ADVANCED LIGHT SOURCE

Five-Year Strategic Plan

FY2023

BERKELEY LAB

U.S. DEPARTMENT OF ENERGY | Office of Science

Contents

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 nearly 1700 users who publish more than 800 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 advance science for the benefit of society by providing our world-class synchrotron light source capabilities and expertise to a broad scientific community. 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 US 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, including the water-energy nexus, energy storage, quantum information science and technology, and advanced semiconductors and microelectronics, and our staff works closely with other US user facilities and the LBNL Energy Sciences and other Areas 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 provide the ALS 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 reached the Critical Decision-3 (CD-3) milestone in November 2022, which approved the start of construction. As part of the strategic planning process, the ALS has identified six 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

Six TAs have been formed around critical growth areas in x-ray science and instrumentation. The TAs are organized around cross-cutting themes and include scientists from the ALS and closely tied LBNL divisions. Members of the TAs collaboratively develop the science and instrumentation strategy for their area, propose new research and development (R&D) activities to advance these strategies, lead ALS responses to funding opportunities, and reach out to the user community to launch initiatives that result in new beamline projects.

2.1.1 Quantum Materials Research and Discovery

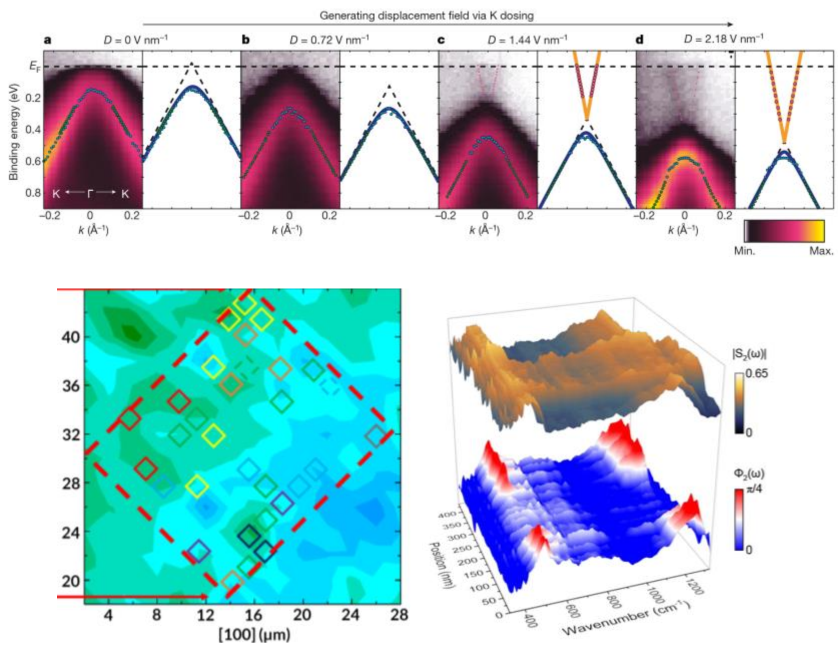

Fig. 1. Top: Changes in the Na_3Bi band structure measured using angle-resolved photoemission spectroscopy (ARPES) at four different levels of K dosing, indicating an electric-field-induced switching of the 2D topological phase [J. Collins et al., *Nature* 564, 3090 (2018)]. Bottom left: Strain map of 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)].

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 discover and understand quantum phenomena in materials, starting with the discovery of superconductivity in 1911, these efforts will continue to provide the foundation for new electronic and information processing technologies. These developments will depend on the posing of new questions to gain a deeper understanding of the electronic and magnetic structure of materials—questions that can only be answered using the world's best characterization tools. Through detailed insight into electronic band structure, spin states, and the morphology of the chemical, electronic, and structural phases that determine a material's response to external stimuli, we gain a more complete understanding of its functionality. 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 also 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. These properties often go beyond the scope of established theories and cannot easily be predicted from the properties of their 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; and molecular materials offer spin and electronic states that can be switched with unprecedented energy efficiency. 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).

