oak Ridge) is much faster and more reliable.

NFS is installed on almost every machine at NSLS-II. Accelerator physicists also rely on NFS, for logins and file sharing. We will implement a separate NFS for beamlines and provide consistency in login environment that will lead to less frustration in general. The accelerator NFS structure will remain the same. We plan to implement an NFS appliance for the beamlines to minimize the ongoing operational effort. Our goal is to reduce the probability of the long waits (>10 sec) for small data to the order of less than 0.1%, a factor of ~50 improvement compared to situations today. We will also aim for an improvement on small data file access speeds by an order of magnitude, from roughly 5 ms today to 0.5 ms, consistent with what is typical at other light source facilities.

• **Improvements in moving and processing experimental data** (FY20-21): This project addresses two issues that currently impede the user science experiments and their productivity. The first is that the users need to visualize and process raw data on-site at NSLS-II either during their experiments or subsequent to their experiments. The second is that the users need to transfer their data back to their home institution either through networks or via personal portable media.

On data transfer – at NSLS-II, all raw data are first stored locally at the beamline where an experiment is conducted, then transferred to NSLS-II central computing facility and/or to the Scientific Data Computer Center (SDCC) in the Computational Science Initiative at BNL, and finally, if needed, transferred to the external user institution. Our goal is to make these data transfers reliable and seamless to the user. We plan to pursue the following tasks in the coming two years to make our objective a reality.

- Develop and demonstrate data transfer from beamline to outside institution through SDCC, by establishing Globus server license and a transfer node, and by establishing full outside-world to beamline connectivity;
- Establish data transfer stations that will have a consistent interface for physical devices (HDD, USB, laptop, etc.); Users will be informed of this capability and of supported devices.

On raw data processing on-site – Users will be able to conduct initial data analysis during beamtime, performed locally at the beamline or at the NSLS-II central computing facility. All subsequent data analysis by users will be performed at the NSLS-II beamline or NSLS-II computer room, or preferably, at the SDCC. We will develop and test a model for the interactions between NSLS-II and the SDCC, including how to access, the business model, what analysis software would be supported, and how analysis workflow could be tailored for specific science/technique areas, among other things.

• **Controls configuration standardization** (FY20-21): A consistent set of standards in maintaining and deploying software and hardware is important to efficiently managing the various controls systems such as software versions and new releases. We plan to upgrade and complete a number of configuration management and release systems to meet the growing needs and complexities in these processes. Success of this project will be measured by (a) zero use of the older systems, (b) software distribution process is uniform and documented, and any exceptions accounted for, and (c) both the internal and external source libraries (GIT) are able to be referenced and indexed from a single place in each instance.
Data Acquisition, Management, and Analysis (DAMA). With the recent advances in photon brightness and X-ray optics and detectors, modern synchrotron experiments at facilities like NSLS-II can produce very large amounts of data in a very short time period, as many users at NSLS-II already experience today. In addition to being able to store the data at such high data rate, the real challenge that these facilities are facing is how to effectively take real advantage of this enormous data rate and harness its benefits that will lead to greater scientific productivity and impact. Recognizing this challenge and potential, the five DOE-BES light source facilities (ALS, APS, LCLS, NSLS-II, and SSRL) have decided to work closely together to jointly address this challenge. A data working group has been formed with representatives from each of the five light source facilities to serve as the resource to the facility management and provide information and recommendations on working together in the areas of data and computing.

Working together to leverage resources across BES light source facilities: Over the years, each of the five light sources has developed its own data acquisition, management, and analysis software packages to serve its users. The main development strategy in DAMA is therefore to leverage these developments, identify those that can be adopted across facilities, and implement a unified data acquisition platform and graphical user interface (GUI) at all five facilities. An example is shown in the schematic below, where components from across the facilities can be combined to form a powerful and unified data acquisition and analysis platform to serve beamlines at all BES light source facilities. These components include Bluesky developed by NSLS-II, Xi-CAM by ALS, TomoPy by APS, and applied math algorithms by CAMARA at LBNL. Here the powerful, flexible, and modular data acquisition package Bluesky from NSLS-II will serve as the basic interface between controls and higher-level GUIs.

Development of joint ASCR-BES strategy to meet the increase in advanced computing needs: It is estimated that multiple order-of-magnitude increase in demand for computing resources is expected at the BES light source facilities combined over the next decade. By 2028, the BES light sources will generate in the exabyte (EB) of data range per year, require tens to 1000 PFlops of on-demand computing resources per year, and utilize billions of core compute hours per year. Therefore unified solutions across the facilities are required in order to leverage efficiencies of scale and to provide facility users with the ability to easily and transparently manipulate data across the BES light sources complex.

Recognizing such needs, a joint Advanced Scientific Computing Research (ASCR) and BES user facilities data and computing workshop was held in June 2019 at LBNL to communicate and understand the needs, and to begin the discussion on whether and how to leverage the ASCR computing facilities to meet the BES needs. The discussions have been focused on four high-priority shared areas:

- Data management and workflow tools that integrate beamline instruments with computing and storage resources, for use during experiments, as well as facile user access for post experiment analysis;
- Real-time data analysis capabilities to significantly reduce the data volumes and provide feedback during experiments to improve data quality and to drive the direction of ongoing measurements; the
application of advanced machine learning algorithms and the integration of simulations and model-based approaches will allow automated steering of data collection;
• On-demand utilization of super-computing environments to enable quasi real-time data processing;
• Data storage and archival resources to house the continually increasing amounts of valuable scientific data produced by the BES Light Sources.

It is proposed that a Data Institute that bridges BES and ASCR facilities could be a way forward in meeting the needs of the BES facilities. Its goal would be to develop
• data management and workflow tools / streaming from the beamline to computing
• adaptive and scalable automated experiment steering capabilities
• novel machine learning, artificial intelligence, and other automated segmentation and registration techniques and approaches

Such Data Institute would build on and institutionalize the progress made by ASCR-BES initiatives, such as the ExaFEL grant and CAMERA, and would be complementary to CAMERA, which focuses on applied math and algorithms, this would deliver production level, customized code for workflow, data analysis, and data management for the over 200 instruments within the BES light source complex.

Expanding Data Acquisition Bluesky Capabilities: The NSLS-II beamline data acquisition system is built to provide an essential infrastructure that can grow and evolve over the life of the facility. NSLS-II has developed a suite of open source software packages that not only supports new detectors and new techniques as they continue to evolve, but also allows the analysis of the quality of the data as it is being collected and the performance of the beamline. The user facing package is called Bluesky and is for experiment control and the collection of scientific data and metadata. Bluesky interacts with the beamline hardware through the standard programming language, Python, using the EPICS interfacing software. In order to promote the use of Bluesky, we are committed to continue running tutorials and training courses both onsite and at other facilities to stimulate active collaborations.

In response to the science needs in using high-throughput and multimodal approaches, we plan to develop a unified centralized Sample Manager system to allow automated tracking of user samples from sample registration and metadata input, to multi-sample data collection, data tracking and management, and data analysis across multiple beamlines. We will also plan to devise a strategy to allow visualizations of multiple datasets with different scales and possibly coordinate systems. Both these will greatly enhance the scientific output of the NSLS-II beamlines, leading to potentially high impact and high productivity from the facility.

Develop and Mature Multi-tier Data Management System: To be able to accommodate high data-rate and high data volume data at beamlines, NSLS-II is implementing a multi-tier data management system to ensure efficient and adequate storage for complex experimental data from beamlines. Initially, this multi-tier system will consist of one or two tiers (depending on the beamline requirements), namely local to the beamline and central NSLS-II storage. This will then be extended by adding connections to CSI for long-term storage and near-computer level storage at SDCC. The investigation, planning and initial prototyping of this expansion took place during FY18-19, with initial implementation by FY20. Based upon current estimates, we will need to have 25 PB available initially in order to support operations up to FY20; this assumes that we will only store data for a period of one year.

Functional Library of Analysis Software Tools: A library of software routines and tools is being developed to meet the needs of specific types of techniques, experiments, and scientific disciplines. NSLS-II is developing the analysis tools in a phased approach consistent with the NSLS-II beamline
development timeline. The software and tools developed are released under the ‘scikit-beam’ umbrella project, which has users and contributors from multiple facilities.

It is important to state that our approach will be to reuse and collaborate on the development of existing software that meets our requirements. During FY18-19 we evaluated existing software that is available (both internally and externally) and developed a project plan for each to meet the requirements of the beamlines. This effort is now merged into the 5-facilities joint effort as described in a previous section. We will continue to work with the APS and ALS to maximize the impact of the software produced by each facility by eliminating areas of overlap.

**Post-Experiment Data Processing Facility:** NSLS-II will work with other stakeholders on computing within BNL to develop and operate a central data processing computing facility as part of the multi-tier data management system. The main goal of this facility is to provide front-end computing and centralized data storage/archiving system for NSLS-II users. This will allow them to access their data on-site during the experiment and also later when they return to their home institutions. The archived data will be made available to users for a length of time that will be determined by policy and resource constraints. This post-processing facility on archived data is an essential component of the NSLS-II scientific capabilities portfolio, and is required to enable effective and efficient workflows from experimental data to publications and solutions.

