ADVANCED LIGHT SOURCE

Five-Year Strategic Plan

FY2020

BERKELEY LAB

U.S. DEPARTMENT OF ENERGY | Office of Science

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1 Introduction

The Advanced Light Source (ALS) is an electron storage ring–based synchrotron radiation facility that is supported by the Department of Energy's Basic Energy Sciences program (DOE-BES). The ALS started operation in 1993 and since then has been upgraded continuously to remain one of the brightest soft x-ray sources in the world. The ALS is optimized for x-ray spectroscopy, microscopy, and scattering using intense beams from soft x-ray undulator sources but also serves a broader community conducting research using hard x-rays, infrared (IR), and vacuum ultraviolet (VUV) radiation from superconducting magnets, conventional dipole magnets, and insertion devices. The 1.9 GeV ring hosts world-class endstations and instrumentation at more than 40 beamlines and serves over 2000 users who publish more than 900 publications per year and conduct basic, applied, and industrial research in energy science, earth and environmental science, materials science, biology, chemistry, and physics. Our mission is to support users in doing outstanding science in a safe environment. Growing, maintaining, and supporting a vibrant and diverse user community is critical for the ALS's success as a user facility. To engage the community, ALS scientists reach out through many channels, via attendance at conferences, the organization of workshops, and participation on boards and review committees.

The ALS is the primary BES-funded soft x-ray facility in the U.S. and our ambition is to provide the U.S. and the international community with world-leading x-ray capabilities that enable consequential scientific discoveries and lead to a detailed understanding of laws governing natural processes and the properties of engineered systems. ALS long-term scientific planning is guided by BES Advisory Committee (BESAC) reports on Grand Challenges (2007) and Transformational Opportunities (2015), and investment in new programs is informed by BES reports, for example on quantum materials, electrical storage, and catalysis science, among many others. The ALS participates in Lawrence Berkeley National Laboratory (LBNL) initiatives, for example "Beyond Moore's Law" and the "Water-Energy Nexus," and we work closely together with other US user facilities and the LBNL Energy Sciences Area to identify new opportunities in x-ray science. The ALS Upgrade Project (ALS-U) is our largest upgrade project since the ALS started operation and will upgrade the ALS to near-diffraction-limited performance in the soft to tender x-ray range, resulting in an increase in brightness and coherent flux of at least two orders of magnitude. Methods based on nanofocusing, diffractive imaging, and coherent scattering will benefit tremendously from the improved performance of the storage ring, and this strategic plan identifies multiple areas where investments into beamline and endstation infrastructure will create opportunities for new scientific discoveries. The ALS-U Project is well underway and reached the Critical Decision-1 (CD-1) milestone in 2018. As part of the strategic planning process, the ALS has identified five Thrust Areas (TAs) centered around cross-cutting themes. These themes guide our long-term strategic planning, as discussed in chapter 2. The chapter also discusses ALS strategic priorities in the areas of accelerator development; the user program; safety; and inclusion, diversity, equity, and accountability (IDEA). A comprehensive list of current accelerator, beamline, detector, optical metrology, and computing projects can be found in chapter 3. New beamline and endstation initiatives are discussed in chapter 4.

2 Strategic priorities

2.1 Thrust areas

Five TAs have been identified that encompass critical growth areas in x-ray science and instrumentation. The TAs are organized around cross-cutting themes and include scientists from the ALS and collaborating LBNL divisions. Members of the TAs collaboratively develop the science and instrumentation strategy for their area and reach out to the user community to launch initiatives that result in new beamline projects.

2.1.1 Quantum Materials Research and Discovery

The discovery, synthesis, and characterization of novel functional quantum materials is the central theme of this TA. Soft x-ray spectroscopy, scattering, and microscopy tools have played a major role in the discovery and understanding of the exotic and fascinating physics of many new classes of spin, quantum, and topological materials over the past few decades: oxide and pnictide superconductors, manganites exhibiting colossal magnetoresistance, graphene and other 2D materials, topological insulators and semimetals, and multiferroics, to name just a few examples. After a spectacular century-long endeavor to understand quantum materials, starting with the discovery of low-T_c superconductivity in 1911, these efforts will continue to provide the foundation for new electronic and information processing technologies. These developments will depend on an ever-improving understanding of the electronic and magnetic structure of materials gained from the world's best characterization tools.

To achieve an understanding of the functional properties of any novel material, researchers need to know the material's electronic band structure and the morphology of those structural, chemical, and electronic phases that determine how a material responds to external stimuli. For example, efficient computing relies on being able to transport electronic information along conducting channels and to process information in electronic gates reliably and at a minimal power cost. Measurements of the band structure and electronic excitations provide information about electrons participating in conduction and about loss mechanisms that reduce the efficiency and reliability of the operation of a device.

Many currently studied materials exhibit emergent behavior—the appearance of unexpected electronic properties and long-range ordered electronic phases that cannot easily be predicted from the properties of the individual building blocks. For example, cuprates exhibit high-temperature superconductivity, which is relevant for lossless power transmission; manganese perovskites produce complex magnetic and electronic phases that can be utilized in information storage and spintronics applications. A recently discovered "zoo" of topological phases that exhibit unique band structures with symmetry-derived protections against scattering and many-particle interactions may become useful in new electronic devices (Fig. 1, top).

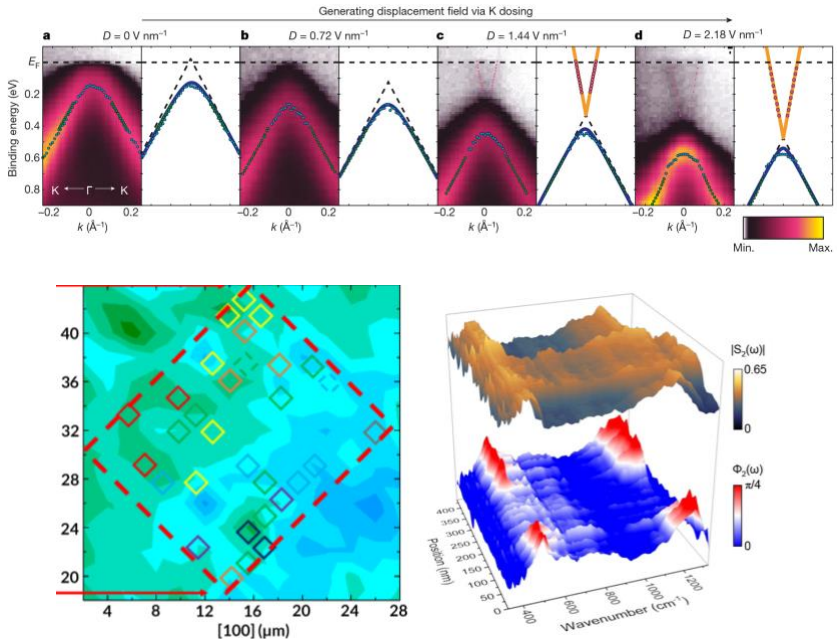

Fig. 1. Top: Changes in the Na_3Bi band structure measured using angle-resolved photoemission spectroscopy (ARPES) at four different levels of K dosing, indicating an electric-field-induced switching of the 2D topological phase [J. Collins et al., *Nature* 564, 3090 (2018)]. Bottom left: Strain map of a composite multiferroic material imaged using microdiffraction [R. Lo Conte et al., *Nano Lett.* 18, 1952 (2018)]. Bottom right: Synchrotron infrared nanospectroscopy (SINS) maps of patterned SiO_2 demonstrating sensitivity to Si–O stretching and bending modes [O. Khatib et al., *ACS Photonics* 5, 2773 (2018)].

To advance the discovery of new materials with novel properties, synthesis needs to be closely integrated with knowledge of the structure and properties of the synthesized material. The ALS offers a comprehensive set of tools to both synthesize materials as well as determine these properties, for instance, angle-resolved photoemission spectroscopy (ARPES) for electronic structure measurements, dichroism spectroscopy to determine chemical and magnetic properties, resonant x-ray scattering to study long-range order, resonant inelastic x-ray scattering (RIXS) to study electron excitations, IR spectroscopy for low-energy excitations, and x-ray photon correlation spectroscopy (XPCS) to determine the temporal response of materials to adiabatic changes in temperature and external fields. Samples are grown in situ using molecular beam epitaxy, pulsed laser deposition, and micromechanical exfoliation.

The Quantum Materials Research and Discovery Thrust Area seeks to advance the discovery and understanding of new quantum materials by developing x-ray methods to measure electronic phases and orders down to nanometer length scales while pushing boundaries in regard to sensitivity, resolution, and the sample environment (temperature, fields, stress, and currents).

High-priority goals (in no particular order) are the development of instrumentation and techniques for the following:

- Efficient measurements of the spin-resolved band structure of quantum materials using spin-ARPES with advanced detection schemes.
- Ultrahigh-energy resolution (sub-millivolt) measurements of exotic electronic phases at ultralow temperatures (sub-Kelvin).

- Magnetic microscopy of quantum materials in high magnetic fields with ≤ 10 nm spatial resolution at cryogenic temperatures.
- Electronic, magnetic, and other ordered phases using nano-ARPES, nano-RIXS, and nano-RSoXS (resonant soft x-ray spectroscopy) with ≤ 100 nm spatial resolution.
- XPCS measurements of electron and spin fluctuations down to nanosecond time scales.
- Multimodal measurements combining x-ray microdiffraction and IR nanospectroscopy with soft x-ray tools together with non-synchrotron methods such as thin-film growth, atomic force microscopy, scanning tunneling microscopy, and transport tools.
- Application of tools to samples and devices under in situ/operando conditions with applied currents, strain, and electromagnetic/optical fields.

The power of these techniques will be dramatically enhanced by the improvements in beam quality delivered by ALS-U. Increasingly, ALS users seek to combine soft x-ray electronic structure techniques with other ancillary tools like scanning probe microscopies, x-ray diffraction (Fig. 1, bottom left) and synchrotron infrared nanospectroscopy (SINS) (Fig. 1, bottom right). Such multimodal methods will enable a broader and more detailed understanding of the role of heterogeneity in novel functional and quantum materials, guided by knowledge of the structure and properties of the synthesized material.

2.1.2 Complex Materials and Interfaces

This TA focuses on how function emerges from the properties of intrinsically heterogeneous materials. Whether bottom-up grown, top-down engineered, or naturally heterogeneous, materials such as fuel cells, batteries, and solar cells are of critical importance to our energy future. In such hierarchical systems, function at the atomic and molecular scale relies on the chemical composition and crystal structure, while at the mesoscale, functions depend upon the transport of electrons, spins, and ions through the material and across interfaces. Composite materials such as concrete or many naturally occurring mineral complexes are also heterogeneous over a range of length scales, determining their response to external forces and ultimately their utility. The ALS provides a range of microscopy, scattering, and imaging tools that allow researchers to determine the electronic, chemical, magnetic, and physical structure of such hierarchical systems. Scanning transmission x-ray microscopy (STXM) can, for instance, quantify nanoscale ion currents in a model system of a lithium-ion battery (Fig. 2, top left) and spin currents in nanostructured magnetic materials. Scattering techniques offer exquisite statistical sensitivity to the morphology and chemical states of multiphase systems, such as an organic solar cell, across a wide range of length scales from nanometers to microns. Element and chemical specificity of the near-edge absorption fine structure allows scientists to differentiate between different chemical components as well as different molecular orientations, which together provide key information about the relationship of structure and function (Fig. 2, top right). At longer length scales, computed tomography visualizes micron-scale and larger functional components and is an excellent tool for both academic and industry users to study the 3D morphology of composite materials, metallic or ceramic compounds, and biological systems (Fig. 2, bottom).

The Complex Materials and Interfaces Thrust Area seeks to advance our understanding of functional, heterogeneous materials by quantifying their properties across a wide range of length and time scales using scattering, spectroscopic x-ray probes, and various imaging techniques.