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—tools such as angle-resolved photoemission spectroscopy (ARPES) for electronic structure measurements, x-ray magnetic circular and linear dichroism (XMCD + XMLD) spectroscopy to determine chemical and magnetic properties, photoemission electron microscopy (PEEM) to study spatially inhomogeneous and patterned electronic and magnetic domains, resonant elastic x-ray scattering (REXS) to study long-range order, resonant inelastic x-ray scattering (RIXS) to study electronic excitations, synchrotron IR nanospectroscopy (SINS) 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 TA seeks to advance the discovery and understanding of new quantum materials by developing novel 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:

- More-efficient measurements of the spin-resolved band structure of quantum materials using spin-ARPES with advanced detection schemes beyond Mott and exchange scattering.
- Ultrahigh-energy-resolution (sub-millivolt) measurements of exotic electronic phases and spin textures at ultralow temperatures (sub-Kelvin).

- Magnetic infrared microscopy of quantum materials in high magnetic fields with ≤ 20 nm spatial resolution at cryogenic temperatures.
- Novel imaging modalities of elastically and inelastically scattered x-rays that can image electronic, magnetic, and other ordered phases down to nm length scales.
- XPCS measurements of electron and spin fluctuations down to nanosecond time scales.
- A novel imaging tool based on reflection geometry that will enable imagining of electronic and magnetic order and phenomena at buried interfaces and heterostructures.
- NanoARPES capabilities at the ultimate reach of spatial resolution (≤ 10 nm) for fundamentally new, direct access to 1D electronic states of single quantum objects and interface and edge states; for access to the natural length scales of electronic heterogeneity in correlated electron systems; and enabling unique sensitivity to electronic phase and coherence by probing within a material's electronic coherence length for the first time.
- 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 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

The Complex Materials and Interface (CMI) TA focuses on understanding how function emerges from the complex properties of intrinsically heterogeneous materials across a wide range of length and time scales, with a particular focus on soft materials and hybrid organic-inorganic systems. Whether bottom-up grown, top-down engineered, or naturally heterogeneous, materials used in applications that range from electrochemical energy storage and conversion to water purification are of critical importance to our energy future. In such hierarchical systems, atomic- and molecular-scale function relies on the chemical composition and crystal structure, while at the mesoscale, physical and chemical functionalities depend upon the diffusion and transport of electrons, spins, and ions through the material and across interfaces and phases. Hierarchical systems, for example, a proton-conducting fuel-cell membrane, require molecular arrangements over a range of length scales for efficient charge transport. The ALS provides a range of scattering, spectroscopy, and imaging tools that allow researchers to determine the electronic, chemical, and physical structure of such hierarchical systems. Scattering and diffraction techniques offer statistical sensitivity to the morphology and chemical states of multiphase systems, such as a phase-separated, proton-conducting polymer membrane (Fig. 2a), across a wide range of length scales from Ångstroms to hundreds of nanometers. Element and chemical specificity provided by the near-edge x-ray absorption fine structure spectra allows scientists to perform operando monitoring electrocatalyst oxidation (Fig. 2b). Structural information from scattering can connect to electronic properties in electronic materials, like 2D perovskites (Fig. 2c). The polarized nature of synchrotron x-rays provides unique capabilities to probe molecular orientation with high resolution of surfaces and buried interfaces (Fig. 2d).