The facility will consist of multiple components, each tuned to a different data processing pattern or activity. The users will be able to make use of which type of computational platform is appropriate for their needs. As an example, for a case where a user has a problem that requires a large amount of physical memory and lots of tightly coupled compute cores, then they will make use of the general user systems within the NSLS-II. But, for a use case that can be parallelized more efficiently and can make use of large parallel HPC like machines, then they will make use of compute clusters situated within CSI. We are currently working with CSI (and have a successful ASCR SBIR) to benchmark some standard codes, such as accelerator physics, ptychography and XPCS, in order to determine which computational platforms would be best suited for the various NSLS-II use cases.

It should be noted that this post-processing facility on archived data is an essential component of the NSLS-II scientific capabilities portfolio. It is required to enable effective and efficient workflows from experimental data to publications and solutions for high scientific productivity and societal impact.

**Closer Interactions with Computational Science Initiative:** We will leverage developments being made by Brookhaven National Laboratory through the Computational Sciences Initiative (CSI) to mitigate the costs involved in providing computational resources, for large scale storage and compute clusters. By partnering with experts within CSI we can develop a ‘flavor’ of HPC resources that are geared more towards the needs of scientists that will use the NSLS-II. One particular example is that we need a more instant on demand access to resources so that we can make use of computational modeling techniques to provide input for both experimental planning and steering. This type of access and usage is significantly different than traditional HPC offerings. Further, leveraging CSI staff for standard computational work will allow NSLS-II staff to concentrate on the problems that are specific to the smooth operation of an experimental facility.

We will continue an active level of general day to day interaction and collaboration between members of the CSI and the Data Acquisition, Management, and Analysis (DAMA) group. In order to encourage this we have allocated office space for the DAMA group within CSI. Another option for closer
integration could potentially include joint appointments, both for permanent staff members and for postdoctoral researchers.

To summarize, we are currently interacting with CSI on: software development and release policies, development of ptychography software, Workflows and Provenance Capture, long-term data storage, computing architectures, GPGPU techniques and developments, cloud computing, application of machine learning, authentication and authorization, and data libraries and catalogues. In addition, we are currently working with CSI to benchmark some standard codes.

**Operations Excellence**

Creating a vibrant research environment includes having the staff, the support, and the infrastructure necessary for staff and visiting users to safely and effectively work at the NSLS-II facility. 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 & diversity, career development and work-life balance, environmental safety and health, facility infrastructure, user services, and communications.

**Workforce Development and Inclusion & Diversity.** Workforce skill mix and matrix assignment of staff resources at NSLS-II will continue to evolve to meet 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 I&D goals for hiring managers, examples of which 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 recent directorate initiatives include requiring each NSLS-II staff member to have an annual I&D goal and creation of a new 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.** NSLS-II considers its talented and enthusiastic staff as the single most important asset of the facility. As a newly developed 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 ramp-up and mature science programs is a critical aspect of NSLS-II facility operations. Recognizing this need of talent management, NSLS-II will implement a staff career development plan that includes the following elements.

- **Scientific Staff Promotions:** 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. As a start, NSLS-II has implemented a new scientific staff review (SSR) process specific to NSLS-II. The new SSR process clarified the case for permanent employment at the level of continuing appointment at NSLS-II, before tenure cases are considered. It has the benefit of strengthened employee/supervisor relationships, and better alignments with staff career
development needs and with our mission. NSLS-II will continue to work with other parts of the Laboratory to further strengthen our staff promotion process and recognitions at the Laboratory level.

- **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 Scientific Staff**: In a recent BNL-wide employees engagement survey about the employees experience at Brookhaven Laboratory, NSLS-II staff provided their views of the Laboratory and various issues related to their working climate, environments, and processes. One of the issues standing out from the rest of the BNL is the difficulties in work-life balance for our scientific staff, especially beamline scientists. NSLS-II plans to address these issues in various ways, including implementation of a Beamline Users Guide to provide the guidance and the expectations on user assistance by beamline staff, implementing a policy to allow ‘unused’ beam time at beamlines, and working with accelerator operations group to develop and implement a more balanced operating schedule for weekends and holidays. In addition, NSLS-II plans to form a new working group consisting of NSLS-II staff to help digest the engagement survey results and make specific recommendations to NSLS-II management.

- **Postdoc and Graduate Student program**: In order for NSLS-II staff to have time to maintain their own scientific research program, they need help from students and/or postdocs. In addition, training of students and postdocs can provide added hands at the beamline and will help grow the experience workforce of the future. To be successful, the facility should have a reasonable number of students/postdocs so they can interact and learn from each other. The biggest challenge to having a team of students and postdocs is funding. Since this cannot readily come from the operating budget, staff are incentivized to find matching funds from other sources such as collaborators or LDRD. Programs such as this exist at ALS and SSRL and NSLS-II will investigate these programs and adopt and adapt them as appropriate.

*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. A Security Plan for NSLS-II is being developed to provide general protection as well as support DOE and user needs to conduct experiments requiring additional security measures. Select members of the NSLS-II leadership team have acquired DOE access authorizations and applications for a few others are pending.

*Buildout of User Laboratories and Offices in LOBs*. As of August 2019, 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 finished. A recently
completed FY16-19 IGPP project ($5.3M) has built out half the lab spaces (10 total) in LOB 4 and 5, in support of the structural biology, imaging & microscopy, hard X-ray spectroscopy, and complex scattering programs, as listed below.

- Cryo-EM screening microscope lab 5LL03, Wet Lab 5LL06 and the sample preparation lab 5LL07 will be used primarily to support the Structural Biology Program. The Cryo-EM screening microscope and sample preparation lab will both support the CRYO-EM/LBMS program. Dry lab 5LL08 will be primarily utilized by beamlines FXI, NYX and XFP.
- Dry lab 4LL04 and Wet lab 4LL08 will primarily be used to support the Complex scattering Program. The Energy and ElectroChem Wet lab 4LL09 will be used to support the Complex Scattering, Hard X-Ray Spectroscopy, and Imaging and Microscopy Programs.

Several other lab spaces have been configured with local funds for use as technician work spaces. LOB 2 is all shell space.

While the previous plan had been to complete the LOB build outs using IGPP for three additional projects funded over the next 7 years, this is no longer possible due to new DOE financial restrictions imposed in May 2018. NSLS-II is working with BNL to develop alternative plans for buildout of the remaining labs in LOBs 4 and 5, but the time horizon will stretch out and total cost will rise substantially. Under the current rules, use of IGPP funds will not be permissible for LOB2 buildout. As a result, LOB2 buildout will require use of BES GPP funds. NSLS-II is working with the Laboratory Modernization Project Office to prepare LOB2 build-out projects for submittal to BES GPP program.

The schedule for the remaining LOB buildouts is critical. With the previous aggressive IGPP buildout plans, the available labs and offices were just keeping slightly ahead of projected staff and user growth. A stretch-out program which delivers at most 1-2 labs per year will cause major disruption to the NSLS-II mission within the next 2-3 years.

**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 and allocation by the Proposal Review Panel, and a fully functional Safety Approval Form system. However, the evolving user science needs require substantial improvements to and possibly a revamp of this PASS system. In FY19, we conducted two external reviews of the PASS system to determine its strengths and limitations both at present, but more importantly, in the future. This information will help to guide BNL in determining whether the PASS system has the functionality, flexibility, and expandability suitable for the current and future needs of all user facilities at BNL, or whether another software solution should be pursued. Based on the reviewers’ comments and recommendations, NSLS-II will make the decision either to continue to use PASS or to develop a completely new system to replace PASS.

As of September 2019, the path forward for PASS will follow the timeline below:

- October 2019: NSLS-II will make its decision on whether to continue to develop PASS to meet the evolving users needs or to develop a new proposal administration system to replace PASS.
- In the case of a new proposal system:
  - NSLS-II will discuss with other BES light source facilities about to decide in FY20 on the appropriate option to pursue, taking into account experiences and developments at these other facilities;
  - NSLS-II will establish a project team in FY20 to define the requirements of the new proposal system, with an estimated scope, effort requirements, and a schedule;
Ideally the chosen development option will be the adopted choice of all five BES light source facilities; NSLS-II will lead, or commit appropriate resources to contribute to, this joint effort;
- During the development, NSLS-II will continue to operate PASS with incremental improvements in FY20-23, before a new system is available and implemented.
- In the case of continuing with PASS:
  - NSLS-II will develop an implementable plan in FY20 to identify a list of needs for improvements, prioritized based on the benefits and impact of the new improvements, and begin to commit resources to implement the plan.
- Overall objective is to have an improved PASS or a brand-new proposal administration software system operational by FY24 to meet the NSLS-II facility users needs.

**Multimodal and Multi-Beamline Proposals.** As part of our initiative to encourage multimodal studies at NSLS-II beamlines, we have started implementing multimodal and multi-beamline user proposals. Such multimodal proposal contains a core scientific background and motivation section that better describes the big picture than individual proposals. This new mechanism became live in May 2019. We plan to continue to monitor the submission and review process of these multimodal/multi-beamline proposals and will act to make improvements as needed to ensure successful multimodal studies at all NSLS-II beamlines.

**Extending the Block Allocation Group Program.** Given the highly successful Block Allocation Group proposals at structural biology beamlines, NSLS-II has extended this program to non-biology beamlines that are based on routine techniques – XAS, XRD, and SAXS/WAXS at ISS, XPD, and CMS beamlines. To date this development has been well received by the user community. NSLS-II will continue to monitor the implementations of these new access programs and make necessary changes to further meet the users needs.