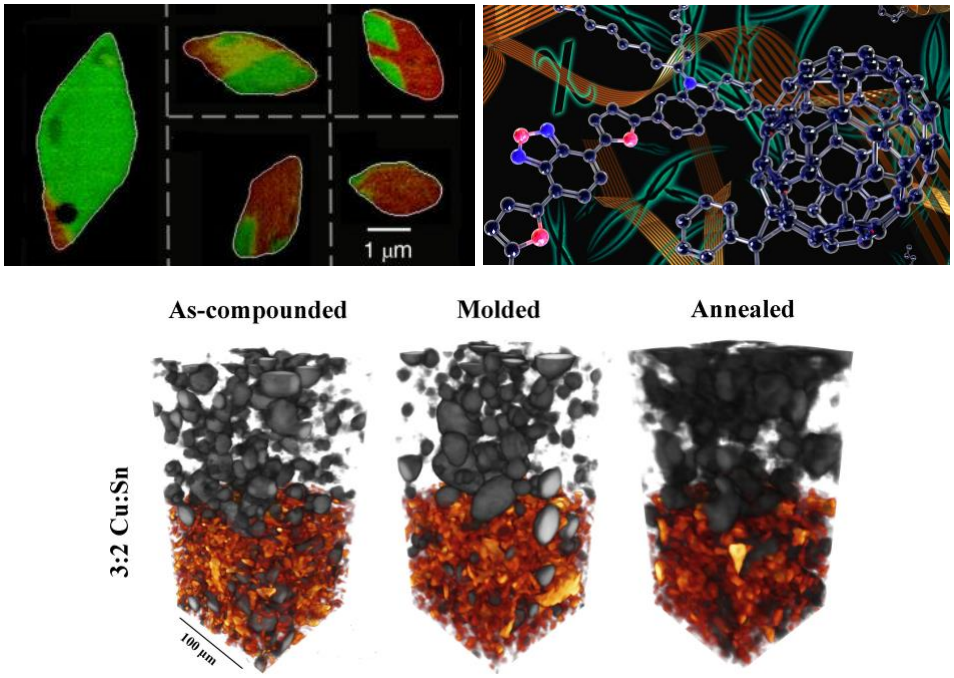

Fig. 2. Top left: STXM images of the lithium distribution in Li_xFePO_4 battery particles at different electrolyte exposures [Y. Li et al., *Nat. Mater.* 17, 915 (2018)]. Top right: Artistic interpretation of an organic solar-cell mixture containing a blend of polymers and fullerenes, which was studied by resonant x-ray scattering [L. Ye et al., *Nat. Mater.* 17, 253 (2018)]. Bottom: Microtomography experiments at the ALS show the distribution of copper (red) and tin (gray) as a function of different processing conditions in conductive plastics. [Q. Yang et al., *J. Appl. Polym. Sci.* 134, 43 (2017)].

High-priority goals are the development of instrumentation for the following:

- Spectromicroscopic and tomographic measurements of functional, heterogeneous materials from the nanometer to millimeter length scales under operando conditions with chemical, magnetic, and morphological sensitivity.
- Microscopy and resonant scattering methods that utilize the tender x-ray energy range to study biological, geological, and energy materials containing elements such as Na, Mg, Al, Si, P, S, Ca, and Fe, among many others.
- Resonant and coherent resonant scattering (such as XPCS) studies of chemical and physical heterogeneity and dynamic processes in soft and hard matter, solid/liquid interphase systems, and membranes, using resonant scattering probes in the soft to tender x-ray range and small- and wide-angle x-ray scattering (SAXS/WAXS) in the hard x-ray range.

The high brightness of the ALS is crucial to reaching nanometer-scale resolution using techniques such as ptychography and to reaching milli- and eventually micro- and nanosecond time resolution using XPCS. The higher brightness (by up to two orders of magnitude) of insertion-device beamlines following the ALS upgrade will dramatically increase the performance of coherent scattering and diffraction imaging techniques, promising near-diffraction-limited resolution in 3D. This TA relies on high-throughput data acquisition, data compression, data visualization, and data analysis techniques and strategies, which the ALS develops together with our partners, including the Center for Advanced Mathematics for Energy Research Applications (CAMERA), the National Energy Research Scientific Computing Center (NERSC), and the LBNL Information Technology Division.

2.1.3 Chemical Transformations

Devices currently in use or being developed for selective and efficient heterogeneous catalysis, photocatalysis, energy conversion, and energy storage rely heavily on diverse multiscale phenomena, ranging from interfacial electron transfer and ion transport occurring on nanometer and picosecond scales to macroscale batteries that charge in hours and catalytic reactors with turnover times of seconds. Soft, tender, and hard x-ray beamlines with innovative scientific and operando instrumentation capabilities can probe dense environments with atomic and chemical contrast spanning a large spatiotemporal range, thereby providing unique fundamental information about these functioning mesoscale chemical devices. Such "nanokinetic" measurements under operando conditions are essential to optimize complex multiscale chemical and electrochemical devices. The multimodal spectroscopic data is interpreted using computational modeling techniques to develop complete models of chemical processes.

The Chemical Transformations Thrust Area focuses on studying the kinetics, energetics, and products of chemical reactions and transformations in diverse environments, ranging from ultrahigh vacuum (UHV) to ambient and even higher pressures, in the presence of liquid and solid interfaces and homogeneous and heterogeneous catalysts. X-rays can penetrate chemical reactors, liquids, and gas-phase environments, and provide very specific chemical and molecular information about the catalysts, reactants, and products participating in a chemical reaction.

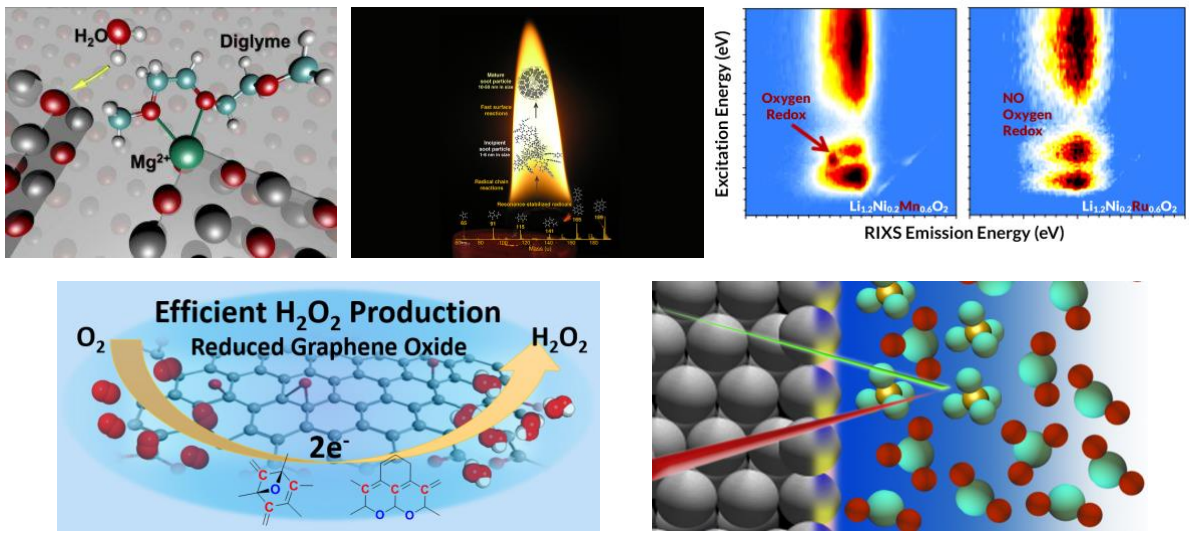

Fig. 3. Top left: A molecular model shows the initial state of battery chemistry that leads to instability in a test cell featuring a magnesium anode. [Y. Yu et al., *Chem. Mater.* 29, 8504 (2017)]. Top middle: VUV mass spectrometry was used to identify fast chemical reactions in flames and soot particles. [K.O. Johansson et al., *Science* 361, 997 (2018)]. Top right: Full-range mapping of RIXS (mRIXS) reveals the novel oxygen states in various energy systems involving unconventional and critical oxygen states. [J. Xu et al., *Nat. Commun*. 9, 947 (2018)]. Bottom left: The efficient production of hydrogen peroxide (H_2O_2) from oxygen (O_2) by a graphene oxide catalyst was studied by x-ray absorption spectroscopy. [H.W. Kim et al., *Nat. Catal.* 1, 282 (2018)]. Bottom right: Operando x-ray absorption spectroscopy (XAS) detects the hidden "fingerprints" of various chemical species that collect just above the surface of a platinum electrode immersed in sulfuric acid to demonstrate the molecular structure of the platinum-sulfuric acid interface. [C.H. Wu et al., *J. Am. Chem. Soc.* 140, 16237 (2018)].

High-priority goals are the development of instrumentation for the following:

- Multimodal spectroscopic and structural measurements of chemical processes at surfaces and under ambient conditions using coherent scattering, IR, and micro- and nano-RIXS/ambient-pressure x-ray photoelectron spectroscopy (APXPS).
- Dynamic measurements of the progress of chemical reactions in jets and electrochemical cells using RIXS and XPCS.
- High-throughput x-ray emission spectroscopy using imaging spectrometers and interferometers.

The high brightness of the upgraded ALS will be needed to study micron and nanoscale systems with high temporal resolution in order to follow a chemical process in real time.

2.1.4 Earth, Environmental, and Biological Systems

Environmental scientists utilize IR, soft x-ray, and hard x-ray beamlines at the ALS with high 2D spatial resolution and chemical sensitivity to disentangle complex processes in environmental systems (e.g., processes governing the distribution and remediation of toxic metal pollutants in soils and mine tailings). The frontier in these studies moves toward capturing these processes in situ under environmentally relevant conditions of temperature, pressure, and pH, with some degree of time resolution, thus moving 2D and 3D studies toward 3- and 4-dimensional datasets. Complex, multimodal, in situ capabilities combining pressure and temperature or temperature and atmospheric composition enable core ALS research in mineralogy and geophysics. Spatially resolved x-ray diffraction in a laser-heated diamond-anvil cell elucidates the stability and reaction pathways of volatile phases such as CO_2 or H_2O within the geochemical context of planetary interiors. In situ diffraction at simultaneous high pressure and high temperature enables the interpretation high-resolution 3D seismic velocity profiles of the Earth in geochemical and geological terms. Highly resolved 2D-strain maps based on Laue microdiffraction enable the recovery of "paleo-strains" in quartz-bearing rocks on the micron scale, thus enabling a quantitative understanding of rock deformation.

Many of the beamlines relevant to the Earth, Environmental, and Biological Systems Thrust Area benefit from close collaborations with external entities. The very successful ALS macromolecular biology and biological imaging beamlines are operated by Participating Research Teams (PRTs), and the ALS coordinates its strategic planning closely with the LBNL Biosciences Area, which includes the Berkeley Center for Structural Biology (BCSB) and the Berkeley Synchrotron Infrared Structural Biology (BSISB) Imaging Program. The macromolecular crystallography PRTs consist primarily of pharmaceutical companies from across the U.S., as well as various academic institutions and the Howard Hughes Medical Institute (HHMI). ALS scientists also closely collaborate with researchers in the LBNL Earth and Environmental Sciences Area and external consortia, such as the Consortium for Materials Properties Research in Earth Sciences (COMPRES), via Approved Programs (APs).

A common thread running through most of the cutting-edge research activities in the Earth, Environmental, and Biological Systems Thrust Area is a move from static postmortem studies to time-resolved and/or in situ/operando/in vivo studies. The high penetration capabilities of hard x-rays and to some extent IR light (with diamond windows) makes these two probes central to these developments. The expansion of such studies to soft and tender x-ray experiments is also of central interest for this TA.

High-priority goals for this TA include the following:

- Cross-platform sample environments for measurement of materials and biological samples under in situ/operando/in vivo conditions but also at extreme pressures and temperatures using IR, scattering, and diffraction techniques.
- 2D and 3D tomographic measurements of geo- and biomaterials on nanometer and micrometer length scales with chemical and structural sensitivity, particularly in the tender x-ray range.
- The study of dynamic biological processes using coherent scattering probes in the infrared and soft, tender, and hard x-ray range.
- Macromolecular crystallography, of small crystals in particular, making use of the high brightness of the ALS.