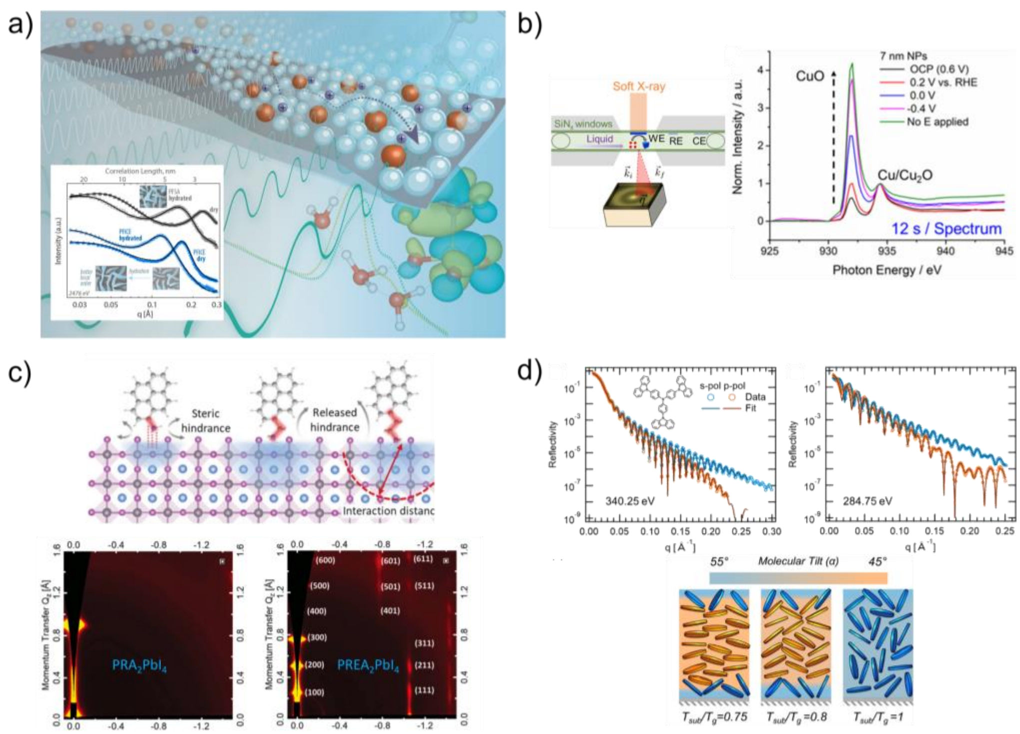

Fig. 2. Overview of recent CMI science highlights. a) In situ tender resonant x-ray scattering near the sulfur K-edge revealed the phase separated morphology of proton-conducting polymer membranes for PEM fuel cells [G. Su et al., *J. Am. Chem. Soc.* 141, 13547 (2019)]. b) The development of an operando RSoXS capability that enables correlated x-ray absorption spectroscopy and SAXS enabled the operando study of CO_2 reduction by copper nanoparticles [Y. Yang et al., *J. Am. Chem. Soc.* 144, 8924 (2022)]. c) Grazing-incidence WAXS experiments on perovskite films that were surface-treated with ammonium helped researchers understand how the pyrene-based ammonium ions influence the perovskite structure. [J. Xue et al., *Science* 371, 636 (2021)]. d) Polarized resonant soft x-ray reflectivity at the ALS was used to measure nanometer-resolved, molecular orientation depth profiles of vapor-deposited thin films of an organic semiconductor [T. Ferron et al., *ACS Appl. Mater. Interfaces* 14, 3455 (2022)].

The ALS has pioneered the development of small- and wide-angle x-ray scattering (SAXS/WAXS), resonant soft x-ray scattering (RSoXS), and tender resonant x-ray scattering (TReXS) capabilities. The higher flux of an ALS-U high-field bending magnet port would enable high-throughput, in situ, and closed-loop autonomous SAXS/WAXS measurements and access to faster time scales, and launching such an upgrade is a high priority for the CMI TA. Moreover, this TA seeks to develop internal and external collaborations that advance tender x-ray scattering capabilities. The CMI TA's scientific priorities span hydrogen, water treatment, polymer upcycling, organic and perovskite-based novel semiconductors, high-precision patterning science, and energy storage and conversion. This scientific breadth provides the basis to nucleate and grow a strong user community consisting of external groups and local research programs that will transition to the coherent ALS-U soft and tender x-ray beamlines. The RSoXS program is continuing to evolve and prepare for future energy-resolved chemical x-ray photon correlation spectroscopy (C-XPCS), which has the potential to monitor the dynamics of specific microphases in hierarchical materials. High-priority goals in the next few years are the development of new instrumentation that will exploit the capabilities of the upgraded ALS to address new science currently out of reach. The high brightness of the ALS is crucial to reaching nanometer-scale resolution using techniques such as ptychography and to reaching milli-, micro-, and nanosecond time resolution using XPCS. Specifically, the development of tender x-ray techniques for the upgraded ALS will be the top priority for the CMI TA in the next five years.

