September 2020

X-ray Science Division Strategic Plan

The X-ray Science Division (XSD) at the Advanced Photon Source (APS) develops cutting-edge instrumentation and techniques to enable and perform world-class research using X-rays. This strategic plan lays out objectives to address the challenges XSD faces to achieve this mission, and provides a framework for how the Division will support our staff, beamlines, and users.

Guiding Principles

To enable great science, XSD requires both state-of-the-art facilities and highly-skilled staff. The continued evolution of our beamline portfolio; the hiring, development, and retention of talented scientists, engineers and technical professionals; and the expansion of the depth and breadth of our user community are essential in keeping the APS at the forefront of scientific research.

Vision

To fulfill our mission, XSD will:

- Develop world-class X-ray capabilities that address problems relevant to current and future scientific needs.
- Attract premier researchers as users of XSD beamlines from a wide range of scientific disciplines by providing top-of-the-line instrumentation, sample environments, supporting laboratories, data analysis methods and outstanding user support.
- Maintain a safe, vibrant, challenging, diverse and inclusive work environment that fosters excellence and innovation, such that the APS continues to be the top choice for scientists, engineers, and technical staff pursuing careers at synchrotron light sources.

Strategy

To achieve the XSD vision, we must concentrate on the following components:

- *Invest in our people*: The XSD staff is key in providing the scientific vision for the future as well as the technical and scientific leadership for the facility. We must attract, retain and invest in our staff, the scientists, engineers and technical support personnel to secure the next generation of leaders and innovators at the APS. We must provide clear career advancement paths, R&D resources, and opportunities for professional growth.
- *Invest in beamlines*: As the APS upgrade nears, the APS beamline portfolio must shift to take advantage of the new and unique source characteristics that will become available. XSD will continue to operate and develop the most innovative, relevant, and effective beamlines that serve the needs of the US scientific community.
- *Invest in R&D*: Continued advancement of methods development and technical support is critical to maintain the APS as a world-leading research facility. The development and evaluation of wavefront preserving optics, engineering of high

stability beamline components, robust nano-positioning instrumentation, advanced beamline controls, *in-situ* / *operando* sample environments, and new detectors are needed to make full use of current and future capabilities. Further, rapid advances in detector technologies are producing ever larger data sets that require new paradigms for data transfer, storage, reduction, and interpretation, not only for effective use of the capabilities of the APS today but even more so after the upgrade. All of these are critical science-enabling technologies that facilitate discovery.

- *Invest in our user community*: The success of the APS is ultimately measured by the impact of the science produced by our users. We therefore must prioritize and allocate resources to ensure the highest level of user support, and invest time in workshops and schools to train the user community in the best strategies for acquiring and analyzing their data. Further, we need to expand outreach efforts in order to attract known and new scientific communities, with particular emphasis on areas that will benefit greatly from the APS upgrade.

Priorities

XSD will focus its resources on four key priority areas:

1. **Brightness and coherence driven beamlines and techniques**

The APS source after the upgrade will provide world-leading beam coherence and high brightness. These beam characteristics greatly enhance experiments in the areas of imaging, microscopy, ptychography, coherent diffraction, and XPCS. The upgraded APS will enable completely new experiments not feasible today. To work towards the upgraded APS, we will give the highest priority to beamline improvements, beamline staffing and beamline technical support that enhance these areas, and work today to establish new methods and techniques that can take full advantage of the upgraded APS source in the future.

2. High-energy beamlines and techniques

The APS is unique amongst the present DOE light sources in providing highly brilliant X-ray beams at high energies (>20 keV). XSD staff have exploited this feature to provide a number of world-leading capabilities in Materials Science, Chemistry, Extreme Conditions, etc. After the upgrade, the APS will have significantly enhanced flux densities at high energies, as well as greatly increased degrees of coherence. Utilizing these unique features will require continued development of novel high-energy techniques and instrumentation.

3. Timing and high-speed imaging capabilities

The current APS bunch pattern, with a routine operating mode employing a large inter-bunch separation, is unique among third-generation synchrotron sources. This has led to the development of a number of novel ultra-fast x-ray imaging, scattering, and spectroscopy capabilities at the APS. The upgrade will support a 48-bunch pattern with a similar large inter-bunch separation. To retain the existing and unique strengths in high-speed measurements at the APS, we will continue to invest in this area, particularly where coupled to new approaches that leverage brightness, coherence and/or high energies.