Earth, environmental, and biological systems are hierarchical over a range of length scales, and structural and chemical information can be interrogated with high precision and sensitivity using high-

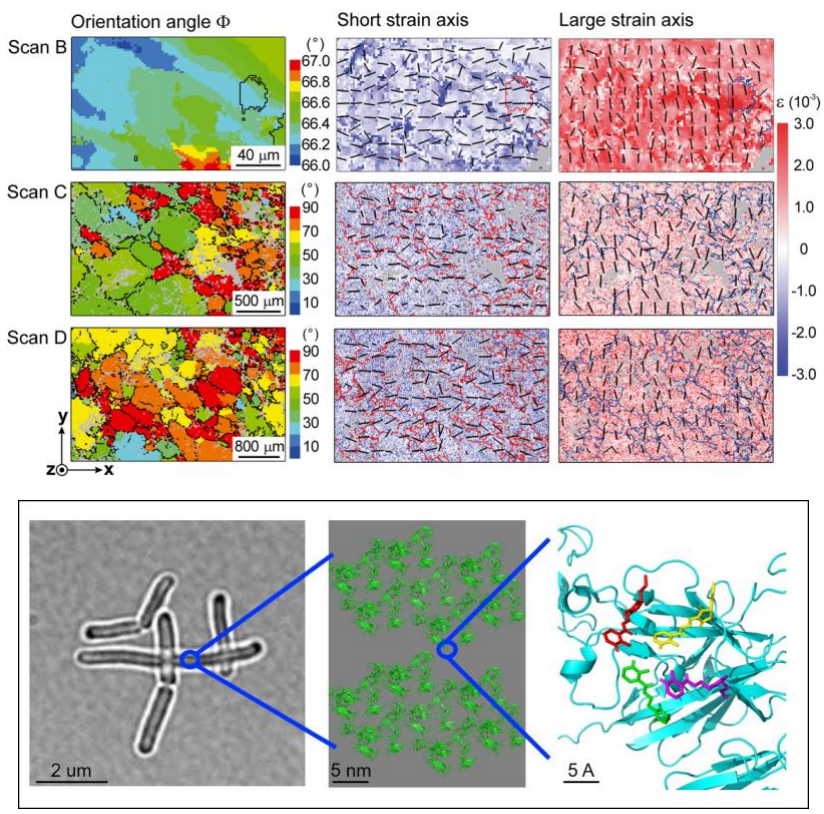

Fig. 4. Top: Maps derived from Laue microdiffraction, displaying orientation (first column) and strain tensors (second and third columns) of deformed rocks from Belgium [K. Chen et al., *Geophys. Res. Lett.* 43, 6178 (2016)]. Bottom: Imaging on the micron scale of biological materials such as microbes can be accomplished with IR and microscopy techniques, with additional spectroscopic information to yield chemical information, while structural information on the nanometer length scale can be obtained with solution scattering methods, and structure at atomic length scales can be obtained with crystallography or x-ray footprinting. Shown in this figure is *Geobacillus stearothermophilus* (left), the layer of proteins coating the surface of the microbe (middle), and the atomic structure of a single surface-layer protein with chemical chelator molecules attached (right). [Baranova et al., *Nature* 487, 119 (2012)].

brightness x-rays. Because of their higher penetration and sensitivity to important mineral-forming and biologically relevant elements, tender x-rays from high-brightness ALS-U insertion devices are of particular interest for this thrust area.

2.1.5 Instrumentation

Facilitating world-class scientific research at ALS beamlines requires continuous, strategic investment in critical technologies that push boundaries and overcome current limitations in experimental capabilities. Orders-of-magnitude gains in coherent power from planned ALS source upgrades will be realized only in the endstations and sample chambers where the quality of the beamline optics and instrumentation has been raised to meet new standards.

The Instrumentation Thrust Area comprises instrumentation experts, beamline scientists, and partners who advise the ALS about instrumentation research and development (R&D) opportunities. We see the potential for significant advancement in x-ray optical technologies and diagnostics, sample environments, controls and computing, and ancillary beamline systems that support the quality and efficiency of our work. Some examples include the following topics.

Beam diagnostics, including beam-position and energy monitors and wavefront sensors, provide essential feedback for the creation of stable, high-coherence beamlines, and they can reduce the maintenance downtime of existing beamlines. We envision the advent of common, multifaceted diagnostic tools, tailored for soft and tender x-ray beamlines and incorporated into new designs or retrofitted onto existing systems.

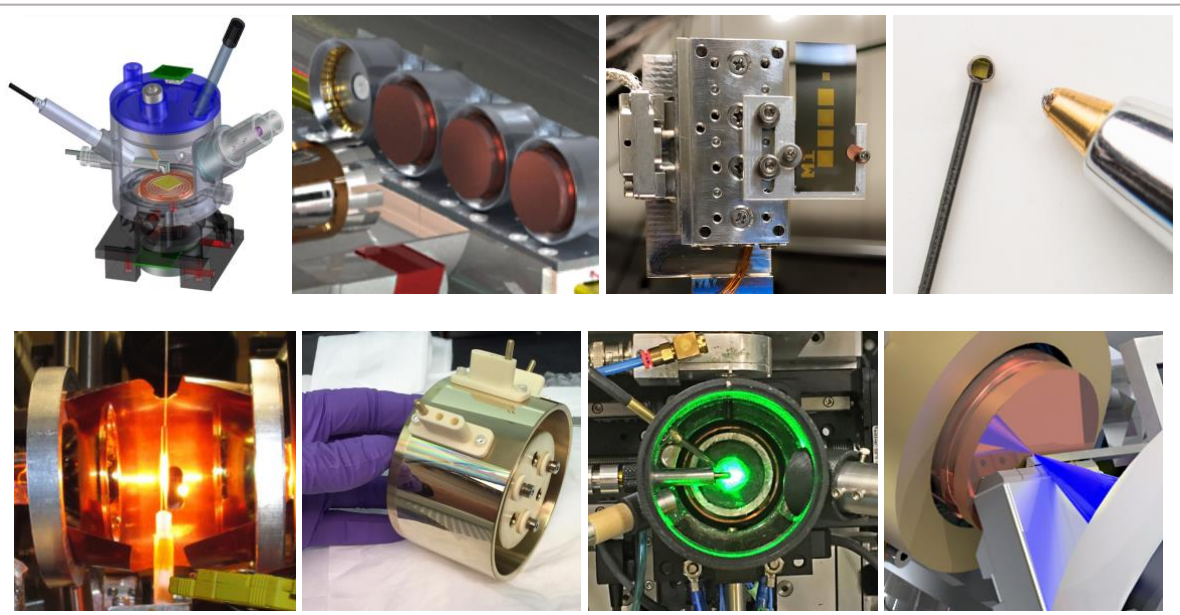

Fig. 5. Instrumentation developed at the ALS.

Adaptive optics for wavefront correction and beam shaping is emerging as an available technology with deployment and refinement taking place at several facilities worldwide. With nanometer-scale surface control becoming possible, we believe that integrated adaptive elements will be required to preserve beam properties in the most demanding beamline applications. Coupled with wavefront-sensing

feedback, a full implementation of adaptive elements at soft and tender x-ray energies will require the development of reliable, automated control systems.

Mirror metrology is a foundational technology that has enabled the creation of optical elements in x-ray optical systems of diffraction-limited quality. Advances in mirror quality follow improvements in metrology, which occur through innovative instrumentation and fastidious attention to systematic errors. Despite significant advances, metrology is challenged to exceed accuracy levels much below 50 nrad and is beset by slow measurement times that throttle throughput. In addition, the demands of highly curved elements, variable-line-space gratings, and the measurement of compound, multi-element optical systems require advances in metrology instrumentation. Development in this area has the potential to benefit numerous future beamline projects.

Mirror stability is among the most significant challenges for existing facilities, such as the ALS, where instrumentation and people operate in close proximity to critical mirror stands and supports. Vibration and drift tolerances shrink proportionally with smaller beam sizes, and ALS-U will reduce the horizontal beam size by a factor of more than 20. Through the exchange of ideas with leading laboratories and by adapting innovations here, we foresee that advanced stabilization methods, including stand engineering, vibration mitigation, and improved feedback, will provide critical support for the success of new and upgraded beamlines across the facility.

ALS beamlines offer a variety of structural, chemical-state, magnetic, and electronic imaging techniques using light from infrared to hard x-rays. Powerful insights arise from combinations of these tools, enabling researchers to probe complex functional relationships. This is especially true for inhomogeneous samples with either engineered or spontaneous heterogeneity. In such complex samples, the direct correlation of diverse properties, determined at fixed sample positions under controlled conditions (e.g. a gaseous environment or applied field), will be immensely more valuable than if applied to multiple similar, non-identical samples. Currently, the coordination of multiple beamlines to achieve this type of measurement is hampered by instrumentation challenges—the lack of compatible sample holders, challenges in preserving sample environments between measurements, and diverse file formats and data-logging systems.

Addressing these incompatibilities will remove bottlenecks to new, sample-centric approaches. High-priority issues for the development of synergistic capabilities are a common electronic notebook that can be shared with researchers across various experimental systems; UHV suitcases for efficient sample transfer between measurement and characterization tools; uniform sample holders or adaptors for different beamlines; sample holders that accommodate multiple leads to enable operando spectroscopy under device conditions; and cooperation with expert user groups at outside institutions and other user facilities at LBNL (NERSC, Molecular Foundry) to enable the broadest participation in multimodal experiments.

2.2 ALS Upgrade and long-range accelerator planning

ALS-U is an ongoing major upgrade of the ALS that will endow the ALS with revolutionary x-ray capabilities. The ALS has been a global leader in soft x-ray science for more than two decades. Recent accelerator physics and technology breakthroughs now enable the production of highly focused beams of soft x-ray light that are at least 100 times brighter than those of the existing ALS. Applying this

technology at the ALS will help us to better understand and develop the new materials and chemical systems needed to advance our energy, economic, and national security needs in the 21st century, securing the United States' world scientific leadership for decades to come.

The upgraded ALS will occupy the same facility as the current ALS, replacing the existing electron storage ring and leveraging about $500 million in existing ALS infrastructure, accelerators, and experimental systems. The new ring will use powerful, compact magnets arranged in a dense, circular array called a multibend achromat (MBA) lattice. In combination with other improvements to the accelerator complex, the upgraded machine will produce bright, steady beams of high-energy light to probe matter with unprecedented detail.

The improved capabilities of the upgraded ALS at new and upgraded beamlines will enable transformative science that cannot be performed on any existing or planned light source in the world. This new science includes 3D imaging with nanometer-scale spatial resolution and measurement of spontaneous nanoscale processes with time scales extending from minutes to nanoseconds—all with sensitivity to chemical, electronic, and magnetic properties. Moreover, the beam's high coherence will enable new classes of optical techniques that will provide the groundbreaking sensitivity and precision needed to detect the faintest traces of elements and subtle electrochemical interactions on the scale of nanometers.

The upgraded ALS is designed to be unsurpassed by any currently envisioned technology and will enable world-leading soft x-ray science for years to come. In June 2016, BESAC released the recommendations of the BES Facility Upgrade Prioritization Subcommittee, whose report deemed the ALS-U project "absolutely central" to contribute to world-leading science and "ready to initiate construction"—the highest possible ratings in the prioritization process. In September 2016, DOE initiated the ALS-U project by approving its "mission need" and assigning it Critical Decision (CD)-0 status, the first milestone in making ALS-U a reality. Most recently, in September 2018, the project received CD-1 approval (alternative selection and cost range), which authorizes the start of engineering and design work.

In order to support the operation of the present and upgraded ALS for an additional several decades, a multi-year prioritized plan for upgrading/replacing legacy accelerator facility subsystems and components was initiated several years ago and will continue in the future. A number of major subsystems, such as for example the booster and storage ring radiofrequency (rf) systems, the accelerator control systems, the timing system, and most of the magnet power supplies, were already replaced with present state-of-the-art technologies, and upgrades of additional major systems, such as the replacement of the linac modulators and rf controls, have been initiated or are planned.

In addition to these projects targeting reliability, a list of prioritized projects, focused on accelerator performance improvements, has been developed, and the highest-priority items in the list are being progressively initiated. In setting priorities, benefits for both the present and the upgraded ALS have been taken into account. Notable examples in this performance-improvement category include new high-performing digital beam-position monitors (BPMs), higher-bandwidth fast orbit feedback, higher-resolution beam-profile monitors, etc.

Additional information on both project categories can be found in section 3.1.

2.3 User program, strategic planning, communications, and workforce development

2.3.1 User program and user services

The quality and impact of the ALS's research depends on an engaged and innovative user community as well as input from other internal and external sources. In collaboration with our scientific staff, our users bring forward key ideas that fuel our facility. As such, our strategic plan is guided by their diverse input, which we seek on a regular basis.

- Our Users' Executive Committee (UEC) serves as an interface between ALS staff and users. We engage them formally and informally several times per year to identify ways to help users be more productive at the facility. The UEC is elected from the user population and generally represents the spectrum of research activities at the ALS.
- Our annual User Meeting is organized by the UEC and includes 10–15 topical workshops and tutorials planned collaboratively by our staff and users (see https://als.lbl.gov/2019-user-meeting-workshops/). The meeting is well attended and provides invaluable advice on emerging opportunities and research priorities. The ALS financially supports the User Meeting in recognition of its impact on the ALS's strategic direction.
- In addition to the regularly held User Meeting, we also convene special ad hoc workshops. For example, a workshop to develop the science case for ALS-U was held in January 2017 and enabled many key users and other outside experts to guide our vision.
- APs provide longer-term, guaranteed access to beamtime for an individual or group proposing a high-quality research program, as evaluated against the General User (GU) population. AP proposals are evaluated by the Proposal Study Panel (PSP), which also evaluates regular GU proposals. APs contribute to the ALS's strategic direction by helping to develop significant new capabilities. The final recommendation on an AP proposal is made by the Scientific Advisory Committee (SAC), which also gauges the R&D plans in terms of the overall ALS program.