- Tender x-ray microscopy will enable operando and multimodal studies of materials with high spatial resolution (<10 nm) and chemical specificity. The ability to quantify morphology and chemical or crystalline phases at high spatial and time resolution will advance many areas of science. A proposed microscope for the ALS-U tender x-ray beamline will be based on the revolutionary Nanosurveyor2 instrument of the COSMIC microscopy beamline, optimized for use at higher photon energies. Nanosurveyor2 provides world-leading spatial resolution and scanning speed in a compact and ultra-stable assembly. The new microscope will be compatible with commercial or custom operando sample environments, use state-of-the-art detectors for fluorescence detection and coherent x-ray scattering, and seamlessly facilitate correlative measurements with other microscopes.
- Novel instrumentation for tender x-ray scattering will enable studies of a broad range of materials relevant to soft matter, geo-environmental science, and bio-inspired materials. A proposed endstation at the ALS-U tender x-ray beamline will perform static characterization through resonant scattering in the 1–5 keV energy range and will offer unique access to a broad range of elemental absorption edges including Na, Ca, P, S, Si, and Ti, providing information on bond orientation or charge/orbital order with chemical specificity. One major focus of the endstation will be studies of spatio-temporal behavior using XPCS. XPCS will shed light on spontaneous fluctuations over time scales ranging from microseconds to seconds. Access to such time scales is important for studying how hierarchical systems with structures at multiple length scales evolve over time and their relation to material performance. The proposed endstation will have SAXS capabilities, x-ray diffraction at higher scattering angles, and x-ray reflectivity geometries. Furthermore, the energy tunability of this beamline will enable complementary x-ray absorption spectroscopy measurements needed to inform XPCS and resonant scattering experiments. Modular sample environments will be developed to enable in situ and multimodal approaches.

Current experimental characterization often lacks effective feedback to materials synthesis, and operando measurements remain challenging. Furthermore, advanced analysis supported by artificial intelligence and machine learning (AI/ML) is needed to decipher high-throughput experiments and multimodal measurements. Advancing multimodal studies is a long-term goal of the CMI TA—for example, seamlessly combining electron microscopy and soft/tender x-ray scattering/spectroscopy. In situ probes—such as a spin coater at beamlines, coupled with Raman, IR, or photoluminescence—also inform advanced manufacturing processes. The CMI TA aims to merge automated sample handling, high-throughput data acquisition, data compression, data visualization, and data analysis techniques and strategies developed together with 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