**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. This is achieved by a strategy that defines long-term goals over the course of five years, mid-term milestones in between, and short-term plans for the following year.

Our long-term goals are:
1. Raise awareness for NSLS-II capabilities among key scientific audiences
2. Support NSLS-II growth into a center for discovery-class research in the nation
3. Grow positive relations with all stakeholders; including DOE and partners
4. Strengthen NSLS-II position as a core facility within Brookhaven Lab; integrate the facility into Brookhaven labs long-term strategy without losing its identity
5. Create a visible, coherent, concise, and engaging external presence for NSLS-II.

The top three goals are strongly supported by the last two goals, which create the base for NSLS-II communication within Brookhaven Lab, the DOE complex, and all other external audiences. More details regarding short-term goals for the next year (FY20) and mid-term goals for the following years are laid out in the NSLS-II Communication Strategy.
New Beamlines and Initiatives
New Beamlines and Initiatives

As stated in the Chapter on Science Program Areas, there have been significant new interests over the past year in the science of quantum information technologies, beyond Moore computing architecture, and artificial intelligence and machine learning. These discussions have been very timely as we shape up our strategies and align our development activities, including new beamlines concepts, with these new initiatives. In this Chapter, we discuss these and other evolving science needs, the new capabilities and beamlines that we plan to develop at NSLS-II, along with a number of programmatic initiatives and partnerships we plan to pursue in order to broaden the range of science to be conducted at NSLS-II.

Our vision is to have in total 40 world-class beamlines operating or under development by year 2030, supporting a broad range of scientific and technology research programs and initiatives as well as R&D partnerships to further enhance the impact of NSLS-II.

Science Case for New Beamlines

Driven by the challenges facing society and the advances in the research tools, the materials science of the 21st century is increasingly focused on inhomogeneous, functional materials with structure on characteristic length scales from the nanoscale to the mesoscale. Further, there is a strong desire to study such materials as they are functioning under real-world operating conditions, i.e. *operando*. As identified in a series of Basic Research Needs workshops and reports, prominent examples include energy storage, catalysis, advanced manufacturing, and more recently, quantum technologies, advanced manufacturing, and microelectronics for beyond-Moore computing. Each of these areas is central to the DOE Office of Science’s mission to transform our understanding of nature and advance the energy, economic, and national security of the Nation. As articulated in these reports and elsewhere, grand challenge science questions arise in each of these areas. It is these that we are seeking to address at NSLS-II. Examples of these include:

- How can we understand the functionality of materials sufficiently to anticipate their behaviour in electrochemical configurations? How can these insights inform the design of chemistries, materials, and structures for future energy storage?
- How do we elucidate the cooperative interactions among the binding site, reacting molecules, and the surrounding environment to enable the design of catalyst structures that precisely control chemical reactions?
- How can we understand and control decoherence of quasiparticles and design long-lived, scalable qubits for quantum information technology?
- How can we measure and quantify the interactions between material and processing technology to better understand the material-process-structure relationship?
- How can we redefine energy-efficient computing by revolutionizing memory and data storage, by reimagining information flow unconstrained by interconnects, and by leveraging new materials with unexploited physical phenomena?

As described in the previous sections, the current suite of NSLS-II beamline capabilities already provides a set of sophisticated tools to address these and other science grand challenge questions. And, we have
laid out an ambitious plan to further enhance these and develop new capabilities at the existing beamlines. However, certain key capabilities are still missing at NSLS-II that impact the type of research that can be done and the range of information that can be obtained to address these questions.

In battery research, current battery architectures feature a complex arrangement of materials each optimized for a different function, for example electron and ion mobility, typically with multiple length scales active effects crucial in the overall performance. Addressing the first question above requires a multiscale understanding of electron and ion transport at interfaces, and to understand the role of crystallographic and chemical structure, and in particular how these change with time with multiple charge and discharge cycles. NSLS-II is presently missing key capabilities in these areas.

In catalysis research, answering the second question above requires understanding the structure and the electronic and chemical configuration of the catalyst and its support and the bonding energetics. Addressing these challenges requires tools of exquisite sensitivity and spatial resolution, tools able to probe both carbon bonds and the crystallographic structure of various host materials on the nanoscale and under operando conditions. As discussed below such tools are presently lacking at NSLS-II.

In quantum information science, deep questions concerning the quantum behavior of solids underlie question the third grand challenge question. Here it is important to understand the quasiparticles that describe the many-electron quantum behavior and how factors such as topology, statistics, strain, defects, temperature etc., determine decoherence times. Exotic, fractional statistics can emerge and even non-abelian exchange statistics that could well be exploited in functional quantum devices. What is required to address these questions are nanoscale probes of the electronic quasiparticles and excitation spectra that can be correlated with structural measurements. Such probes are presently lacking at NSLS-II.

In advanced manufacturing, the “Strategy for American Leadership in Advanced Manufacturing”, as outlined in an October 2018 publication by the National Science and Technology Council, highlighted the need for developing world-leading materials and processing technologies. With its high-brightness source, NSLS-II is ideally positioned to contribute to this national goal. However, most scattering projects still focus on ex-situ measurements on materials prepared under a variety of different conditions, often studied during post-processing anneals or operando conditions. While these are important studies, progress can be slow with months between synchrotron runs. Moreover, during processing, materials undergo many transient states before the structure and properties get 'frozen in'. Understanding and control of these transient states is what's needed for rational design and optimization of material feedstocks and processes. For these reasons, there is growing interest, especially among industrial researchers, in studying the whole out-of-equilibrium processes associated with additive manufacturing. In addition, the large materials and processing parameter space requires real-time experiments by changing processing conditions on-the-fly based on the outcome of analyzed x-ray measurements. This mode of operation requires integration of processing instrumentation, fast data acquisition using large-format area detectors, computational infrastructure for large data-set processing, engagement of experts in modeling and simulations, and on-line data analysis and feedback workflows that incorporate AI/ML approaches. It also requires beamlines capable of handling large-scale industrial processing instrumentation and facilities for testing product reliability under accelerated aging conditions.

In microelectronics, it has become clear that the Moore’s law that has been driving the microelectronics industry to reduce the dimension of the technology node by roughly a factor 1.4 every two years is approaching its fundamental and economic limit – due to the quantum physical limit and the leakage current towards the physical limit. Furthermore, the computing use landscape has evolved significantly from pure digital computing applications to the applications of big data and pattern recognition. Both
these changes are driving the needs for novel 3D integration of microprocessors and memories and for novel computing platforms such as neuromorphic devices that have the potential to be more energy efficient for big data and image recognition. Dedicated nanoscale probes will be required to characterize/image the strain fields and/or structural phases in potential nano-devices in-situ and ideally under operating conditions. Such probes would greatly help the development of 3D integrated microchips and neuromorphic memories for the next generation of computers.

NSLS-II will hold a community strategic planning workshop at Stony Brook and BNL, October 21-23, 2019. This 3-day workshop will aim to engage the broad scientific community to discuss the scientific grand challenges, the research needs, and how NSLS-II may help to meet the research needs and address the scientific challenges in the specific areas of quantum information science and quantum materials, soft matter research, catalysis and chemical sciences, materials and engineering sciences, molecular and cell biology, and biological and earth & environmental sciences. More information about this exciting workshop can be found at https://www.bnl.gov/newscience2019/.

**Beamline Development Strategy**

The current NSLS-II beamline portfolio (see Figure below) occupies ~60% of insertion device (ID) straight sections and ~30% of the BM/3PW/IR ports, and thus the facility overall is about half-built. Among the remaining open ports, there are 11 insertion device straights plus three canted undulator sources, and 22 available BM/3PW/IR ports. Given the high demands on the existing beamlines and the needs for additional scientific capabilities at NSLS-II, one of our main development initiatives for the next five years is to start build out the remaining beamlines.

In addition to beamlines, we very much recognize that scientific research and development in the 21st century has been rapidly evolving and has become increasingly interactive and interdisciplinary. The success often relies on a large team of researchers with complementary expertise to work together to achieve the best possible research objectives. One of our strategic approaches is to integrate the scientific community interest and expertise in NSLS-II facility operations, leading to mutually beneficial partnerships that promote innovation and support the strategic mission of our stakeholders. The second half of this Chapter will outline our ongoing strategic initiatives to enhance the NSLS-II productivity and impact, as well as to jointly pursue and bring funding to develop new capabilities or new beamlines at NSLS-II.

Given that the majority of the highly-demanded ID ports are already under development and the overall facility is half full, it is important to develop a high-level strategy for allocation of the remaining open
beam ports. We have been actively engaging the NSLS-II SAC and the community at large to discuss this topic. During these interactions, we have considered several factors in order to make informed decisions on future strategic development directions. These include the following:

- **Capabilities gaps**: Key science questions that we seek to address in our stakeholders’ mission areas include: How can we understand the functionality of materials sufficiently well to inform the design of new technologies to meet future energy storage needs? How can we understand the processing of these materials and the emergence of functionality from the out-of-equilibrium state? How do we elucidate the cooperative interactions of catalyst structures to precisely control chemical reactions? And, how can we understand and control decoherence of quasiparticles and design long-lived, scalable qubits? The suite of beamlines presently operating at NSLS-II offers an array of tools which already contribute to the solution of these grand challenges. However, there are important additional capabilities that are required to address some of the most challenging aspects of these major questions. In particular, it is important to understand the electronic structures associated with low-energy states and excitations of energy related materials, to be able to probe the morphology and strain of multi-grain samples, to study the chemical states of light elements and to probe the magnetism and magnetic interactions in materials systems - and to do all of this with nanoscale resolution.