The ALS user services web interface is the first face of the ALS seen by ALS users. Provision of a modern user services business system, for coordination of user registration, proposal administration, beamline scheduling, safety management, and tracking and reporting outcomes, is essential to ensure safe and efficient user operations at ALS. ALSHub, the ALS user portal, provides a single point of entry to a personalized, easy-to-use interface which allows users and staff to do the following:

- Register and notify the ALS of a user's arrival date
- Track the status of user agreements, training, and ALS building access
- Submit and view current and past beam time applications
- View the ALS and beamline schedules
- Submit and view current and past experiment safety documents
- Report and search for publications
- Complete all safety and security requirements and provide feedback to ALS

Recent software developments have provided ALS users with a suite of modern and effective tools accessed through the ALSHub interface, including the ALS Scheduler (a centralized scheduling application), the Experiment Safety Assessment Form (ESAF) system to manage user experiments, and

upgraded publication report and search tools. At this point, the ALS will undertake a rolling program of assessing and, if necessary, upgrading each component to ensure that the user services system remains fit for its purpose. The ALS continues to reach out to other user facilities, both within LBNL and nationally, to develop consistent best practices for user services software. During the next 5 to 10 years, it is anticipated that the ALS may do the following:

- Establish Federated Identity Management as part of a development across LBNL user facilities.
- Update the primary ALSHub and user-registration interface to increase integration with changing LBNL human resources and foreign-visit software applications and efficiently meet DOE requirements.
- Replace or update the current proposal administration system. We envisage the replacement product will allow users to select resources across multiple LBNL user facilities. This project will likely be in conjunction with the Light Source Common Software Committee and/or with other LBNL user facilities.
- Participate in coordinated exchange of user data, including digital identifiers, to add metadata to scientific data collected at the ALS. This will be necessary to enable streamlined mechanisms of data analysis and storage.

2.3.2 Strategic planning

The ALS strategic planning process is designed to a) identify new opportunities in synchrotron radiation science, b) recognize and balance the instrumentation needs of our user community, and c) determine technologically advanced and cost-effective solutions to achieve ALS goals.

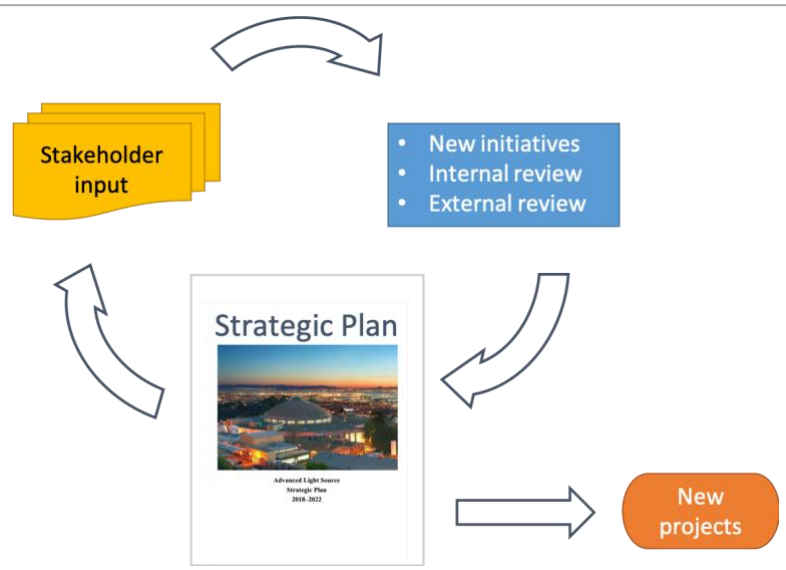

Fig. 6. Schematic of the strategic planning cycle based on using stakeholder input to develop new initiatives that, following internal and external reviews, are included in the ALS strategic plan and lead to new projects. The strategic plan is our way to communicate with ALS stakeholders and seek their feedback.

The ALS uses the following prioritization criteria when assessing new projects:

- Will user research enabled by the project likely have high impact and lead to transformational scientific discoveries?
- Does the project serve a strong community of users in the area of basic energy sciences?
- Will the project significantly enhance the technical capabilities of beamlines or the accelerator in support of user research?
- Is the solution cost effective, appropriate, and technically advanced?

In our planning process we utilize the expertise of the ALS scientific staff who are distinguished scientists and stay in close contact with the user community and experts in the field of synchrotron instrumentation to identify new science opportunities and develop new beamline and accelerator initiatives. ALS scientists are knowledgeable about current research trends and many serve as members of review boards at other light sources, as members of scientific planning committees, and participate in workshops and conferences. The ALS has formed TAs that are charged with incubating new ideas in strategically important areas of x-ray research. Scientists in TAs can seek ALS and LBNL internal resources, including collaborative fellowships or Laboratory Directed Research and Development (LDRD) funds, to develop these ideas. The recently formed ALS Science Council, an ALS internal review board, advises ALS management about prioritizing resources, for example for beamline and endstation projects, and supervises the ALS fellowship programs (see section 2.3.5) and the ALS Colloquium, a regularly occurring set of seminars featuring diverse and high-profile speakers.

The ALS SAC is composed of national and international experts from many disciplines and meets twice per year to provide high-level advice to LBNL and ALS management. All of our strategic plans and priorities are discussed in detail with the SAC. With oversight from the SAC, the ALS regularly organizes crosscutting reviews of all beamlines organized by entire subdisciplines to seek focused advice on how to optimize our capabilities to address important research problems.

2.3.3 Communications

The ALS Communications Group is responsible for highlighting the facility's capabilities and amplifying highly impactful research carried out by our users and staff to a diverse set of audiences. By promoting our capabilities and scientific outputs to current and potential users, DOE, other synchrotron facilities, and the general public, we attract a talented and innovative user pool and garner the support of the public and government agencies for our work. The Communications Group coordinates closely with all functional areas of the ALS to stay apprised of achievements, updates, and plans that need to be communicated to a range of audiences.

The ALS's primary distribution channels for news and updates include the ALS website and a monthly newsletter, ALSNews, which has more than 7,000 subscribers. The group also collaborates with LBNL's Strategic Communications department to increase the visibility and reach of ALS research outputs to the media and general public. Another primary distribution channel is social media, which the ALS will continue to expand and use in combination with multimedia to better reach a breadth of audiences, including the general public and younger demographics. Recently, the ALS has also offered online forums to apprise users of critical news and opportunities involving ALS-U and receive feedback. As the

transition to ALS-U approaches, it will be increasingly important to use several diverse mechanisms for communicating critical updates with users.

Three years ago, the ALS overhauled its website, transitioning to a more modern platform with updated features that would allow potential and existing users and other site visitors to more easily find proposal information and resources, contact relevant staff, and link scientific outputs to specific beamlines. The Communications Group will continue to build out features that make the content more accessible and to highlight capabilities and pathways for collaboration with our scientists.

Another focus of the Communications Group moving forward is internal communications. ALS staff are distributed across multiple LBNL divisions and work in multiple physical locations, and at any given time there are a number of visiting scientists and users onsite as well. TV monitors placed throughout the ALS provide updates on scientific accomplishments, upcoming seminars, and other announcements. To expand these offerings, a revamped intranet will be launched to collect essential resources in one place, and an internal newsletter will be introduced as well that will provide a more direct and frequent way to convey information to staff.

Finally, the Communications Group focuses on outreach, which encompasses students and visitors from the general public, government officials, and potential users. The ALS works with LBNL's Government and Community Relations Office to host high-profile officials and other visitors, as well as to provide requested information to Congress and the California State Legislature, and to plan events on Capitol Hill. Moving forward, the ALS will continue to engage in these outreach efforts, with an increased emphasis on ALS-U and its benefits for the scientific community. Government and Community Relations also includes LBNL's K–12 programs, which the ALS participates in to educate local students and expose the next generation of potential scientists to synchrotron career options. The Communications Group also works with ALS scientists to ensure that they have the resources they need to reach out and attract new users. In collaboration with our scientists and User Office, the Communications Group will help develop specific outreach strategies to ensure a strong base of users who are prepared to take advantage of the enhanced capabilities of the upgraded ALS.

2.3.4 Inclusion, diversity, equity, and accountability

The ALS has a strong commitment to diversity, equity, and inclusion and supports a culture in which the entire ALS community, including staff, users, affiliates, and visitors, feels welcomed and valued.

LBNL and the ALS believe that inclusion, diversity, equity, and accountability (IDEA) are key enablers to accomplishing the Lab's vision of bringing science solutions to the world. As critical components of the Lab's stewardship efforts, they unlock innovation, produce high-performing teams, and drive meaningful impact and outcomes. LBNL and the ALS strive to

- create an environment in which everyone belongs (inclusion);
- welcome and engage all people and perspectives (diversity);
- ensure fair access to opportunities (equity); and
- take responsibility for making progress (accountability).

The ALS's efforts in IDEA comprise a new framework that encompasses several task forces and an IDEA Committee, which advises ALS leadership. Task forces address a focused set of issues related to ALS culture and consist of volunteer members. The chairs of these task forces, along with the IDEA chair, an IDEA facilitator, and at-large representatives of ALS staff comprise the IDEA Committee, which coordinates task force activities and makes recommendations on policy changes to the ALS director. The IDEA framework is flexible, allowing task forces to sunset or be created to address new priorities.

Fig. 7. IDEA task force structure.

Initially, the IDEA Committee and its task forces will work to improve ALS policies and culture with regard to career and professional development; onboarding; recognition; recruiting and hiring; social activities; education and communication; and work–life balance.

2.3.5 Fellowship programs

The success of the DOE synchrotron radiation facilities depends strongly on developing a knowledgeable and highly trained community of users and beamline scientists who apply existing and innovate new tools, often collaboratively, to pursue a diverse array of research frontiers. It is very important to establish a strong pipeline of talented candidates to become facility staff—at the ALS and at other facilities—in the future. Aside from the user-training activities that happen daily on the experiment floor, the ALS sponsors two related programs that directly impact the professional development of young scientists, from college undergraduates to advanced postdoctoral associates:

- **ALS Doctoral Fellowship Program.** This program supports about a dozen doctoral fellows. This program is highly competitive and attracts superb young talent to the ALS. The ALS offers each Fellow stipend support of about 50% of a typical graduate student's pay. The Fellow's thesis supervisor generally provides the balance of financial support as well as university benefits. In addition to training, other goals of the program are to engage the thesis advisor deeply in ALS research activities and to provide a career-development opportunity and supervisory responsibility to ALS staff scientists. The program was established in 2003 and has developed an impressive list of alumni—some now ALS staff and users.
- **ALS Collaborative Postdoctoral Fellowship Program.** This program takes a collaborative approach similar to the doctoral program described above. The strength of the ALS in applying x-rays to frontier research problems attracts a very strong pool of applicants. The financial arrangements are more diverse than for the doctoral program, but the funds are similarly leveraged and a primary intent is again to engage faculty as well as principal investigators in other LBNL divisions in strong collaborations.

The ALS Science Council oversees the fellowship programs, helping to maintain a high degree of leveraging and ensuring strong alignment of the programs with the facility's strategic plan. Applications for doctoral fellowships are evaluated once per year, and postdoctoral fellowships are evaluated quarterly.

2.4 Safety

As part of Integrated Safety Management (ISM), the ALS Safety Program continuously evaluates its effectiveness and identifies opportunities to improve. These improvements are integrated with, and support, the ALS Strategic Plan.

Enhancing beamline safety. While safety at the beamlines is the primary responsibility of the beamline scientists, the floor operators play a key role in ensuring that beamline activities are conducted with the appropriate radiation safety controls. Accordingly, the scope of floor operator responsibilities and oversight regarding beamline operations and configuration is being enhanced through training, updated procedures, improved communications, and expanded roles. A lead floor operator position has been created to assist the operations supervisor in accomplishing these tasks. Software is being developed to provide an electronic means of tracking beamline status and work authorizations. Beamline-shielding drawings are now being evaluated on a yearly basis during the annual beamline radiation surveys. Engineering controls are being created to replace administrative radiation-safety controls.

Annual Beamline Safety Day. Previously, an annual ALS safety stand-down was carried out division-wide on a single day for safety activities while shutters were closed. A new program has been initiated to focus on one beamline at a time. User beamtime is suspended at that beamline in order to dedicate the time to daylong safety-oriented activities. This day combines the annual beamline safety inspection, the annual beamline radiation surveys, and training on beamline radiation safety and beamline-specific ALS procedures. It involves beamline staff, floor operators, ALS safety management, and beamline line-management supervisors, as well as ALS and LBNL subject-matter experts.