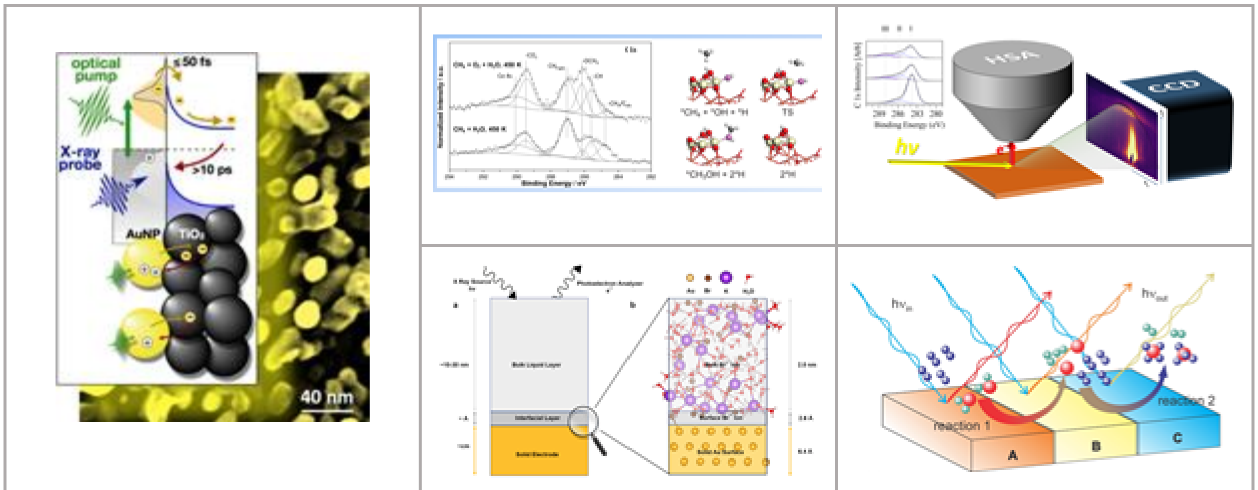

Fig. 3. Left: Optical laser pulses excite electrons in gold nanoparticles (AuNP) attached to a TiO_2 substrate. Short x-ray pulses measure how many electrons are injected from the AuNP into the substrate and monitor their return back to the AuNP [M. Borgwardt et al., *J. Phys. Chem. Lett.* 11, 5476 (2020)]. Top middle: Ambient-pressure x-ray photoelectron spectroscopy (APXPS) investigation of catalytic methane-to-methanol conversion reveals the significant promoting role of water in the process [Z. Liu et al., *Science* 368, 513 (2020)]. Bottom middle: Development of an analytical model informed by density functional theory (DFT) calculations that sample molecular dynamics configurations, enabling the direct simulation of measured APXPS spectra [J. Qian et al., *J. Chem. Phys.* 153, 044709 (2020)]. Right top: Multimodal approach using x-ray scattering and APXPS reveals correlations between structural and chemical transformations under operating conditions [H. Kersell, et al., *Rev. Sci. Instr. 92, 044102 (2021)*]. Right bottom: A grand challenge experiment that could be realized by imaging RIXS with multiple but correlated components and reactions probed simultaneously across a wide x-ray beam exposure [Y.-D. Chuang et al., *J. Synchrotron Radiat.* 27, 695 (2020)].

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 devices that operate on time scales of seconds to hours. Soft and tender x-ray beamlines with innovative scientific instrumentation and operando capabilities can probe dense environments with atomic and chemical contrast spanning a large spatiotemporal range and can detect correlated and inhomogeneous components simultaneously through advanced large-area imaging techniques, thereby providing unique fundamental information about these functioning mesoscale chemical devices. The utilization of hard x-rays in operando conditions contributes complementary quantitative structural and morphological information at length scales ranging from the atomic (a wide variety of x-ray diffraction techniques) to the nanometer (SAXS) to the micrometer (tomography) and has the potential to probe kinetic properties at millisecond to hour time scales. Such "micro- to nano-kinetic" measurements under operando conditions are essential to optimizing complex multiscale chemical and electrochemical devices. We aim to integrate these experimental multimodal spectroscopic capabilities with computational modeling techniques to develop complete models of chemical processes.

The Chemical Transformations TA 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. The high brightness of the upgraded ALS will enable the study of micro- and nanoscale systems with high temporal resolution in order to follow a chemical process in real time.

High-priority goals are as follows:

- Increased access and improved capabilities for users of high-brightness tender x-rays, which would facilitate in situ/operando ambient-pressure x-ray photoelectron spectroscopy (APXPS) experiments and sub-nm-length-scale x-ray scattering experiments at higher operating pressures and providing deeper probing depths.
- Development of imaging RIXS instrumentation to realize microscopic experiments across a large area with spatial and temporal resolutions down to the nanometer and nanosecond scales. Such instrumentation would enable the simultaneous detection of correlated chemical reactions with high spatial and time resolution.
- To address chemical dynamics and reactions in liquid environments by developing a dedicated combined APXPS and RIXS setup with microseconds to seconds temporal resolution and specificity to bulk and surface properties.
- Development of a suite of state-of-the-art, multimodal techniques deployed at bend-magnet beamlines advancing our scientific capabilities for probing interfacial chemistry, in particular for probing beam-sensitive chemistries:
    - APXPS research combined with an IR port would enable new multimodal science that simultaneously probes chemical states and vibrational dynamics.
    - Fast x-ray absorption spectroscopy in transmission (FAST) combined with ML would enhance the science of chemical transformations and materials discovery through new knowledge, synergy with other experiments, and materials projects.
- Realizing high-pressure soft x-ray spectroscopy experiments for in situ/operando studies of high-pressure chemistry in energy devices. Soft x-ray experiments typically require a UHV environment, but recent ALS innovations have shown that it is possible to host the samples in localized high-pressure conditions for soft x-ray experiments. It is anticipated that liquid-flow systems can operate under 10–250 bar pressure for soft x-ray absorption spectroscopy and RIXS experiments, and preliminary tests have been performed on hydrogen storage materials under H_2-pressures of 5–10 bar.
- Development of a unique high-resolution RIXS tool (<5 meV) in the 100–200 eV region for heavy elements and critical materials studies.
- Development of AI/ML algorithms to process large data sets to meet the requirements for handling multimodal, high-throughput, and spatially and temporally resolved data.

2.1.4 Earth and Environmental Systems

Earth and environmental scientists use hard, tender, soft x-ray, and IR beamlines at the ALS with high 2D and 3D spatial resolution and chemical sensitivity to disentangle complex processes in the geosphere, atmosphere, and hydrosphere. Capturing these processes in situ, in two and three dimensions, and under environmentally relevant conditions of temperature, pressure, and pH, with commensurate time resolution, has become critical. Complex, multimodal, in situ capabilities in variable environments enable core ALS research in geoscience. Spatially resolved x-ray diffraction (XRD) in a laser-heated diamond-anvil cell elucidates the stability, sequestration mechanisms, and reaction pathways of volatile phases such as CO_2 or H_2O within the geochemical context of planetary interiors (Fig. 4a). Hard x-ray microtomography allows 3D imaging of geological samples at the micron scale, such as pore spaces and their connectivity in oil- and gas-hosting shales or characterizing the texture of pyroclastic fragments to understand volcanic eruption types (Fig. 4b). Laue microdiffraction enables the discovery of new rare minerals which are otherwise difficult or impossible to study with other techniques, and 2D strain maps based on Laue microdiffraction enable the recovery of paleo-strains in rocks at the micron scale (Fig. 4c), which provides a quantitative understanding of rock deformation with implications for seismogenesis. X-ray fluorescence elemental mapping and x-ray absorption spectroscopy (XAS) in the hard and tender x-ray energy ranges allow mapping of the top nine elements present in the Earth's crust (O, Si, Al, Fe, Ca, Na, K, Mg, and Ti) to determine the distribution of major and trace metal(loids) and their chemical speciation at the micron scale, notably in groundwater, soils and associated critical minerals (rare earth elements), and geomicrobiological samples (Fig. 4d), for bioremediation applications, for instance, using sample cryogenic cooling capabilities compatible with cryo-electron microscopy and micro-CT cryogenic capabilities. Soft x-ray nanoprobes such as STXM are used to investigate marine particles, aerosols (Fig. 4e), and biominerals and can by complemented by x-ray ptychography, which provides high spatial resolution in 3D and spectral sensitivity to obtain metal oxidation state and crystal orientation, respectively. PEEM enables the characterization of meteorites and growth mechanisms of nanoscale precursors of biominerals. Finally, IR spectroscopy and imaging are frequently deployed for the study of diamond inclusions of high-pressure phases, meteorites, and other space sample returns like interplanetary dust.

A common thread running through most of the cutting-edge research activities in the Earth and Environmental Systems TA (EESTA) is a move from static postmortem studies to in situ, operando, and time-resolved 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. Furthermore, Earth and environmental systems are hierarchical over a range of length scales. Morphology, chemical speciation (including oxidation state), and elemental distribution can be determined with high spectral resolution and detection sensitivity using high-brightness x-rays. Because of their higher penetration and sensitivity to the major elements present in Earth's crust minerals, tender x-rays from a high-brightness ALS-U insertion device are also of particular interest for this TA. The future Tender fluorescence nanoprobe beamline is expected to reach the top nine elements that constitute the Earth's crust. The core focus of the EESTA is to enable a correlative and multiscale approach between x-ray and electron microscopy techniques to, for instance, further our understanding of the structure and function of microbial consortia in metal-contaminated environments to predict the stability and reactivity of these toxic metals.