- **Capacity estimates**: For some high-throughput beamlines and high-end beamlines, while the required capabilities exist, the user community using such instruments can be extremely large and very diverse. This often leads to very different sample environment and associated ancillary equipment that need to be moved in-and-out, or beamline reconfigured, making operations of the beamline very inefficient. In these cases, a separate new beamline will not only increase the operational efficiency but also allow dedicated endstation instrument that is optimized for the specific science applications. Among the existing suite of NSLS-II beamlines, such capacity challenges are most evident in the areas of hard X-ray nanoprobe, X-ray diffraction, and ambient-pressure photoelectron spectroscopy.

- **National and global context**: Since the inception of NSLS-II – the first synchrotron designed to reach ~0.6 nm-rad horizontal emittance, there has been increased interest worldwide in pursuing synchrotron sources at ever lower emittance, including using the multi-bend achromat (MBA) lattice concept. MAX-IV in Sweden is the first MBA-based light source facility, and several MBA storage rings are now in construction around the world. In the US, the Advanced Photon Source (APS) will upgrade to an MBA design in the 2022-23 timeframe. The Advanced Light Source (ALS) is also progressing a conceptual design on an MBA upgrade on a somewhat later schedule.

- **NSLS-II strengths and opportunities**: In this international context, NSLS-II has several strengths: As a green-field, large circumference storage ring, designed for high-brightness beamlines, it has a large, ultra-stable floor, the ability to take beamlines outside the experimental hall, and world-leading and competitive coherent flux from the infra-red to soft and multi-keV x-rays and beyond. In addition, it has built up experience and expertise in the use, and operation, of ultra-bright beamlines including technique development and data analysis. Finally, the facility remains half built out and there are significant opportunities to develop additional capabilities, optimized and tailored to meet the research needs.

On the basis of scientific need, strategic strengths of NSLS-II, and the international context, our strategy for the next round of beamline build-out will be on the most-demanded additional cutting-edge imaging capabilities while supplemented by additional capacity beamlines tailored to meet the evolving needs of the scientific community.
NEXT-II Project

Following our beamline development proposal solicitation and peer-review process, we have identified and selected six new beamlines as the next suite of beamlines to develop at NSLS-II. Among them, three beamlines (CDI, ARI, and SXN, as described below) have been included in a Major Item Equipment (MIE) proposal submitted to DOE-BES for dedicated construction funding starting in FY20. This MIE project, named NSLS-II Experimental Tools-II or NEXT-II, has received the Critical Decision 0 (CD-0) mission need approval by DOE-BES in December 2019. Dedicated construction funding is expected in FY20, and a CD-1 review is being planned for March 2020. It is expected that the NEXT-II will be a multi-year project to be completed in the FY24 timeframe. The three beamlines included in the CD-0 proposal are described below in more details.

**Bragg Coherent Diffraction Imaging (CDI).** Bragg Coherent Diffraction Imaging (CDI) will be a state-of-the-art beamline that takes full advantage of the world-leading coherent photon flux in a 6-15 keV energy range at NSLS-II. It will enable cutting-edge research on structural evolution in a wide-range of materials systems under in-situ conditions. By taking the advantage of largely empty reciprocal space at large momentum transfers, Bragg CDI will be a largely full-field diffraction imaging beamline that has the unique capability to single out materials of interest in highly complex systems, leading to imaging of defects, dislocations, and strain fields in single grains of heterogeneous materials with relatively high signal-to-noise ratios. Additional capabilities include Bragg ptychography to allow mapping single grains in extended polycrystalline specimens, and time-resolved measurements for both reversible and naturally occurring processes. The CDI beamline is well aligned with all three NSLS-II science focus areas and the strengths of the NSLS-II source, and complements the multimodal capabilities at the existing beamlines e.g. HXN, CHX, CSX, and ISR.

We plan to design and construct the CDI beamline on an open low-beta ID port that has the possibility to extend beyond the ring building. In FY19, we have started its full conceptual design along with refined cost and schedule estimates. In FY20, we will continue to advance the beamline engineering design, complete the conceptual design report within the NEXT-II project, and prepare for the NEXT-II CD-1 review. Assuming the NEXT-II project kicks off in FY20, we will aim to finalize the engineering design and start long-lead procurements of CDI in FY21, with a goal to complete its construction in the FY23-24 timeframe.

**ARPES and RIXS Nano-Imaging (ARI).** The ARI beamline will be a cutting-edge soft X-ray facility with two experimental capabilities - Angle-Resolved Photo-Electron Spectroscopy (ARPES) and Resonant Inelastic X-ray Scattering (RIXS), combined using a nanofocused soft X-ray beam on the same sample spot with a spatial resolution of ~100 nm. Its chief science mission is to address the basic R&D needs in the development new quantum materials as driven by the basic research needs for new quantum information science and technologies. With this combined capability of nano-ARPES and nano-RIXS and leveraging the NSLS-II strengths in long-working-distance spectrometers and exceptional stability, it will be possible for the first time to provide a complete picture of near-Fermi-edge excitations and interactions with collective modes at the nanoscale in complex condensed matter systems. The ARI beamline will offer synergy with existing soft X-ray programs at CSX, IOS, ESM, and SIX, and with strong research interests at BNL and in the condensed matter research community.
The development plan for the ARI beamline included the R&D for its multiplexing spectrometer and conceptual design activities using NSLS-II operating fund. With NEXT-II project kicking off in FY20, we will finalize the conceptual design of the ARI beamline and prepare for a successful CD-1 review as part of the NEXT-II project. It is expected that the ARI beamline will be completed in the FY24 timeframe.

**Soft X-ray Nanoprobe (SXN).** The Soft X-ray Nanoprobe (SXN) beamline (formerly known as the Spectro-Microscopy Facility or SMF) will be a world-leading soft X-ray beamline consisting of two scanning transmission X-ray microscopes STXMs – one low-energy STXM with full polarization control that covers the energy range from Li K-edge at 45 eV to Si K-edge at 1.5 keV, and one high-energy STXM from C K-edge 250 eV to Au/Pt M-edges at 3.5 keV. Both instruments will have best-in-class focused soft X-ray beam sizes down to 10-15 nm, wide temperature range sample environments to LN$_2$ temperatures, modular sample holders compatible with other imaging beamlines as well as TEM, and integrated ptychography capabilities to reach better than f5 nm spatial resolution. The unique capability of the low-energy STXM will allow access to the Li K-edge, enabling direct imaging of Li chemistries and distributions in Li-ion batteries for the first time. Both STXMs will fill the spectral gap in soft X-rays and complement existing cutting-edge X-ray imaging and microscopy tools at HXN, SRX, TES, XFM, and FXI, allowing multiscale imaging of hierarchical structural and chemical organizations in complex systems. The SXN beamline will also fill a capacity gap in the national STXM user base and be able to quickly accommodate a very broad user community from energy materials and soft matter research, to geo-environmental and biosciences.

Our current conceptual plan is to develop the SXN beamline, as part of the NEXT-II, on a canted greenfield ID port shared with the ARI beamline. In FY20, we will continue to mature and complete the beamline conceptual design, and prepare for a successful CD-1 within the NEXT-II project. We expect that early long-lead procurement may start as early as in FY21, and the completion of the beamline construction in FY23-24 timeframe. Depending on the total funding level within NEXT-II, we will also consider engaging other funding agencies such as DOE-BER or NSF to procure funding for a high-energy STXM at the SXN to meet the needs of the environmental science and/or soft matter research communities.

**Other New Beamlines**

In addition to the three beamlines included in the NEXT-II project, we have identified three other beamlines that should be developed at NSLS-II. These beamlines are: Quick RIXS (QIX), Infrared Near-Field Nanospectroscopy (INF), and Processing and Liquid Scattering (PLS). Among these, QIX concept has evolved into a novel concept of multi-modal soft X-ray spectroscopy beamline that includes resonant inelastic X-ray scattering, photoelectron spectroscopy, and infrared endstation (INSPIRE), which will be a new endstation at the upgraded IOS beamline 23-ID-2.

Furthermore, during the various strategic planning brainstorming sessions in the past two years, NSLS-II arrived at a number of additional new beamline concepts that would expand our beamlines portfolio at NSLS-II. These concepts are preliminary and most require further discussions and developments before they can move forward.

We outline below in this section the three additional ‘beamlines’ mentioned above, and the additional beamline concepts from the brainstorming sessions. Our plan forward on these new beamline concepts...
will be to engage the broad scientific community at the October 2019 Workshop, as described in the
*Science Case for New Beamlines* section, to revisit the science case and refine the potential technical
scope of each of these new concepts. Such strategic planning discussions will help identify potential
funding routes for some of these new beamlines so that a path forward can be developed.