Improved communications. Reorganization of the beamline staff structure will improve safety communications through a more granulated line-management structure. Monthly meetings with beamline staff (in Photon Science safety and business meetings) and postdocs and students (in ALS safety circles) provide a mechanism for bi-directional discussions regarding safety and for communicating lessons learned. The ALS Division Safety Committee has been revamped to foster communication with scientific and technical staff, including personnel matrixed to the ALS from other divisions. The ALS training program continues to grow, with new courses for scientific and technical staff regarding radiation, cryogen, and electrical safety, and beamline-specific user training for accessing and securing radiation hutches. An onboarding curriculum for new staff is being developed. Online communication is also being enhanced with a new ALS safety website.

Continued user support. The ESAF, which is the online ISM evaluation form for users, will be applied to the Molecular Biophysics and Integrated Bioimaging (MBIB) beamlines to achieve floor-wide user coverage. Improvements are being made in the ESAF to enhance early communication between users and ALS safety staff. Online training will be developed to improve user understanding of the ESAF process.

Incorporation of ALS-U work into the ALS ISM process. Work for the preparation and installation of equipment needed for ALS-U must be carried out with regard to standard work authorization, ALS safety procedures, and without impacting the accelerator safety envelope and ALS operations. A work evaluation and permitting process is being developed between ALS and ALS-U staff to ensure that this is done in an efficient and safe manner.

3 Accelerator and instrumentation projects

3.1 Accelerator projects

This section enumerates and describes the accelerator projects planned for the next five years. The projects are divided into reliability and performance improvement categories, which are described in two separate subsections. Tables for each of the two categories provide the basic information at a glance, and details about the projects can be found in the text.

3.1.1 Reliability improvement projects

Table 1. Accelerator reliability projects.

Project title	Type of project	Expected completion	Notes
Replacement of the legacy linac modulators	AIP	Q4 FY20	Funded and initiated
Upgrade of the low-level rf (LLRF) controls for the electron gun, linac, and booster	AIP	FY23–24	To be initiated
Septum-magnet spare preparation	OPS	Q2 FY20	Initiated
Equipment protection system (EPS) upgrade	OPS		Being initiated. Completion date depends on funds and resource availability.
Radiation safety system (RSS) upgrade	OPS		Being initiated. Completion date depends on fund and resource availability.
Online radiation-shielding configuration control	OPS	FY21	Initiated
Storage ring HVAC and utilities upgrade	AIP	FY20–21	Initiated
Storage ring radiation shielding ALARA upgrade and seismic retrofit	OPS	2030	Partially initiated

AIP: accelerator improvement project; OPS: operations project

A number of projects in this category will be completed or initiated during the next five years. Particular attention and priority is being placed on those accelerator systems that will continue to operate beyond ALS-U. These include the present ALS injector chain (gun, linac, booster, and most of the electron-transfer lines), equipment protection systems (EPSs), radiation safety systems (RSSs), most of the utilities, and a number of beam diagnostic systems. Projects in this reliability category include the following:

Replacement of the legacy linac modulators. The two 26-year-old units will be replaced with state-of-the-art commercial devices. The contract for the new units has been assigned to a commercial manufacturer (Scandinova Systems AB) and will be delivered to LBNL at the beginning of 2020. Installation and commissioning of the units is planned for the July 2020 shutdown.

Upgrade of the low-level RF (LLRF) controls for the electron gun, linac, and booster. New digital systems will replace the obsolete analog systems presently in operation. Such upgrades will improve reliability but also, and in a significant way, the overall performance and stability of the system. The project will be initiated in FY20, and the new LLRF controllers will be installed and commissioned after the completion of the linac modulator replacement.

Septum-magnet spare preparation. The ALS uses two pairs of thin and thick septum magnets, one pair for beam extraction from the booster, and the other for injection into the present storage ring. With ALS-U, the pair in the booster will continue to operate, while the pair injecting the storage ring will be removed. These septa are complex, high-power, custom devices. A complete set of spare components for the septa is presently available, but they are not assembled into a fully functional unit. The scope of this project is to refurbish and assemble the spare components into a complete pair of septa to allow for a reduction in downtime in case of failure from the present four to five weeks to less than a week. The project has been initiated and will be completed in FY20.

EPS upgrade. Each of the ALS sectors is equipped with an EPS system to protect front-end and beamline components during operation. The present system is fully operational, but it is based on obsolete components and on a not-fully-optimized architecture and distribution. The plan is to redesign the front-end systems to overcome these limitations and to gradually replace them sector by sector. The project is being initiated and will continue in the years to come with the completion date depending on resource and fund availability.

RSS upgrade. Each of the ALS beamlines is equipped with an RSS system to protect personnel from radiation exposure during operation. The present system is fully operational but it is based on obsolete relay logics. The plan is to redesign the RSS systems using state-of-the-art programmable logic controller (PLC) technology and to gradually replace them. The project is being initiated and will continue in the years to come with completion date depending on resources and funds availability.

Online radiation shielding configuration control. ALS beamlines use a complex and custom set of radiation shielding that requires careful configuration control to avoid undesired personnel radiation exposure. The present system is based on a number of physical forms that need to be filled out and linked together depending on the particular beamline at which the radiation shielding operation is being performed. This project goal consists of moving the whole system to a computer-based online application to mitigate the risk of human error while performing this critical operation. The project has been initiated and will be completed in FY21.

Storage ring HVAC and utilities upgrade. The present temperature-control system inside the ALS storage ring shielded area is obsolete and needs to be replaced. In addition, the existing system is located in a position that interferes with the installation of the accumulator—the new ring that will be added as part of the injector chain for the upgraded ALS—and needs to be relocated. The upgrade is being initiated and needs to be completed before the installation of the accumulator in FY20–21.

Similarly, some of the utility systems need to be modified within the same time frame to allow for future operation of the upgraded ALS and of its subsystems.

Storage ring radiation shielding ALARA upgrade and seismic retrofit. The ALS beamline floor is not a radiation area due to the effective shielding that keeps radiation doses below the required limit. Nevertheless, there is a continuous effort to reduce radiation doses on the ALS floor to as low as reasonable achievable (ALARA). As part of this, there is a plan to reinforce the internal side of the concrete shielding in each sector with the addition of a floor-to-ceiling lead "belt." Furthermore, new California codes require the retrofit of the ALS storage ring concrete shielding wall to satisfy new seismic standards. The ultimate deadline for this retrofit is 2030, but the current tentative plan is to perform this seismic operation in conjunction with the radiation shielding addition one sector at a time in sequential order. The actual completion of these projects depends on resource and fund availability.

3.1.2 Performance improvement projects

Table 2. Accelerator performance projects.

Project title	Type of project	Expected completion	Notes
ALS rf distribution system upgrade	AIP	FY20–21	Funded and initiated.
High-resolution BPM at Beamline 7.2	OPS	FY20–21	Preliminary design funded and completed. Final design and fabrication start date depends on fund and resource availability.
High-bandwidth kHz-class fast orbit feedback upgrade	AIP	FY21–22	Funded and initiated.
Photon BPMs for soft x-rays	OPS		To be initiated. Start date depends on fund and resource availability.
Commissioning of the in-vacuum Leda undulator for the Gemini beamline	AIP	FY20	Funded and initiated.
Machine-learning applications for the ALS accelerator	OPS		First phase funded and initiated. Continuation after FY20 depends on fund availability.

AIP: accelerator improvement project; OPS: operations project

A number of accelerator projects targeting performance improvements to ultimately provide users with a better-quality photon beam are planned in the years preceding the ALS-U dark time. These projects will provide benefits and performance improvements to the present ALS and further enhance the performance of an upgraded ALS.

ALS rf distribution system upgrade. The numerous rf systems that allow the synchronized operation of the ALS facility accelerators (gun, linac, booster, and storage ring) receive their operating frequency from a single source represented by a high-stability, high-quality rf synthesizer. Downstream of that, the rf distribution system takes this master frequency and splits, down-converts, up-converts, and formats it to properly feed all the different "client" systems. The upgrade will replace the legacy components with state-of-the art technology counterparts to create a new setup fully integrated with the (recently upgraded) ALS high-performance timing system. The project has been initiated and will be completed in FY20–21. The upgraded rf distribution will provide much higher operational flexibility and performance stability to both the current and upgraded ALS.

High-resolution BPM at Beamline 7.2. Measurement of the transverse size of the electron beam in a storage ring is necessary to provide this beam quantity to the systems in charge of ensuring the photon-source stability required by users' experiments. At the ALS, two dipole beamlines (3.1 and 7.2) are dedicated to such a measurement. In 7.2, the vertical root-mean-square (rms) beam size is less than 10 microns, and with the upgraded ALS, the beam size in both the horizontal and vertical planes will be smaller than 10 microns all around the ring. To properly measure such small beam sizes, a profile monitor with micron-class resolution is required. The preliminary design of an upgrade of BL 7.2 using a visible-light diffraction/interference technique has been completed; final design and fabrication will start when funds and resources become available. Modified versions of this new beamline will also be implemented in the accumulator and storage ring of the upgraded ALS.

High-bandwidth kHz-class fast orbit feedback upgrade. The present ALS is equipped with two feedback systems to maintain beamline source points fixed with micron/submicron precision. One of the feedbacks, the slow orbit feedback, compensates for slow beam orbit drifts, mostly driven by thermal cycles (day/night, seasonal, etc.). The second system, the fast orbit feedback, is designed to mitigate the effects of faster variations. The present ALS fast orbit feedback has a bandwidth limited to about 60 Hz. A project to upgrade this feedback to kHz-class bandwidth has been initiated and is structured in three main parts: upgrading the ALS BPMs and their cell controllers to digital high-performing electronics (this part has been recently completed); replacement of corrector power supplies with high-bandwidth components (48 new fast power supplies have been ordered and will be delivered in FY19); replacement of 48 aluminum vacuum-chamber spool pieces (located inside the corrector magnets) with stainless-steel counterparts to reduce eddy-current attenuation of high-frequency (kHz) magnetic fields (this part has been initiated and will be progressively completed in FY21 or early FY22). Most of the new system (with the exclusion of the vacuum chambers) will be reused in the upgraded ALS.

Photon BPMs for soft x-rays. The ultimate performance in terms of photon-beam stability at the beamlines can be obtained using photon BPMs (pBPMs) in the beamline front end, integrated into the electron-beam orbit feedback. The present ALS does not have pBPMs, and monitors operating in the soft x-ray regime (core of the ALS) with arbitrary types of insertion devices do not presently exist. The goal of this activity would be to develop a scheme capable of operating in this photon spectral region and to implement it in the ALS and later in the upgraded ALS. The start of this project is conditional on resource and fund availability.

Commissioning of the in-vacuum Leda undulator for the Gemini beamline. Leda, the in-vacuum undulator recently installed in the ALS ring for the Gemini beamline, will be commissioned with the electron beam in the first quarter of FY20. Leda will continue to operate at the upgraded ALS.

Machine-learning applications for the ALS accelerator. Machine-learning (ML) techniques are finding applications in nearly every field of human activity, including particle accelerators. At the ALS, a new activity (that hopefully will become a multi-year program) has been initiated to develop ML accelerator applications to control and improve the performance of the ALS. The first step that was undertaken at the ALS in this direction consisted of a project, funded by the DOE Accelerator and Detector Research (ADR) area of the Basic Energy Sciences program and the DOE Advanced Computing Science Research (ASCR) program, to develop a new scheme using deep-learning techniques to compensate for beam-size variations induced by insertion devices. The first test results were very promising, and the ML-based compensation scheme will be put into operation for users in FY19. Additional applications are also under evaluation and will be developed and tested in the future.

3.2 Photon-science projects

3.2.1 Beamline instrumentation projects under construction or in commissioning

The ALS has commissioned eight new and upgraded instruments in the last two years, including the following:

2017

- A magnetic spectroscopy station with a 4 T superconducting “octupole” magnet (American Recovery and Reinvestment Act).
- A soft x-ray branchline (purchased in the Wisconsin Synchrotron Radiation Center "fire sale") installed at 9.0.1 to extend the breadth of the ALS/LBNL Chemical Sciences Division chemical dynamics program capabilities.
- The COSMIC (COherent Scattering and MICroscopy) imaging branch at 7.0.1.2 and an endstation for soft x-ray ptychographic imaging with sub-10 nm resolution (DOE Scientific User Facilities Division midscale funding).
- A new superbend beamline at 12.2.1 to upgrade the chemical crystallography program previously on 11.3.1.
- An upgrade of the 7.3.3 SAXS beamline to allow push-button control of detector distance for flexible, high-throughput operation.