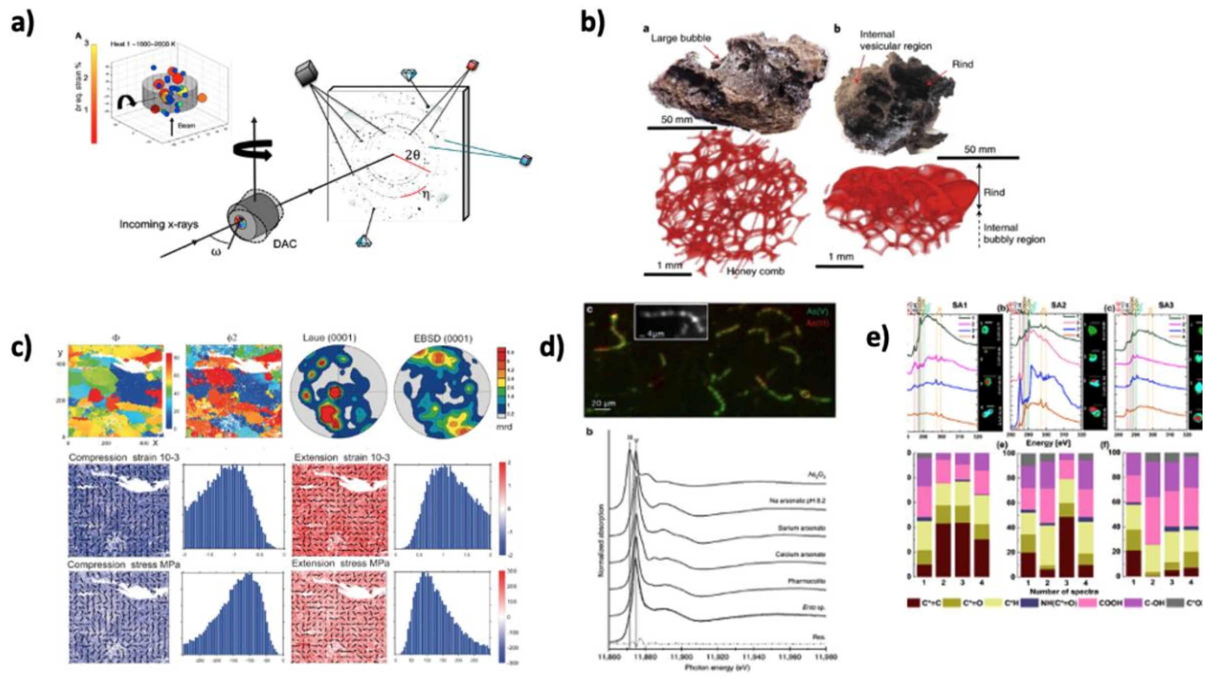

Fig. 4. a) Schematic and main result of a multigrain XRD experiment in a diamond anvil cell. The multigrain technique bridges the gap between a perfect single crystal and a perfect powder, allowing quantitative determination of orientation and the spatial relationship between several individual grains (up to ~100) originating from a pressure- and temperature-driven phase transition or chemical reaction [B. Chandler et al., *Science Adv.* 7, eabd3614 (2021)]. b) Vesicular pyroclasts with unbroken and reticulite-like fractured regions (top). X-ray microtomography of fragments to examine their texture, providing insights on vesiculation and volcanic gas cooling processes (bottom) [A. Namiki et al., *Nat. Geosci.* 14, 242 (2021)]. c) Microstructure of a metamorphically deformed quartz sample obtained by Laue x-ray microdiffraction. Top: Orientation distribution is given by Euler angles Φ and φ2, and the (0001) pole figures. Bottom: maps of the magnitude of the principal residual strain axes, with the arrows indicating the direction of the local strain axis. The histogram shows the distribution of strain magnitudes. [H-R. Wenk et al., *Geophys. J. Inter.* 222, 1363 (2020)]. d) X-ray fluorescence elemental (inset) and chemical maps of arsenic in sponge-associated filamentous bacteria (Entotheonella sp.) at 95 K (top) and arsenic K-edge XANES (95 K) of Entho. sp. (LSQ fit 47% sodium arsenate, 39% pharmacolite and 14% As_2O_3) demonstrating that this bacterium mineralizes As(V), suggesting it acts as a detoxifying organ for the sponge (bottom) [Keren et al., *Nat. Comm.* 8, 14393 (2017)]. e) Free tropospheric aerosols that nucleate ice clouds were examined at the ALS. (a-c) C K-edge STXM/NEXAFS spectra obtained from four representative types of particles for each sample. The carbon map to the right of each spectrum shows the STXM/NEXAFS composition illustrating the internal particle heterogeneity. (d–f) Relative contribution obtained from each of the C-functionalities observed for the respective spectra. Here, the numbers indicate the identity of particle's spectra, C-map, and relative contribution in each sample. [N.N. Lata et al., *ACS Earth Space Chem.* 5, 3499 (2021)].

Research in Earth and environmental sciences in the US is funded by several separate federal agencies, including DOE, the National Science Foundation (NSF), the National Aeronautics and Space Administration (NASA), and the US Geological Survey (USGS), with by far the largest amounts being contributed by NSF and NASA. This broad federal funding represents a tremendous opportunity for the ALS, since it not only allows the ALS to contribute to a very broad range of geoscience but also offers opportunities to raise supplemental funding for research and development, one being the NSF-funded Consortium for Materials Properties Research in Earth Sciences (COMPRES). The EESTA is seeking and fostering collaborations with LBNL's Earth and Environmental Sciences Area and to respond to DOE