**Inelastic Scattering, Photoemission, and Infrared Endstation (INSPIRE).** Relying on a new endstation
and optics upgrades to the IOS (23-ID-2) beamline, INSPIRE will offer a unique combination of state-
of-the-art ambient pressure XPS, XAS, IR, and XES/RIXS capabilities for advanced energy and catalysis
systems under the same close-to-realistic operating conditions, at chemically relevant time scales. It will
capitalize on a focused beam spot of 1 µm x 10 µm with spectral brightness enabling very fast RIXS (~1
sec) and AP-XPS (~tens of millisecond) data acquisition. INSPIRE will also potentially benefit from the
future neighboring INF beamline to use synchrotron IR to perform simultaneous AP-XPS/IR and
RIXS/IR experiments, which would provide unprecedented advantages in spectral range and brightness
compared to conventional lab IR sources. These techniques will provide complementary information on
surface chemical states, chemical bonds, valence states and ligand coordination, making INSPIRE a tool
of choice for catalysis and chemical sciences and their vibrant user community.

INSPIRE evolved from QIX (Quick Inelastic X-ray scattering), which in the 2016 beamline development
proposal process was proposed as a new endstation at IOS. In FY19, we organized a workshop on the
science that INSPIRE will be enable using combined RIXS, AP-XPS, and IR spectroscopy capabilities.
In FY20, we will allocate small amount of the NSLS-II operating funds to further the engineering design
of the INSPIRE endstation, with a goal to start the construction of the INSPIRE endstation in FY21. The
INSPIRE endstation project will be designed with modularity to enable a phased construction process to
balance the demands of user operation with instrumentation development, with an estimated completion
of late FY24, depending on available funding levels.

**Processing and Liquid Scattering (PLS).** The PLS beamline will be a versatile x-ray scattering facility
to support a world-class program for operando studies of soft matter interfaces, especially polymer thin-
films during processing, and liquid surfaces and interfaces. This independent beamline would make use
of the existing PPLS hutch and of the current PPLS instrument (commissioned in FY19-20) that will be
used in a time-shared mode with SMI. The PLS beamline will provide new scientific opportunities at
NSLS-II that are not currently addressed by existing beamlines, as its unique design allows the sample
to remain level while the beam is tilted downward over a wide angular range. The high flux and tight
focus of the NSLS-II source will enable unprecedented time-resolved studies of soft matter specimens
undergoing industrially-relevant formation, processing, additive manufacturing, as well as structural
transformation, weathering, degradation, and aging. These studies will encompass polymers, liquids,
liquid crystals, granular materials, gels, and biomolecular materials, all of which lack the three-
dimensional crystallinity characteristic and are increasingly called upon to address national needs in
energy, health, the environment, and national security. This facility will also be well suited for studying
the synthesis of new materials at the liquid/vapor and liquid/liquid interfaces (discussed in section XX).
The PLS beamline is also well suited to take advantage of new funding opportunities associated with
BES and DOE interests in the Energy-Water Nexus, in particular the DOE Energy-Water Hub, and in
molten salts, currently funded by an EFRC.

Our development plan is to implement the PLS as a canted undulator beamline at 12-ID. We plan to
leverage the significant interests in the advanced manufacturing community and industry to explore the
external funding opportunities in partnership and close collaborations with NIST and the Department of
Defense (DoD) services laboratories. In FY18, we have refined the PLS conceptual design, particularly
the concept of the processing instrument, and pursue joint research projects with these groups using
existing NSLS-II beamlines to demonstrate benefit to the community. Our goal is to form a realistic approach to pursue funding of the PLS beamline in FY20. Recognizing the level of uncertainties in the timeline for funding, we are upgrading and installing an existing liquid-scattering instrument in a time-sharing mode with the SMI main beamline (see PPLS section on Page 15).

**Infrared Near-Field Nanospectroscopy (INF).** The infrared near-field nanospectroscopy (INF) will be a new infrared beamline for nanospectroscopy and vibrational spectroscopy of materials central to address current challenges in quantum materials and chemical catalysis. Apertureless near-field nanospectroscopy, based on synchrotron infrared light scattered from an atomic force microscope (AFM) tip, offers broadband spectroscopy of materials with better than 10 nm spatial resolution across the important range of wavelengths from 2µm to 100µm that probes many intrinsic electronic and vibrational excitations. Applications of this novel method will include a wide range of studies in such areas as phase transitions and intrinsic inhomogeneities in Mott insulators, metal to insulator transitions, high Tc superconductors, magnetic and multiferroic domains in complex oxides and heterostructures, elementary excitations in low dimensional and plasmonic materials, spectroscopic and chemical catalysis of nanoparticle catalysts, and phonon vibrations in oxide nanoparticles or organic thin films.

NSLS-II plans to develop the INF beamline on the 23-BM floor space, utilizing the 24-BM bending magnet as its IR source. The scope of the INF beamline consists of three endstation programs – near-field IR spectroscopy for condensed matter and materials physics, near-field IR spectroscopy of nanomaterials for catalysis, and IR reflection-absorption spectroscopy (IRRAS) of catalytic systems under ambient pressure in combination with the IOS branch in partnership with CFN, and will also provide conventional mid-IR micro-spectroscopy of materials with ~50% time share. These state-of-the-art instruments are well aligned with the new national initiatives in quantum information science and neuromorphic computing, and will place NSLS-II at the forefront of synchrotron IR nano-spectroscopy, extending conventional IR micro-spectroscopy far beyond the diffraction-limit. In FY20 we will continue to exploit the substantial funding interest in quantum information science and in neuromorphic devices by federal and state agencies to pursue potential construction funding for the INF beamline. Once funding is in place, the construction of INF will proceed as rapidly as possible, with the goal to complete the construction by FY22.

**Additional New Beamline Concepts.** During strategic planning brainstorming discussions in past two years among NSLS-II staff as well as with NSLS-II SAC and other stakeholders, it has become evident that a number of scientific capabilities gaps exist in the current suite of NSLS-II beamlines, even with the potential future addition of the new beamlines discussed above. These gaps limit the range of research that can be done at NSLS-II and may impede our ability to attract future new programs impacting national initiatives to NSLS-II. Such gaps include:

- Multidimensional Multimodal Diffraction
- Integrated In-situ and Resonant Hard X-ray Studies 2
- Multimodal High Pressure Tools
- Micro Computed Tomography
- In-situ and Operando Nanoprobe
- Cryo X-ray Nanoprobe
- Metrology and Test Beamline (possibly with MCT endstation)
- Catalysis and Growth Village (soft and tender X-rays)
• Additive Manufacturing Scattering Facility (hard X-rays)
• Soft X-ray STXM for Soft Materials
• Tender and Hard X-ray Resonant Inelastic Scattering Nanoprobe
• Massively Automated Crystallography
• High-flux Serial Crystallography
• Fixed Energy MX
• Long-wavelength Automated Crystallography.

Some of these new, as well as other new beamline concepts will be further developed in FY20, based on the community input at the upcoming NSLS-II Strategic Planning Workshop in October 2019. Our objective is to arrive at a strawman roadmap for the next ~10 new beamlines (including the three in the NEXT-II project) that will complement the capabilities of the existing 29 beamlines in our current portfolio. Together these beamlines will enable powerful new studies of a wide-range of materials and systems, in a way not possible before, from quantum information and microelectronics technology and catalysis and energy systems, to biological and environmental sciences.

Strategic Partnerships

In addition to new beamlines, we will leverage our facility strengths to develop new user communities that have not traditionally been associated with synchrotron light sources. We will work with these communities to broaden the usage of synchrotron techniques and increase the scientific as well as the societal impact of NSLS-II. A number of initiatives that are underway in this direction are described below.

**BNL Cryo-EM Facility:** Scientists have long used x-ray crystallography to determine the structure of proteins and deduce their internal workings. Recent advances in cryo-electron microscopy (cryo-EM) have opened up the possibility of resolving the structure of the large multi-protein complexes that perform vital functions within cells. In the future, scientists will combine both techniques in their studies. A complete picture of these complexes is needed to fully understand the vital processes they perform and forms the basis for the development of novel drugs or biotechnology.

To provide maximum impact, Brookhaven National Laboratory is in the process of establishing a cryo-EM facility located at a new building connected to NSLS-II. We have successfully secured $15M from New York State to fund the construction of this cryo-EM facility, including two cryo-microscopes (one low-resolution screening and one high-resolution microscope) and a satellite building (see figure at right) connected to LOB5 of NSLS-II to house these and future microscopes. The first screening microscope has already arrived and has been installed and commissioned as of September 2019. The high-resolution microscope will be scheduled for delivery in late 2019 or early 2020. The satellite building is under construction as of September 2019 and occupancy is expected in March 2020.
The new cryo-EM facility will be operated in close collaboration with the Structural Biology program of NSLS-II with cryo-EM-dedicated operating funding support from DOE-BER. Staff hires are in progress. User access to this facility will leverage the existing NSLS-II user administration and proposal system, based on the beamtime proposal management and review process already existing at NSLS-II.

**Nanoscience Partnership with CFN.** NSLS-II plans to continue the strong partnership with the BNL’s Center for Functional Nanomaterials (CFN) to pursue joint ventures to establish and maintain world-leading nanoscience capabilities in X-ray scattering, photoelectron microscopy, and operando spectroscopy. During the 2016–18 period, CFN and NSLS-II have completed critical build-outs of the four partner instruments, bringing them to full operations and building highly productive user populations. Development plans for the next five years are described below.

- **AP-XPS Station.** The CFN strategy for developing operando capabilities for catalysis and energy storage, leveraging the unique capabilities of NSLS-II, relies on performing photoelectron spectroscopy at pressures approaching one bar. An ambient pressure photoelectron spectroscopy (AP-XPS) endstation has been operating and supporting NSLS-II users at the IOS beamline. This partnership will continue in FY20-21.