2018 and 2019

- The COSMIC scattering branch at 7.0.1.1 and an endstation for coherent scattering and XPCS.
- An upgraded bend-magnet beamline for tender-energy spectroscopy at 9.3.1 for hard x-ray photoelectron spectroscopy (HAXPES) and APXPS.
- An upgraded beamline for soft x-ray spectroscopy at 7.3.1 for in situ and operando XAS measurements.

Table 3. Photon-science projects in commissioning (green) and design, procurement, construction (blue).

Source point	Project Title	Target commissioning	Partners & Funding	Scope and Notes
9.3.1	Tender energy spectroscopy	In user operation	JCAP, JCESR, ALS EQU	Upgrade vacuum crystal monochromator & optics; tender energy ambient pressure XPS at the solid/solid and solid/liquid interface
7.3.1	Soft x-ray spectroscopy	Limited user operation	JCAP, ALS EQU	Update monochromator; increase capacity for in situ/operando SXR spectroscopy; complements undulatorbased capacity on 8.0.1 and AMBER
7.0.1.1	Coherent scattering - XPCS	Now	DOE midscale, ALS EQU	Half-length undulator and SXR beamline for XPCS studies of spontaneous fluctuations in spin, quantum, and topological materials
6.0.1	AMBER	Starts end of 2019	PNNL, JCAP, JCESR, ALS EQU	Repurpose undulator; multimodal SXR in situ/ operando spectroscopy studies of catalysis, earth & environment, and energy conversion
6.0.1	AMBER-2	2020	ALS EQU	2nd branch for high-throughput spectroscopy
2.0	GEMINI	Starts end of 2019	HHMI, LBNL, LBNL/MBIB	In-vacuum undulator monochromator; microfocus optics for macromolecular crystallography; advanced detectors; robotic sample handling
6.0.2	QERLIN	BL and ES start 2020	Moore Foundation, ALS EQU	Repurpose undulator; soft x-ray RIXS beamline & double dispersion design for high throughput & resolution; spin & quantum materials

ALS EQU: ALS equipment funding; XPS: x-ray photoelectron spectroscopy; SXR: soft x-ray; BL: beamline; ES: endstation

Table 3 summarizes ALS beamline and endstation projects with a total cost over $0.5M presently being commissioned or under construction. The first three projects are in commissioning and will provide some access to commissioning users in 2019. Two additional beamline projects, AMBER (Advanced Materials Beamline for Energy Research) and Gemini, will finish construction in 2019, and the commissioning of the beamlines and endstations will start soon after. The QERLIN (Q- and Energy-ResoLved INelastic scattering) beamline is under construction, and the commissioning of the beamline and the endstation will start in 2020.

COSMIC (now). Since 1995, the ALS has led the world in developing soft x-ray (SXR) scanning transmission x-ray microscopes (STXMs). STXMs on ALS Beamlines 5.3.2.1/2 and 11.0.2 are in very high demand and are highly productive. Commissioning of COSMIC began in 2017 and will maintain this world leadership. One branch of COSMIC is optimized for ptychographic diffractive imaging with state-of-the-art scanning systems, high-data-rate charge-coupled device (CCD) detectors matched to a high-bandwidth data system, and diverse in situ sample environments. COSMIC provides images with <5 nm resolution, ultimately combining 3D tomographic reconstruction with full chemical contrast. A second branch of the COSMIC beamline and associated endstation is devoted to probing spatial correlations in spin and quantum materials in the time domain by enabling SXR XPCS and various speckle metrology experiments.

Beamline 7.3.1 upgrade (now). To increase our soft x-ray spectroscopy capacity and thereby to address burgeoning user demand for these capabilities, we have updated and restarted ALS bend-magnet Beamline 7.3.1 and installed a soft x-ray spectroscopy endstation for operando spectroscopy. The beamline accesses K-absorption edges up to aluminum.

Beamline 9.3.1 upgrade (now). ALS has developed a new tender x-ray energy variant of APXPS on ALS Beamline 9.3.1 to probe electrochemical reactions with operating electrodes/electrolyte systems (Fig. 3). The new vacuum crystal monochromator and optics have been delivered, and user operation has started.

AMBER beamline (2019). AMBER will be enabled by the repurposing of Sector 6. This beamline will be optimized for advanced-materials preparation and multimodal, high-throughput, operando analysis of chemical and energy systems, thereby improving ALS capabilities and increasing capacity in this area. AMBER will provide in situ sample preparation with RIXS and XAS spectroscopies. AMBER is developed in partnership with Pacific Northwest National Laboratory (PNNL) and the Joint Center for Artificial Photosynthesis (JCAP) and the Joint Center for Energy Storage Research (JCESR) Energy Hubs. Construction of the first branch will finish in 2019. Work has started on a second branch, which will broaden the technical capability of the beamline for high-throughput operando RIXS.

QERLIN (2020). A strength of ARPES is that it measures the coupling of electrons and holes to low-energy excitations. However, it can be difficult to identify which excitation(s) lead to a particular emergent property. It is crucial to measure the dispersion relations of the low-energy excitations directly, with high resolution, with SXR contrast, through crucial regions of the phase diagram, and over a large region of Fourier space. For this reason, one of the highest ALS priorities is to build and commission a new SXR RIXS beamlines called QERLIN. The QERLIN beamline is enabled by the repurposing Sector 6 following decommissioning of the ultrafast slicing sources, and is based on a novel optical design that involves multiplexing the incident beam across the face of the sample and the scattered beam across a high-resolution pixelated detector. This will provide a resolving power of >10,000 and will probe an entire map of photon energy in vs photon energy out in parallel—a 100-fold increase in throughput.

Gemini beamline (2020). The macromolecular crystallography beamlines at the ALS have enabled outstanding scientific productivity, providing high-performance hard x-ray diffraction capabilities that have kept pace with the changing needs of the structural biology community. To continue to provide the highest possible performance, HHMI has funded a new high-brightness protein crystallography facility called Gemini in ALS Sector 2. A high-brightness in-vacuum undulator beamline has been installed and the commissioning of the beamline and endstation has started. The beamline is designed to eventually serve two branchlines simultaneously located in a single hutch. One of the branches will be served with diamond beam-splitters and operate at fixed wavelength; the other will allow variable-wavelength operation for multi-wavelength anomalous dispersion measurements.

3.2.2 New ALS-U and ALS beamline projects

Table 4. ALS-U (blue) and ALS (gold) projects prioritized for development.

Source point	Project title	Target commissioning	Partners & funding	Scope and notes
8.0.1	Tender x-ray beamline	After ALS-U dark time	ALS-U	Beamline for tender-energy coherent scattering and microscopy
10.0.1	FLEXON beamline	After ALS-U dark time	ALS-U	Beamline for soft x-ray photon correlation spectroscopy and nano-focus elastic and inelastic scattering
7.0.1	COSMIC upgrade	After ALS-U dark time	ALS-U	Beamline for soft x-ray microscopy, ptychography, tomography
7.0.2	MAESTRO upgrade	After ALS-U dark time	ALS-U	Beamline for nanoscale angle-resolved photoemission spectroscopy (ARPES)
4.0.3	High res. ARPES	TBD	ALS	High energy-resolution, low temperature beamline for ARPES and spin-resolved ARPES
4.0.2	Magnetic spectroscopy & microscopy	TBD	ALS	Brightness upgrade of beamline and high-field low temperature STXM for magnetic studies

Table 4 contains a new set of projects selected for development by the ALS and also through ALS-U. The table includes four prioritized ALS-U project beamlines and two proposed ALS beamline upgrades. The planning process for ALS-U and ALS beamlines was informed by a number of workshops organized by ALS-U and the ALS and by five crosscutting reviews in 2017–2018 that reviewed ALS beamlines. In order to maximize the scientific impact of the ALS upgrade, a coherent strategic plan for ALS and ALS-U beamlines was developed during the last year, and all new beamlines will be designed to make use of the improved performance of the ring after the upgrade.

The ALS-U beamlines were selected in an ALS-U–supervised beamline selection process. A working group of LBNL scientists created 15 initial beamline proposals based on reports from a series of workshops attended by synchrotron radiation scientists and ALS users. The output of these workshops is documented in the report, “Solving Scientific Challenges with Coherent Soft X-Rays.” A down-select process guided by an LBNL internal steering committee and advised by an ALS external ad hoc committee with participation from the ALS scientific advisory and ALS-U technical advisory committees created a final set of scenarios from which the ALS-U Project selected the final list of project beamlines. To receive broad input and communicate progress in the beamline selection process, ALS and ALS-U organized user forums hosted by the ALS UEC and solicited input and feedback from the user community. Updates about the status of the selection process were given at the ALS User Meeting and at advisory committee meetings.

The ALS-U Project plans to build two new beamlines—a soft x-ray beamline in Sector 10 dubbed “FLEXON” (FLuctuation and EXcitation of Orders in the Nanoscale) and a tender x-ray beamline in Sector 8. It will also upgrade two existing soft x-ray beamlines in Sector 7, COSMIC and MAESTRO (Microscopic And Electronic STRucture Observatory). The ALS has prioritized the upgrade of two additional beamlines: 4.0.3, a beamline for high-energy-resolution ARPES, and 4.0.2, a beamline for magnetic spectroscopy and scattering.

ALS-U FLEXON beamline. Sector 10 will house the FLEXON beamline, a high-brightness coherent soft x-ray beamline for probing the roles of multiscale heterogeneity in quantum materials. FLEXON will integrate multiple complementary techniques to provide multimodal probes required for revolutionary progress in understanding the complex physics of quantum materials. One branch will be optimized for high efficiency and medium-energy resolution for XPCS and nano-RSoXS. The second branch will provide x-rays with high-energy resolution in a nanofocused spot and will be optimized for nano-RIXS. XPCS experiments will achieve an improvement in time resolution of three to four orders of magnitude over the current ALS, while the nano-RIXS and nano-RSoXS capabilities will enable measurements with 100-fold improved spatial resolution.

ALS-U tender x-ray beamline. Sector 8 will house a new tender x-ray beamline designed to address challenges at the frontiers of diverse scientific areas, ranging from soft condensed matter and biomaterials to energy science and earth/environmental science. One branch will feature coherent scattering capabilities enabling operando and in situ studies of materials in the tender energy range. The second branch will be optimized for STXM. The brightness of the upgraded ALS in this energy range, when coupled with advanced detectors and experimental systems, will allow for coherent x-ray scattering with microsecond time resolution and scanning spectromicroscopy with spatial resolution of a few nanometers.

ALS-U COSMIC upgrade. The ALS-U Project upgrade of COSMIC will consolidate the ALS's insertion-device STXM instruments (currently occupying 7.0.1.2 and 11.0.2.2) on a single straight section. Following the upgrade of the beamline optics, the full brightness of the upgraded ALS will be available for zone-plate-based microscopy, ptychography, and 3D tomography, all of which require coherent illumination of the zone plate and the sample. The upgrade will lead to an up to 100-fold increase in measurement speed and an improvement in spatial resolution down to 1 nm.

ALS-U MAESTRO upgrade. The MAESTRO beamline makes use of zone-plate and reflective focusing optics to investigate the electronic, chemical, and morphological structure of in situ deposited materials using scanning probe and full-field ARPES instrumentation. The upgrade will improve the ARPES collection efficiency by more than an order of magnitude.

ALS Beamline 4.0.3 upgrade. This proposed ALS beamline upgrade will prepare the beamline for electronic band structure studies of quantum materials at very low temperature (1 K). The development branch of the ALS Photon Science Group (PS-D) is preparing a modular upgrade plan for the beamline that we expect to execute over the next years.

ALS Beamline 4.0.2 upgrade. This proposed ALS beamline upgrade will renew the optics of the beamline, which serves the magnetism and quantum materials community. The monochromator will be replaced with a state-of-the-art-system, and mirror systems will be upgraded with brightness-preserving optics. PS-D is developing work packages that will allow us to start the upgrade when engineering and technical resources become available.

While the ALS continues to innovate new and to upgrade existing experimental systems, the facility carefully balances its suite of instruments with the staff it is able to support so as to maintain efficient and sustainable operations. The design, commissioning, and operation of most of the projects listed above will be handled by existing ALS scientific staff who have been managing the beamlines and

instruments being upgraded, or in some cases being shut down. Overall, these projects are intended to be net staffing neutral.