4. Beamline operations and development

The APS serves a large number of users across diverse fields, who benefit greatly from excellent beamline capabilities and outstanding staff expertise. The increasing complexity of these experiments requires a workforce from a variety of disciplines and backgrounds to develop instrumentation adapted to the experimental needs. We will continue to optimize and invest in valuable, sought-after programs and facilities, including but not limited to high-throughput approaches, complex sample environments, multi-modal characterization, and analysis tools. These core capabilities underpin many of the materials and chemistry initiatives at Argonne and within the wider APS user base.

Implementation

The APS X-ray Science Division develops novel X-ray instrumentation and techniques, and is responsible for the operation of APS-supported beamlines. XSD will need to maintain the productivity of these beamlines while simultaneously transitioning to a portfolio of beamlines and instruments that will more fully exploit the unique characteristics of the upgraded APS. Accomplishing this transition will require directing investments towards beamlines and technologies aligned with APS-U. Where possible we will seek to leverage these efforts through collaborations with Collaborative Access Teams, Argonne Divisions, and other light sources both within and beyond the DOE complex. One goal will be to establish entirely capabilities enabled by the upgrade and empower them to be ready to solve grand scientific challenges of the future. Another goal will be to strengthen successful programs that are in high-demand for the science in the US, and adapt them permanently to the challenges and the new opportunities provided by the upgrade.

Goals and Action Plan for FY2021

- *Maintain active and productive user programs on XSD operated beamlines by implementing remote access and automation at the beamlines in response to the current pandemic, including sample environments that can be operated remotely. Continue the development of novel innovative instrumentation that further advances the beamline capabilities.*
- *Develop the full final designs for the APS-U feature beamlines and enhancements with particular emphasis placed on completing the end-station instruments.*
- *Work with APS-U staff on completing construction and commissioning of the 25-ID ASL and 28-ID IDEA beamlines, and start preparation for construction of 4-ID POLAR beamline. After 25-ID commissioning, transfer spectroscopy programs from 20-ID, and start consolidation of time-resolved spectroscopy programs from 11-ID-D and 7-ID onto this beamline. Decommission 4-ID-C and transition some capabilities to 29-ID.*
- *Complete upgrade of 2-ID to enable fully independent operation of the D and E stations in order to enhance nano-scale scanning-probe capabilities essential for APS-U*

- *Enhance APS metrology facilities to provide the capabilities for characterizing APS-U optics by upgrading the long-trace profiler and replacing the Fizeau interferometer.*
- *Implement scientific computing strategies that leverage on-demand high-performance computing resources at the APS and Argonne in the context of APS and APS-U. Collaborate with the other DOE light sources to develop unified approaches for efficient and transparent data workflow, processing, analysis and management across the complex. Develop novel machine learning and artificial intelligence methods to transparently reduce, analyze, and visualize data close to the source, and to take full advantage of 'big data' opportunities that increased detector speeds and source brightness will provide.*
- *Continue to refine strategy for beamline optics, detectors, instrumentation, controls, and computing, keeping it aligned with current and future APS priorities, while developing approaches for beamline and instrument design that incorporates all aspects of X-ray technologies. Expand deployment of Bluesky control software on beamlines.*
- *Continue to strengthen collaboration with Argonne's programmatic divisions in the development of novel x-ray methods and complex in-situ/operando sample environments (MSD, CSE), specialized supporting laboratories (NE), nanofabrication of x-ray optics and instrument development (CNM), and development of new data pipelines, analysis methods, and machine learning approaches (DSL, MCS, CPS).*
- *Develop long-term plan for increased support of biological and environmental research at the APS, including a transition plan for BER supported activities at SBC.*
- *Address on-going obsolescence issues at the beamlines through a coordinated multi-year plan to replace key components.*
- *APS management, XSD management, XSD group leaders and senior scientific and technical staff will together continue to develop a long-term vision for the XSD beamline portfolio with input from the APS user community, consistent with the roadmap for the APS-U beamlines.*