- **AC-LEEM/XPEEM Upgrade.** The CFN state-of-the-art aberration-corrected AC-LEEM/XPEEM, with a spatial resolution better than 3 nm in LEEM and 8 nm in XPEEM mode at the ESM beamline has started GU operations in FY18. CFN plans to upgrade this instrument with: a state-of-the-art solid-state detector, which will replace the current multi-channel plate setup; and a closed-cell sample environment for operation at significantly increased gas pressures. The energy range at ESM (15-1500 eV) is ideal for nanoscale XPEEM in closed cells, thus providing world-leading capabilities for operando spectromicroscopy at high gas pressure and in liquids. We will also collaborate towards the tight integration of the two endstations at ESM, including the development of common sample preparation facilities and standardized sample transfer systems.

- **X-ray Scattering Upgrades.** CFN will continue to develop a world-class nanoscience X-ray scattering program at CMS and SMI beamlines. These instruments provide complementary capabilities for structural studies of complex nanomaterials. Over FY18 and FY19, CFN has developed and deployed automation hardware and software, including coding data pipelines for automated analysis, developing machine-learning methods for x-ray analysis, and through collaboration with NSLS-II and the DoE CAMERA project, developed and demonstrated autonomous experimentation methods for use at x-ray scattering endstations. Simultaneously, the CFN has deployed a one-of-a-kind x-ray detector with a through-hole to greatly broaden the q-space at SMI for simultaneous SAXS/MAXS/WAXS measurements of complete scattering arcs. These cutting-edge instruments enable advanced research in nanomaterials synthesis and functional characterization in catalysis, batteries, energy processing, light manipulation and sensing. The CFN remains committed to these x-ray scattering partnerships. In the coming years, CFN will continue to advance the data analytic and autonomous experimentation capabilities at the CMS and SMI beamlines. The CFN will also develop and deploy materials synthesis and processing platforms for use at the beamlines, allowing material formation and reordering to be studied in real time. These platforms will be connected to the autonomous methods being developed and made available to the general user program.

- **Complementary laboratory-based instruments** for screening and materials development. The CFN will acquire and/or upgrade its lab-based instruments for X-ray scattering, LEEM, ambient-pressure XPS, and IR spectroscopy to complement the synchrotron-based partner instruments at NSLS-II. These facilities will allow users to screen samples and experimental conditions prior to scheduled NSLS-II beamtime, maximizing productivity of synchrotron-based instruments.
**Industrial Research.** Industrial research is an essential and integral part of the research program portfolio at NSLS-II. Establishing a vibrant industry research program is a key component of the NSLS-II mission. This program promotes interactions and partnership along the discovery to deployment research pipeline, and provides immediate connection and relevance to the general public. Based on discussions at the focused workshops on industrial research at NSLS-II, we have identified three key areas to pursue in order to strengthen industrial research: enhanced support for industry users, flexible and timely access to beam time, and common protocols among National Laboratory facilities. To promote the industrial research partnership and add to industry perspectives, representative scientists from industry have been included in the NSLS-II proposal review panels and on the NSLS-II science advisory committee. Proprietary research policy and procedure has been established to guide proprietary research. In addition, proprietary users can submit proposals at any time during a given cycle through rapid access to take advantage of the dedicated fraction of beam time for rapid access proposals on select NSLS-II beamlines. Initial industrial usage started in FY17 at a number of NSLS-II beamlines. Since then industry usage of NSLS-II has been increasing steadily, with increasing industry user demands on NSLS-II beamlines.

In FY20-24, we plan to continue the development of a strong industrial research program along several directions, including pharmaceuticals, microelectronics, and petrochemicals. Our development plan in the next five years includes the following elements:

- Continue developing scientific capabilities tailored to industrial applications, e.g. *in-situ* and *operando* capabilities with automated specimen handling in industry-relevant conditions,
- Promoting close partnerships with industry partners, e.g. collaborations with beamline staff, participating in beamline programs through partner users, and pursuing SBIR/STTR funding,
- Developing and implementing flexible and timely access modes to accommodate industry needs within the framework of the *NSLS-II User Access Policy*,
- Enhancing staff support to industrial users by allowing matrixed staff at beamlines to work with industry users with a goal to provide not only data but also solutions,
- Implementing the Technical Service Agreement (TSA) mechanism to allow NSLS-II staff to allocate small fraction of their efforts to conduct proprietary or non-proprietary research projects at NSLS-II under a TSA contract with a company,
- Enhancing directorate-wide communications and outreach to the industrial community via a dedicated industry webpage, targeted workshops, training, and conferences and meetings of interest to various types of industrial users, as well as reaching out to other industrial liaison offices of universities and organizations,
- Tracking industrial research by user statistics, publications, funding sources, and corporate impact statement to better understand industry users’ needs and identify the impact of NSLS-II,
- Coordinating within DOE complex on common protocols for industry access to user facilities,
- Organizing dedicated industry research workshops, coordinated among other BES light source facilities, to highlight the impact of industry research at BES facilities and improve user experience for industry users.

**Materials in Radiation Environments.** Nuclear materials, including nuclear fuels and structural materials for nuclear containment systems, are of critical importance for the next-generation nuclear reactors and the nation’s overall energy production landscape. These materials and material systems are traditionally difficult to study experimentally, largely due to the extreme complexity of the interplay between radioactivity and radiochemistry at multiple length scales – from atomic to millimeter scales. Furthermore, it is very challenging to characterize these systems in-situ, beyond what can be done today typically using electron microscopy which is often destructive, in order to obtain accurate information about naturally occurring radiochemistry and structural degradations that may happen in real nuclear
systems. NSLS-II plans to work with the nuclear energy community and DOE Nuclear Energy and BES to address these critical challenges in the nuclear materials and systems. In collaboration with the BNL Nuclear Science and Technology (NST) department and in partnership with Idaho National Laboratory (INL), NSLS-II proposes developing a dedicated Materials in Radiation Environments (MRE) beamline based on a superconducting wiggler to enable in-situ multiscale imaging of radiochemistry and radiation-induced structural changes and degradation in a wide range of nuclear fuel and structural materials.

This unique facility would house three hard X-ray instruments – X-ray diffraction and diffraction tomography, X-ray spectromicroscopy, and full-field X-ray imaging in an external building of ~17,000 sq. ft. The external building will allow a self-contained secure environment to enable research on hot nuclear materials – from segments of actual fuel pellet to highly radioactive materials due to irradiation. In addition, the facility will house an ion accelerator to enable studies of these and other materials while they are being irradiated by ion radiation. In FY20-21, we will implement and operate the NST partnership-supported XRD tomography set-up at the XPD beamline, and to develop and implement software tools for 3D reconstruction and analysis. We will plan to develop a refined schedule in support of the potential decision on MRE funding CD-0 from DOE-NE. If CD-0 is granted, we will then work closely with NST staff and their collaborators at INL to develop a conceptual design for MRE and ramp up project activities if funding becomes available.

**Additive Manufacturing.** The BNL additive manufacturing (AM) strategy is currently focused on polymeric materials and metals. In FY19, the two AM working groups identified ways to better coordinate cross-disciplinary efforts that leverage local expertise and facilities as well as engaged partners from universities, government labs, and industry. As part of the networking effort, in FY19 BNL joined the America Makes partnership, managed and operated by the National Center for Defense Manufacturing and Machining (NCDMM). Several case studies were completed to demonstrate the value of in-situ synchrotron characterization for advancing additive manufacturing processes and teams are being identified to apply for external funding. Almost every funding agency (DOE, DOD, DOC, NSF, NASA) has funding programs in AM. Moreover, in FY20, the DOE is sponsoring a workshop on Basic Research Needs in Transformative Manufacturing, which will likely result in a funding call.

Members of the AM working groups engage in research focused on measuring, modeling, and controlling the spatial and temporal heterogeneities that are inherent in AM processes, with the intent of elucidating mechanisms and thereby provide better control and monitoring of AM processes to enhance the performance of printed components. Understanding out-of-equilibrium processes can be exploited to create materials with novel internal structures, inaccessible by conventional fabrication pathways. These enhancements will allow BNL researchers to surpass various technological hurdles that currently limit the success of AM in replacing conventionally manufactured parts and devices. Equally important is the development of accurate process models for structure-property-processing relations, which are a pre-requisite for part qualification in critical applications.

Research will leverage state-of-the-art synchrotron techniques at the NSLS-II, nanoscale analytical tools at the Center for Functional Nanomaterials (CFN) and engage the Computational Science Initiative at BNL for data visualization, material simulations, and Artificial Intelligence approaches.

**Polymeric materials AM.** This working group focuses on in-situ x-ray characterization during processing and operando x-ray characterization of a wide range of polymeric materials: amorphous and crystalline, thermoset and thermoplastic, nanocomposites (nanoparticles and fibers), elastomers, organo-gels, and hydrogels. In FY19, a compact on-line 3D printer was put into operation on the CHX and SMI beamlines. The instrument was described in a special issue of Synchrotron Radiation News that highlighted...
synchrotron research in additive manufacturing (Synch. Rad. News 32, 20 (2019)). The on-line 3D printer was used by staff and collaborative user groups including Henkel Corporation, AFRL, Stony Brook, Harvard, and Kent State Universities for projects respectively on adhesives, high-strength nanocomposites, batteries, soft robotics, and cell scaffolds. In FY20, with user community input obtained at a 2019 CFN/NSLS-II Users’ Meeting workshop on “Opportunities for synchrotron studies in advanced manufacturing research”, a second-generation on-line 3D printing platform will be constructed that can accommodate an order of magnitude heavier printheads and achieve an order of magnitude higher print rates. This new printing platform is compatible with the CHX and CMS beamlines as well as the new PPLS instrument on the SMI beamline. Through a coordinated inter-facility effort, a similar on-line 3D printing platform is being developed for the MSN-C Functional Materials beamline at the CHESS synchrotron.