3.3 Detector development

The ALS Detector Development Program focuses on the development of novel soft x-ray detectors that enhance the productivity of the ALS and enhance the facility's scientific reach. The program is also involved in efforts to help plan and optimize detector capabilities for the upgraded ALS. Soft x-ray detection has challenges not present in hard x-ray detection: signal-to-noise issues (with one-tenth the energy of hard x-rays), in-vacuum operation, and detection efficiency (shallow penetration of soft x-rays into a detector). Several of the techniques and beamlines described above (ptychography, STXM, COSMIC, QERLIN, etc.) are enabled by detectors developed by this program.

The FastCCD, developed in collaboration with the detector group at the Advanced Photon Source (APS), is now deployed at the ALS, APS, Linac Coherent Light Source (LCLS), National Synchrotron Light Source II (NSLS-II), and the European X-Ray Free-Electron Laser Facility (XFEL). It is used for scanning microscopies at the ALS, and several new deployments at ALS beamlines are planned. The VeryFastCCD, the next generation of the FastCCD, is being developed in a collaboration with SLAC National Accelerator Laboratory (SLAC) as an LCLS-II soft x-ray detector and will be an obvious upgrade for scanning microscopies at the ALS as brightness increases.

The SpectroCCD, a very-fine-pitch (5 x 45 μm^2) detector for (1D) RIXS, has proven key to obtaining the resolution needed for momentum-resolved RIXS (qRIXS). The detector is being commercialized through the DOE Small-Business Technology Transfer (STTR) program and has now been deployed on the qRIXS endstation at Beamline 8.0.1. QERLIN presents the challenge of high spatial resolution for 2D RIXS, at a comparatively high rate. Here, the group has leveraged its experience in pioneering CMOS (complementary metal-oxide semiconductor) detectors for electron microscopy to develop a 5 x 5 μm^2 soft x-ray, high-rate CMOS detector.

Future soft x-ray detector advances will be needed to cope with the higher rates provided by improvements in optics and sources, notably due to ALS-U. For example, we are actively collaborating with the University of California (UC) Space Sciences Laboratory to investigate and develop hybrid detectors that combine channel plate sensors that feed pixelated CMOS TimePix detectors for several of these applications—fast XPCS, time-resolved spectroscopy, and high-resolution RIXS. Initial testing of the TimePix2 detector already has produced promising results. The next-generation TimePix3 detector under development will enable full-speed readout of the entire array.

Workshops every one to two years at ALS User Meetings and elsewhere are forums to collect community need and interest, and, together with the Photon Science Group, drive our priorities. ALS operating funds are used to deploy the detectors we develop and to adapt them to specific experiments and beamlines.

3.4 X-ray optics and metrology

This section describes the tools and techniques that are being developed to enable the construction of a new generation of beamlines and endstations, as outlined in section 3.2. One of the challenges will be to cope with beam sizes in the horizontal direction that are 30 times smaller than the beams we have

today. This requires horizontally focusing mirrors to be of much higher quality, and to have a surface figure under load that deviates from the theoretically perfect figure by less than 1 nm. The absorbed power load is typically a few hundred watts. Such tolerances require large improvements in fabrication quality and in mirror cooling technology. Fortunately over the last decade, major advances in fabrication have been made, and even fairly complex figures can now be made to the requisite tolerance. Significant advances, though, are required in mirror cooling, and this is an area of active research.

The major challenges relate to cooling and suppression of vibration. High-power mirrors at the ALS traditionally have used an internally cooled copper structure. Calculations show that at the new tolerance levels we need, this basic structure is inadequate. This type of structure will be replaced by highly optimized water-cooled silicon mirrors, or silicon mirrors cooled by liquid nitrogen to around 124 K, the point at which the expansion coefficient becomes zero. Both routes require significant R&D to prove the technology before deployment in beamlines. Not only do the high-power mirrors in high-brightness beamlines have to be upgraded, all horizontally focusing mirrors in these beamlines need mirrors built to this new tolerance.

In addition to manufacturing and thermal tolerances, vibration becomes a major factor in the performance of a beamline at this tolerance level. One area of work is centered on reduction of cooling-fluid-induced vibration by performing R&D on the modeling of turbulence in cooled systems, the use of optimum geometry and diffuser structures to reduce vibration, and the implementation of stiffer support mechanisms. Part of this ongoing work is to survey the vibration we currently have on the ALS floor and in some of our insertion-device beamlines.

Another area of concern is the slow drift of optics due primarily to ground motion and relaxation of support mechanisms. For regular alignment of the beamline, we intend to use multilayer imaging devices that can be inserted into the beamline; this will allow us to find the beam center, and together with electron BPMs, the beam angle. A combination of this type of device and photodiode and photoemission monitors will allow us to track the position down the beamline. Unlike present-day ALS beamlines, each component will be movable using motor-controlled systems. The combination should allow us to do routine realignment of the beamlines in a simple way, compared to the manual methods we use today.

All of the techniques outlined above most probably will not be sufficient to ensure preservation of the beam brightness and reduction of noise and drift to the required levels. To go beyond this, we are developing wavefront sensing and adaptive wavefront control. The wavefront sensing uses grating-based interferometry, and feedback will be used to adjust pre-figured mirrors that have integral piezo systems to create high-order corrections to the surface height. The aim is for these systems together to work with a bandwidth of >150 Hz, i.e., to a regime where mechanical vibrations are small.

The result of this work should be a new toolbox of techniques in mirror cooling, mounting, alignment, stabilization, and beam monitoring that should significantly improve the quality of beam that is delivered to users.

An integral component of the optics program at the ALS is the X-Ray Optics Laboratory (XROL). This group assures the quality of the optical components installed in beamlines or used in endstations. For example, we must ensure that the mounting system of mirrors does not cause undue deformation in operation, and that the system under adjustment or water flow has the desired characteristics. The

XROL delivers the state-of-the-art optical metrology required to build and maintain high-performance operation of ALS beamlines. For example, the upgraded Long Trace Profiler (LTP-II) and Developmental Long Trace Profiler (DLTP) are capable of 1D surface-slope profiling with a proven accuracy of tangential slope measurements with flat optics of about 60 nrad (rms) and with significantly curved optics (radius of curvature of ≥15 m) of around 200 nrad, limited by the profiler's systematic errors. The increasing brightness of ALS is driving our program to even higher measurement accuracy. For next-generation optics, we need an absolute slope accuracy of 50 nrad and a height accuracy of <0.5 nm in many cases. In close collaboration with optics teams from other DOE BES facilities as well as with our colleagues around the world, we are developing new methods that should take us to these goals within a few years.

Specific optical metrology challenges to be addressed are the development of the required ultrahigh-accuracy x-ray mirror and diffraction-grating characterization instruments. Major XROL efforts will be directed to R&D on a new optical surface measuring system (OSMS) capable of 2D surface-slope metrology with an accuracy below 50 nrad (absolute). Another promising technique is stitching interferometry, similar to the MSI/RADSI (microstitching interferometry/relative-angle determinable stitching interferometry) system recently developed at the Ultra-Precision Machining Laboratory at Osaka University.

A third component of our work is to develop unique optical elements, where required by the ALS experimental program. For example, we require diffraction gratings with very high efficiency and resolution for RIXS. Maximizing efficiency requires the use of multilayer coatings, which in turn require the grating facets to be atomically smooth. We have developed this technology, and it will be deployed for the first time in the high-resolution QERLIN RIXS spectrometer. In addition, we will be developing reflection zone plates as simple high-efficiency monochromators, and ultrahigh-resolution zone plates using zone patterning techniques to go beyond 10 nm focused resolution, in collaboration with colleagues in the Center for X-Ray Optics (CXRO).

Finally, we are conducting research on methods, based on Fourier transform interferometry, that go well beyond the resolution offered by grating-based spectrometers and monochromators. In principle, resolving powers of well over 10^5 can be reached in a fairly compact system, but major challenges exist in the mechanical control of the required delay stage and beam-division systems.

3.5 Data management and computing

About two years ago, a Data Working Group (DWG) composed of members from the five BES light sources was charged by the light-source directors to evaluate and quantify the long-term needs for data analysis, management, and storage across the five BES light sources. The estimates present a daunting challenge: in 10 years, the DWG estimated that, collectively, these facilities will produce around one exabyte (quintillion bytes) of data per year and will require on-demand computing resources of 1000 petaFLOPS (quadrillion floating-point operations per second). The ALS alone is estimated to require much less than this—a mere 30 petabytes (quadrillion bytes) per year and 10 petaFLOPS, numbers that even by themselves will require serious effort to achieve.

The DWG outlined computing challenges in four main 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 data volumes and provide feedback during experiments to improve data quality and to drive the direction of ongoing measurements.
- On-demand utilization of supercomputing environments to enable 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.

With challenge comes opportunity, and the ALS is enthusiastic about pursuing these opportunities. The challenges bulleted above are endemic to light sources and other kinds of facilities around the world, and it makes sense to collaborate to find solutions. Recently, BES management encouraged such a collaboration among the BES light sources and also defined a structure to find solutions. This collaboration will necessarily include ASCR-supported high-performance computing and networking facilities and, as importantly, the expertise of their respective staffs.

To address the approaching data challenges, the ALS is developing data-driven acquisition solutions, data workflows for near-real-time analysis, graphical user interfaces for analysis, advanced data transfer solutions combined with machine learning solutions. These emerging capabilities are described in more detail below.

3.5.1 Data management tools

The ALS Computing Program, together with beamline scientists and users, is developing data management tools that assist users and staff during the full data lifecycle from acquisition to storage and analysis. These tools include software that runs at the beamline to detect, package, and transfer new data; database servers that register data with its associated metadata to allow subsequent search and organization; and workers, message-passing systems, and workflow tools that allow automated processing to be launched on data sets using local and remote resources (such as supercomputing centers) as data arrives. Stored metadata will cover information about experiments, the beamline environment, and pointers to raw and derived data that is stored in a variety of locations. An easy-to-use web portal will allow users to view or download results during or after their beamtime.

Table 5. List of data management tools currently under development.

Tools	Description
Implementation of Bluesky	The ALS is developing procedures for beamline automation and simplification of common tasks and is integrating the Bluesky (NSLS-II) toolchain in a data acquisition graphical user interface that will execute complex acquisition "plans" through simple button clicks.
Graphical User Interface Xi-CAM	ALS and CAMERA are developing this Python and Qt-based graphical user interface as an integrated platform for synchrotron data acquisition, management, visualization, and analysis. The program plans to: a) add scripting tools to pre-existing LabView controls, b) enable parameterized analysis using metadata from Databroker databases, c) enable exploratory analysis using interactive visualization tools, and d) support workflow-driven data processing powered by Dask.
Implementation of CAM-Link data processing workflows	CAM-Link, developed by the ALS and CAMERA, will support data movement and execution workflows across one or more facilities. CAM-Link will provide: a) an automatable process for authentication and authorization enabling distributed end-to-end pipelines, b) interfaces for analysis routines communicating across multiple facilities, c) resource provisioning support for backend resources such as remote job schedulers, d) interfaces for moving data and extracting metadata information, and e) tools enabling the execution of analysis workflows and real-time feedback.
Networking and computing infrastructure	The ALS will design a reference architecture for beamline networking and computing hardware utilizing existing ALS network, LBLnet, and ESnet structures while taking advantage of the ScienceDMZ model.
Experiment metadata database	The ALS is designing a metadata repository and accompanying portal to store metadata about user experiments. The system will coordinate with various metadata capture tools (sample data, electronic notebook, etc.) to gather information about experiments, which can be reviewed later.

3.5.2 Machine learning

Machine learning (ML) concepts provide a novel and transformative mechanism to develop powerful real-time processing solutions for large and complex data sets. Applications at the ALS range from improving the electron beam stability, which all users will benefit from, to assisting and guiding scientific discovery at individual beamlines.

Table 6. List of machine-learning-enabled software tools currently under development.

Tools	Description
Electron beam size stabilization	The ALS is developing a ML model based on a complete set of metadata from the storage ring and implementing a neural-network-based correction loop. Vertical beam variations have decreased by an order of magnitude since the ML-enabled loop is operating.
Pattern recognition for images and volumes	ALS and CAMERA are developing ML based tools to extract quantitative information from acquired 2D and 3D data. ML tools aid users in transitioning to more autonomous modes of data analysis, e.g., providing tools for feature extraction, detection, segmentation, and classification at beamlines acquiring image and volumetric data.
Pattern recognition of scattering patterns	ALS and CAMERA are developing convolutional neural network tools to aid the high-throughput analysis of x-ray scattering data. A trained model successfully recognized grazing-incidence small-angle x-ray scattering patterns with a rate of 98% from simulated data.

Look-up tables imperfectly correct changes in the transverse beam size in the storage ring following undulator gap moves. A recently developed neural network (NN) for the accelerator was trained by varying the gaps of all undulators inside the ALS storage ring and recording the resulting beam-size changes. The results of the trained NN are shown in Fig. 8. The area with a white background represents the NN being disengaged and results in high fluctuations in the vertical beam size due to undulator and ID gap changes. When the NN was activated, the loop counteracted the effect of the undulator motions and stabilized the vertical beam size by an order of magnitude.

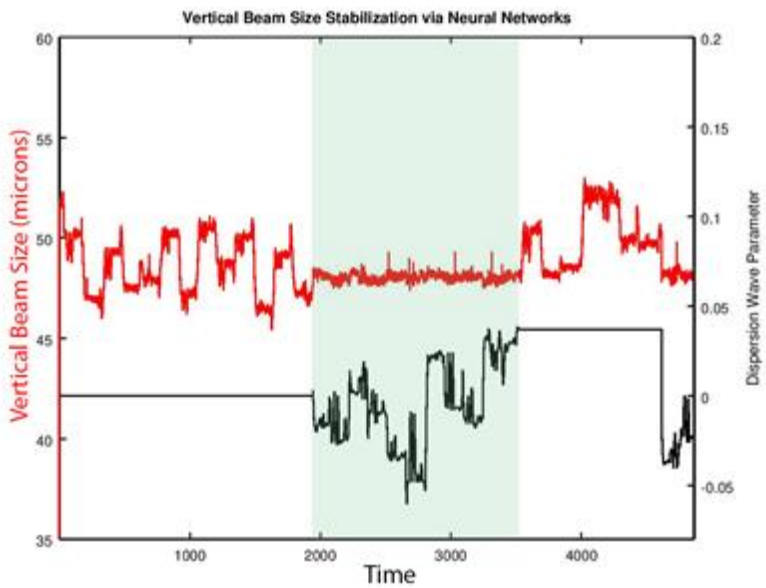

Fig.8. The vertical size of the electron beam (red) is shown to stabilize under application of a feed-forward neural network (NN). The green area shows the duration during which the NN was actively stabilizing the beam size and tuning the dispersion wave parameter (DWP), a parameter that compensates for the influence of the undulator moves.

4 Initiatives and emerging beamline and endstation development opportunities

Guided by the TA priorities discussed in section 2.1, the ALS seeks to develop new beamline instrumentation over a time window of five to ten years, which will significantly enhance our existing capabilities in synchrotron science. These proposed instrumentation upgrades have been endorsed by ALS crosscutting reviews and have strong user community support. The ALS is seeking partners to support and realize these initiatives, which target important growth areas in x-ray science at the ALS. The ALS intends to prioritize and execute projects from this list as resources become available.

Table 7. Emerging beamline and endstation development opportunities (not in any order of priority).

Source point	Project title	Scope and notes
9.3.2 or 9.1.1	APXPS	Bending-magnet beamline optimized for soft x-ray ambient-pressure photoemission spectroscopy
11.0.2	MESB-U	Upgraded beamline for operando RIXS and APXPS combined with nano-focusing and coherent scattering
Endstation	High-res. ARPES	Low-temperature, high-resolution ARPES and momentum microscopy instrument
Endstation	Low-T SINS	Low temperature and nanometer-resolved infrared spectroscopy setup for quantum materials research
Endstation	Q-STXM	STXM endstation optimized for high-field, low-temperature magnetic microscopy
Endstations	Instrumentation for high-brightness beamlines	Nano-focus scattering and coherent scattering endstations

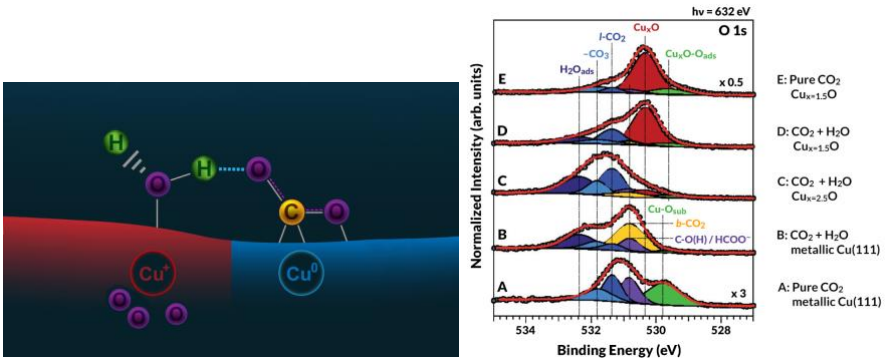

Fig. 9. Oxygen chemistry at the surface of a Cu catalyst used for CO_2 conversion into liquid fuel measured using APXPS at Beamline 9.3.2 [M. Favaro et al., *PNAS* 114, 6706 (2017)].

Beamline 9.3.2 APXPS. Beamline 9.3.2 serves a strongly growing community utilizing soft x-rays to study surface catalytic reactions and electrochemistry using x-ray photolectron spectroscopy at ambient pressures, a priority of the Chemical Transformations TA. The obsolete beamline optics need to be updated by building a replacement beamline at port 9.3.2 or at 9.1.1. Plans are being developed for a start after the ALS-U dark time.

Beamline 11.0.2 upgrade. This high-brightness beamline initiative is a priority of the Chemical Transformations TA. The upgraded beamline targets operando-RIXS and APXPS paired with coherent scattering and nanofocusing and would offer tools to study chemical reactions dynamically in liquid jets and at surfaces with down-to-nanoscale spatial resolution and down-to-microsecond temporal resolution. Initial R&D is conducted through an LDRD.

High-resolution ARPES endstations. The ALS seeks to develop new endstations for electronic structure measurements at very low temperatures below 1 K and in combination with efficient spin detection, a priority of the Quantum Materials Research and Discovery TA. One of the anticipated endstations would be a spin-momentum microscope, a high-throughput setup for momentum-, energy-, spin-, and position-dependent photoemission spectroscopy. The second endstation would have an optimized sample environment and spectrometer for ultrahigh-resolution electron spectroscopy at very low temperatures to map the electronic structure of novel exotic phases.

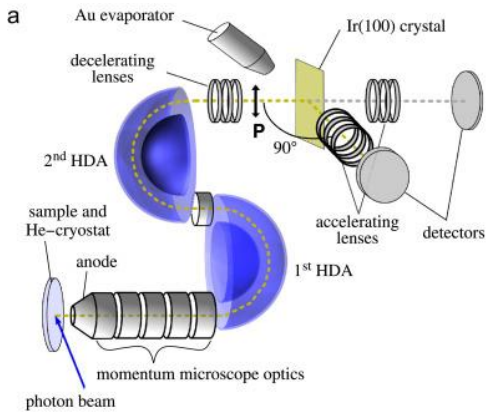

Fig. 10. Schematic design of a spin-momentum microscope by C. Tusche et al., *Ultramicroscopy* 159, 520 (2015).

Cryogenic SINS. The ALS is seeking to develop a cryogenic endstation for broadband infrared nanospectroscopy in the far-IR in a UHV environment that will enable exploration of new nanoscale physics in novel materials near phase transitions. SINS combines the high brightness, broad spectral bandwidth, and spatial coherence of synchrotron infrared radiation with the high spatial resolution and sensitivity of scattering-type, scanning near-field optical microscopy (s-SNOM) to achieve broadband infrared spectroscopy with nanometer spatial resolution.

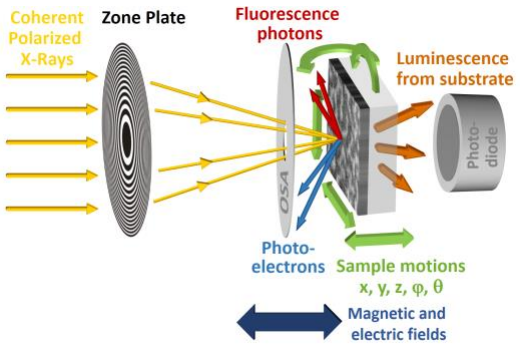

Fig. 11. Zone-plate-based Q-STXM microscope to conduct high-field and temperature-dependent measurements of quantum and functional materials using luminescence detection.

Q-STXM endstation. This low-temperature high-field STXM would be optimized for studies of the electronic, chemical, and magnetic properties of spin systems exhibiting nanoscale phases and would serve the magnetism, spintronics, and quantum materials community. This endstation is a priority of the Quantum Materials Research and Discovery and the Multiscale Structure and Dynamics STAs. An LDRD proposal has funded successful exploratory work.

Endstations for high-brightness beamlines. The ALS seeks to develop additional endstations that will complement the initially deployed endstations at the ALS-U project beamlines and will further leverage the two-order-of-magnitude increased brightness of the storage ring.

5 List of abbreviations

ADR	Accelerator and Detector Research
AIP	accelerator improvement project
ALARA	as low as reasonably achievable
ALS	Advanced Light Source
ALS EQU	ALS equipment funding
ALS-U	Advanced Light Source Upgrade Project
AMBER	Advanced Materials Beamline for Energy Research
AP	Approved Program
APS	Advanced Photon Source
APXPS	ambient-pressure x-ray photoelectron spectroscopy
ARPES	angle-resolved photoemission spectroscopy
ASCR	Advanced Scientific Computing Research
BCSB	Berkeley Center for Structural Biology
BES	Basic Energy Sciences
BESAC	Basic Energy Sciences Advisory Committee
BL	beamline
BPM	beam-position monitor
BSISB	Berkeley Synchrotron Infrared Structural Biology
CAMERA	Center for Advanced Mathematics for Energy Research Applications
CCD	charge-coupled device
CD	Critical Decision
CMOS	complementary metal-oxide semiconductor
COMPRES	Consortium for Materials Properties Research in Earth Sciences
COSMIC	COherent Scattering and MICroscopy
CXRO	Center for X-Ray Optics
DEI	diversity, equity, and inclusion
DLTP	Developmental Long Trace Profiler
DOE	Department of Energy
DWG	Data Working Group
EPS	equipment protection system
ES	endstation
ESAF	Experiment Safety Assessment Form
FLEXON	FLuctuation and EXcitation of Orders in the Nanoscale
FLOPS	floating-point operations per second
GU	General User
HAXPES	hard x-ray photoelectron spectroscopy
HHMI	Howard Hughes Medical Institute
HVAC	heating, ventilation, and air conditioning
IDEA	inclusion, diversity, equity, and accountability

IR	infrared
ISM	Integrated Safety Management
JCAP	Joint Center for Artificial Photosynthesis
JCESR	Joint Center for Energy Storage Research
LBNL	Lawrence Berkeley National Laboratory
LCLS	Linac Coherent Light Source
LDRD	Laboratory Directed Research and Development
LLRF	low-level rf
LTP	Long Trace Profiler
MAESTRO	Microscopic And Electronic STRucture Observatory
MBA	multibend achromat
MBIB	Molecular Biophysics and Integrated Bioimaging
MESB-U	Molecular Environmental Science Beamline-Upgrade
ML	machine learning
mRIXS	mapping of resonant inelastic x-ray scattering
MSI	microstitching interferometry
NERSC	National Energy Research Scientific Computing Center
NLK	nonlinear kicker
NN	neural network
NSLS-II	National Synchrotron Light Source II
OPS	operations project
OSMS	Optical Surface Measuring System
pBPM	photon beam-position monitor
PLC	programmable logic controller
PNNL	Pacific Northwest National Laboratory
PRT	Participating Research Team
PS-D	Photon Science Development (branch of the Photon Science Group)
PSP	Proposal Study Panel
Q-STXM	STXM endstation optimized for high-field, low-temperature magnetic microscopy
QERLIN	Q- and Energy-ResoLved INelastic Scattering Beamline
qRIXS	momentum-resolved resonant inelastic x-ray scattering
R&D	research and development
RADSI	relative-angle determinable stitching interferometry
rf	radiofrequency
RIXS	resonant inelastic x-ray scattering
rms	root-mean-square
RSoXS	resonant soft x-ray scattering
RSS	radiation safety system
s-SNOM	scattering type, scanning near-field optical microscopy
SAC	Scientific Advisory Committee
SAXS	small-angle x-ray scattering

SINS	synchrotron infrared nanospectroscopy
SLAC	SLAC National Accelerator Laboratory
STTR	Small-Business Technology Transfer
STXM	scanning transmission x-ray microscopy
SXR	soft x-ray
TA	Thrust Area
TBD	to be determined
UC	University of California
UEC	Users' Executive Committee
UHV	ultrahigh vacuum
VUV	vacuum ultraviolet
WAXS	wide-angle x-ray scattering
XAS	x-ray absorption spectroscopy
XFEL	European X-Ray Free-Electron Laser Facility
XPCS	x-ray photon correlation spectroscopy
XPS	x-ray photoelectron spectroscopy
XROL	X-Ray Optics Laboratory