Looking to the future, in FY20, a concept design paper for a beamline for studying Advanced Manufacturing Processes (AMP) will be developed. This beamline will provide state-of-the-art coherent/incoherent SAXS/WAXS capabilities with microbeam in combination with a unique endstation optimized for large equipment (industrial-scale) and capable of in-situ/operando studies. In-house and user case studies have demonstrated the power of coherent/incoherent scattering techniques for understanding the out-of-equilibrium processes during polymer processing at beamlines CMS, CHX and SMI. However, the equipment required for industry relevant studies, including Big Area Additive Manufacturing (BAAM) as pursued at the ORNL Manufacturing Demonstration Facility, is out sizing sample space available at existing beamlines. The proposed beamline concept will also include capabilities for efficient use of large-scale growth chambers, e.g. for in-situ studies of the growth of quantum materials, which are also too large for existing beamlines. The combination of coherent and incoherent scattering techniques with cubic meter size equipment would be unique in the world.

Metals AM. The metal Additive Manufacturing strategy develops along two parallel thrusts for structural and functional components. The thrusts have been aligned to the ongoing effort and needs of the metal AM community; these clearly emerged also from the Industrial Additive Manufacturing Workshop on Metals and Ceramics held at BNL on April 25, 2019, and in which the capabilities of NSLS II had a primary role. The timing for the workshop was ideal because of growing interest from the metals AM communities from both academia and industries. The metals community is enthusiastic and sees the NSLS-II HEX beamline will be an ideal platform for characterizing printed metal components and their response to tensor stress forces.

The structural component applies synergistically material analysis and artificial intelligence to achieve failure prediction evaluations of 3D printed parts and obtain an improved overview of the effects of the laser-based printing process. This is done in collaboration with BNL’s CSI. During FY19, proof-of-principle experiments at 28-ID-1 (PDF) beamline, in collaboration with external partners, have established capabilities and helped us better understand issues and phases formation in Nickel superalloys. In addition, we have begun a strategic integration with the programs and capabilities of other synchrotron facilities, through a collaboration with APS Sector 11; in FY20, the goal is to extend our integration effort with the new capabilities at CHESS. Along this line, the latest developments in planning an AM sample environment at the high-energy beamline HEX (27-ID, under construction) benefit from an ongoing discussion with several potential users including NIST, which has shown some interest in collaborating on the design and integration of in-situ monitoring equipment dedicated to 3D printing, including controls for sample stage / laser motion coordination and in-situ thermography. While it is clear that High Energy XRD has a distinctive role in the development of AM technologies, other 3D characterization techniques need to be taken into consideration, for example, the demand for high-frequency XRD and large field of view X-ray imaging both of which are used to elucidate time-
dependent evolutions within and around the melting pool and which lead to specific phases forming. Equally important is the use of High Energy SAXS to enhance our understanding of the annealing process.

The Functional Component of our strategy focuses on performance characterization of high-precision 3D printing solutions and new materials. In FY19, an interdepartmental collaboration between Sustainable Energy Technologies Department, NSLS II and Physics, along with Obsidian AM, LLC, has been awarded an High Energy Physics DOE STTR Phase I project which is applying a novel plasma-based AM technology to print metallic filter circuits, operating in the GHz bandwidth, with bulk-like metallic electric behavior of the printed conductors for application in bolometric detectors. The project builds on the NSLS II expertise in microwave technology and IR spectroscopy; it will rely on the 22-IR-2 (MET) beamline for infrared & THz spectroscopy. Ancillary laboratory instruments will also be used, to characterize transmission, reflection and absorption of the 3D printed materials in a wide frequency band, ranging from the infrared to the GHz range. During FY20, effort will be directed to align the high-precision printing applications with the BNL’s Quantum Information Science (QIS) Initiative and the needs of the Department of Defense (DOD). Given the potential to run the plasma-based 3D printing process with multiple materials, independently or at the same time, discussion has started with the industrial partner to contemplate a future test setup for in-situ analysis and enhancement of the printing process at NSLS II; this step may support the investigation of multiple materials deposition, possibly leading to study new materials and alloys for high-precision and special applications.

**Partnerships in quantum information technologies and next generation microelectronics.** Given the substantial interests in the scientific community on quantum information science and beyond-Moore computing, NSLS-II will work within BNL and with the broader community to join forces to pursue research and development in these two areas. Leveraging our advanced materials studies capabilities and expertise, we plan to apply a number of synchrotron techniques in structural and chemical characterization of the materials systems of interest, such as quantum qubit and cavity materials, 3D nanofabricated microelectronics such as 3D monolithic integration devices, and novel quantum materials for neuromorphic AI applications such as memristor devices based on the unique properties of transition metal oxides.

Considerable work already started in FY19. In quantum information science, a working group has been formed among NSLS-II and CFN scientists to study a variety of materials systems for the purpose of improving the performance QIS devices including qubits, cavities, quantum transducers, emitters, repeaters and quantum sensors, as driven both by new device designs and materials research. Research on novel materials is also key to developing next-generation QIS devices. This work is based on a collaboration among regional research institutions – BNL, IBM, MIT, Princeton, Yale, and SBU. This collaboration will continue in FY20, with a goal to identify a number of key research themes that will help form the basis for a funding proposal to DOE in the area of quantum information science.

In microelectronics, there are also ongoing research using the cutting-edge nano-imaging capabilities at NSLS-II. This includes 3D nano-CT imaging at the FXI beamline of microchips to identify defects and potentially harmful nano-features, and the nano-XRD strain mapping on nanosheet transistors by IBM at the HXN beamline. In FY20, we plan to form a new collaborative research team involving IBM, SUNY Polytech Institute in Albany, and SBU, to identify additional areas of research that will take our cutting-edge nano-imaging capabilities in novel microelectronic devices, including devices that are more energy efficient for neuromorphic computing and AI applications. Such collaboration may also include additional partners as research progresses in the coming year.
Summary and Outlook
Summary and Outlook

NSLS-II has progressed rapidly in the past four years since its first beamline started its general user operations. These four years have been truly exciting, with now 28 beamlines in operations and user science programs rapidly ramping-up. Looking ahead, the next five years will be again be exciting times for NSLS-II and for our community as we continue to ramp up our accelerator and beamline capabilities and develop and mature our science programs. The innovative research conducted at NSLS-II will have high scientific and technological impacts not only in the fields of quantum condense matter, complex materials and processes, catalysis and materials sciences, and structural biology, but also in the emerging science initiatives on quantum information technology, next-generation microelectronics, artificial intelligence, advanced manufacturing, and multiscale integrative materials and bio-systems.

As the first low-emittance storage-ring in full user operations, NSLS-II will continue to play a key leadership role in the synchrotron community in advancing high-brightness synchrotron technology and associated R&D, in pioneering high-brightness science to address challenging problems in the society, and in cultivating and developing the evolving scientific community to maximize the scientific impact of high-brightness synchrotrons. In this regard, we plan to continue to develop new beamlines and new instruments, and to secure new funding to develop additional new beamlines at NSLS-II to provide the needed new capabilities for the society.

This 2020 NSLS-II Strategic Plan outlines our vision, strategy, and approach, our science program areas and crosscutting support programs, our development plans and initiatives to meet the science needs and enhance the impact of NSLS-II.

To summarize, our strategic goals for the next five years are:

- Maintain reliable accelerator operations and deliver mature performance of the storage ring;
- Effectively operate the 29 beamlines for general users, including seamless access to data and compute resources during and post experiments, and near real-time analysis on all beamlines;
- Upgrade select beamline capabilities to meet the evolving science needs, including a 5-nm focused beam size for hard X-rays, and optimized suite of detectors;
- Complete construction of the three beamlines in the NEXT-II project, and develop additional new beamlines as part of the strategic vision to reach 40 beamlines by year 2030;
- Pursue enabling technologies R&D including instrumentation needed to deliver 5 nm focus to user experiments, AI-based data science and machine learning, and strategic partnerships.

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

<table>
<thead>
<tr>
<th>Acronym</th>
<th>Description</th>
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<tbody>
<tr>
<td>3PW</td>
<td>Three-Pole Wiggler</td>
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<tr>
<td>AC-LEEM</td>
<td>Aberration Corrected Low Energy Electrons Microscope</td>
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<tr>
<td>ADR</td>
<td>Accelerator &amp; Detector Research</td>
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<tr>
<td>AFM</td>
<td>Atomic Force Microscope</td>
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<tr>
<td>AFRL</td>
<td>Air Force Research Laboratory</td>
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<td>ALS</td>
<td>Advanced Light Source</td>
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<td>AM</td>
<td>Additive Manufacturing</td>
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<tr>
<td>ANL</td>
<td>Argonne National Laboratory</td>
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<tr>
<td>AP-PES</td>
<td>Ambient Pressure Photo-Electron Spectroscopy</td>
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<tr>
<td>APS</td>
<td>Advanced Photon Source</td>
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<tr>
<td>AP-XPS</td>
<td>Ambient Pressure X-ray Photo-emission Spectroscopy</td>
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<tr>
<td>ARL</td>
<td>Army Research Lab</td>
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<tr>
<td>ARPES</td>
<td>Angle-Resolved Photo-Electron Spectroscopy</td>
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<td>ASCR</td>
<td>Advanced Scientific Computing Research</td>
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<tr>
<td>ASIC</td>
<td>Application-Specific Integrated Circuit</td>
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<td>ASU</td>
<td>Arizona State University</td>
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<tr>
<td>BAT</td>
<td>Beamline Access Team</td>
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<tr>
<td>BCDI</td>
<td>Bragg Coherent Diffraction Imaging</td>
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<td>BDP</td>
<td>Beamline Development Proposal</td>
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<tr>
<td>BER</td>
<td>Biological and Environmental Research</td>
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<td>BES</td>
<td>Basic Energy Science</td>
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<td>BL</td>
<td>Beamline</td>
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<td>BM</td>
<td>Bending Magnet</td>
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<tr>
<td>BNL</td>
<td>Brookhaven National Laboratory</td>
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<tr>
<td>CAMERA</td>
<td>Center for Advanced Mathematics for Energy Research Applications</td>
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<tr>
<td>CBMS</td>
<td>Center for Biomolecular Structure</td>
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<tr>
<td>CD-1</td>
<td>Critical Decision 1</td>
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<tr>
<td>CDI</td>
<td>Coherent Diffractive Imaging</td>
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<td>CFN</td>
<td>Center for Functional Nanomaterials</td>
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<td>CLS</td>
<td>Canadian Light Source</td>
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<tr>
<td>CMOS</td>
<td>Complementary Metal–Oxide–Semiconductor</td>
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<tr>
<td>CMPMS</td>
<td>Condensed Matter Physics and Materials Science</td>
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<tr>
<td>COMPRES</td>
<td>Consortium for Materials Properties Research in Earth Sciences</td>
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<tr>
<td>Cryo-EM</td>
<td>Cryogenic Electron Microscopy</td>
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<tr>
<td>CSI</td>
<td>Computational Science Initiative</td>
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<tr>
<td>CWRU</td>
<td>Case Western Reserve University</td>
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<tr>
<td>DAMA</td>
<td>Data Acquisition, Management, and Analysis</td>
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<tr>
<td>DAQ</td>
<td>Data Acquisition</td>
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<tr>
<td>DBA</td>
<td>Double Bend Achromat</td>
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<td>DESY</td>
<td>Deutsches Elektronen-Synchrotron</td>
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<tr>
<td>DFT</td>
<td>Density Functional Theory</td>
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<tr>
<td>DoC</td>
<td>Department of Commerce</td>
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<td>DoD</td>
<td>Department of Defense</td>
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<td>DOE</td>
<td>Department of Energy</td>
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<tr>
<td>ECA</td>
<td>Early Career Application</td>
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<tr>
<td>ECBC</td>
<td>Edgewood Chemical and Biological Center</td>
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<td>EMSL</td>
<td>Environmental Molecular Science Laboratory</td>
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<tr>
<td>EPICS</td>
<td>Experimental Physics and Industrial Control System</td>
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<td>EPU</td>
<td>Elliptical Polarized Undulator</td>
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<tr>
<td>ESS&amp;H</td>
<td>Environment, Safety, Security &amp; Health</td>
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<tr>
<td>FHE</td>
<td>Flex-Hybrid Electronics</td>
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<td>FIP</td>
<td>Facility Improvement Project</td>
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<td>FNAL</td>
<td>Fermi National Accelerator Laboratory</td>
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<td>FY</td>
<td>Fiscal Year</td>
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<tr>
<td>GHS</td>
<td>Gas Handling System</td>
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<tr>
<td>GPGPU</td>
<td>General-Purpose computing on Graphics Processing Units</td>
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<tr>
<td>GU</td>
<td>General User</td>
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<tr>
<td>GUI</td>
<td>Graphical User Interface</td>
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<tr>
<td>GUV</td>
<td>Guests, Users, Visitors center</td>
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<tr>
<td>HEP</td>
<td>High Energy Physics</td>
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<td>HFIR</td>
<td>High Flux Isotope Reactor</td>
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<td>HOM</td>
<td>High Order Mode</td>
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<tr>
<td>HPC</td>
<td>High Performance Computing</td>
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<td>HVE</td>
<td>High Viscosity Extrusion</td>
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<tr>
<td>I&amp;D</td>
<td>Inclusion and Diversity</td>
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<tr>
<td>ID</td>
<td>Insertion Device</td>
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<tr>
<td>Abbreviation</td>
<td>Full Form</td>
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<td>IGPP</td>
<td>Institutional General Plant Projects</td>
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<td>INL</td>
<td>Idaho National Laboratory</td>
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<tr>
<td>IO-XAS</td>
<td>In-Operando X-ray Absorption Spectroscopy</td>
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<tr>
<td>IR</td>
<td>Infrared</td>
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<tr>
<td>IRRAS</td>
<td>Infrared Reflection-Absorption Spectroscopy</td>
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<td>IT</td>
<td>Information Technology</td>
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<td>Information Technology Division</td>
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<td>JGI</td>
<td>Joint Genomics Institute</td>
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<td>KB</td>
<td>Kirkpatrick Baez</td>
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<td>LBNL</td>
<td>Lawrence Berkeley National Laboratory</td>
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<td>LCLS</td>
<td>Linac Coherent Light Source</td>
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<tr>
<td>LDRD</td>
<td>Laboratory Directed Research and Development</td>
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<tr>
<td>LEEM</td>
<td>Low Energy Electron Microscope</td>
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<tr>
<td>LOB</td>
<td>Laboratory Office Building</td>
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<tr>
<td>MAXS</td>
<td>Medium Angle X-ray Scattering</td>
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<td>MBA</td>
<td>Multi-Bend Achromat</td>
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<td>MBE</td>
<td>Molecular Beam Epitaxy</td>
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<td>MCT</td>
<td>Micro Computed Tomography</td>
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<tr>
<td>MEMS</td>
<td>Micro-Electro-Mechanical System</td>
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<td>MIT</td>
<td>Massachusetts Institute of Technology</td>
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<td>MLL</td>
<td>Multilayer Laue Lens</td>
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<td>MOF</td>
<td>Metal Organic Framework</td>
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<td>MRE</td>
<td>Materials in Radiation Environment</td>
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<td>MRI</td>
<td>Magnetic Resonance Imaging</td>
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<td>MX</td>
<td>Macromolecular Crystallography</td>
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<tr>
<td>NASA</td>
<td>National Aeronautics and Space Administration</td>
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<td>NE</td>
<td>Nuclear Energy</td>
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<td>NIH</td>
<td>National Institute of Health</td>
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<td>National Institute of Standard and Technology</td>
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<td>Naval Research Laboratory</td>
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<td>NSF</td>
<td>National Science Foundation</td>
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<td>NSLS-II</td>
<td>National Synchrotron Light Source II</td>
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<td>NST</td>
<td>Nuclear Science and Technology</td>
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<td>NYSERDA</td>
<td>New York State Energy Research &amp; Development Authority</td>
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<tr>
<td>PASS</td>
<td>Proposal Administration, Safety, and Scheduling</td>
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<tr>
<td>PNNL</td>
<td>Pacific Northwest National Laboratory</td>
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<td>PPLS</td>
<td>Polymer Processing and Liquid Scattering</td>
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<td>QA</td>
<td>Quality Assurance</td>
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<tr>
<td>R&amp;D</td>
<td>Research and Development</td>
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<tr>
<td>R2A2</td>
<td>Roles, Responsibilities, Authorities, and Accountability</td>
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<tr>
<td>RF</td>
<td>Radio Frequency</td>
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<tr>
<td>RIXS</td>
<td>Resonant Inelastic X-ray Scattering</td>
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<td>SAC</td>
<td>Science Advisory Committee</td>
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<td>Small Angle X-ray Scattering</td>
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<td>SBIR</td>
<td>Small Business Innovation Research</td>
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<td>SBU</td>
<td>Stony Brook University</td>
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<td>SNS</td>
<td>Spallation Neutron Source</td>
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<td>Synchrotron Radiation Workshop</td>
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<td>SSR</td>
<td>Scientific Staff Review</td>
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<td>SSRL</td>
<td>Stanford Synchrotron Radiation Lightsource</td>
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<td>STTR</td>
<td>Small Business Technology Transfer</td>
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<tr>
<td>STXM</td>
<td>Scanning Transmission X-ray Microscope</td>
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<td>TEC</td>
<td>Total Estimate Completion</td>
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<td>TEM</td>
<td>Transmission Electron Microscopy</td>
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<tr>
<td>TXM</td>
<td>Transmission X-ray Microscope</td>
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<td>UEC</td>
<td>User Executive Committee</td>
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<td>USCEO</td>
<td>User Services, Communication, Education &amp; Outreach</td>
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<tr>
<td>VIPIC</td>
<td>Vertically Integrated Photon Imaging Chip</td>
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<tr>
<td>WAXS</td>
<td>Wide Angle X-ray Scattering</td>
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<tr>
<td>XAS</td>
<td>X-ray Absorption Spectroscopy</td>
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<td>X-ray Emission Spectroscopy</td>
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<td>X-ray free-electron laser</td>
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