Energy Earthshots and critical materials and minerals priorities, but also outside the DOE complex among NSF-, NASA-, and USGS-funded PIs and organizations. Such an inclusive approach will help ALS beamlines with a focus on Earth and environmental sciences to participate in a variety of recent and anticipated funding opportunities from within DOE (e.g., carbon reduction and critical minerals) and outside DOE (e.g., NSF's Earth in Time vision and NSF's Division of Earth Sciences program solicitation for a synchrotron community facility).

High-priority goals for this TA include the following:

- Develop cross-platform sample environments for measurement of materials under cryogenic/operando conditions using hard and soft x-ray imaging, spectroscopy, diffraction, and scattering techniques.
- Expand in situ capabilities in terms of P-T-atmospheric conditions to offer appropriate tools to respond to DOE's carbon mineralization and critical mineral priorities. Expanding in situ, operando, and cryogenic imaging and spectroscopy capabilities will be crucial to address these two areas.
- Optimize and expand existing measurement facilities across the spectrum for collaborations and general use to address NSF's Earth in Time decadal report and vision.
- Drive the science case and specifications for the new ALS-U Tender nanoprobe, including educating the community, acquiring funding, and performing R&D.
- Develop and implement new capabilities such as multigrain analysis and structure solution to be broadly available to the Earth and environmental science community.
- Develop an infrastructure for computing and data access which facilitates correlative analysis of data acquired by users across multiple beamlines and methods.

2.1.5 Biosciences

Over the next five years, the ALS will continue to provide unique opportunities to address and respond to national priorities such as climate change and human health, exemplified by the COVID-19 pandemic. Key to the ALS impact to these global challenges are strong and vibrant programs in biology. With the synergy of Biosciences TA (BioTA) capabilities with other regional resources, LBNL is exceptionally positioned to address these and other pressing topics (e.g., diseases, biofuels, and biomaterials).

Most of the BioTA-related programs receive funding external to the ALS and rely on Participating Research Team (PRT) beamlines. BioTA is a forum for ALS and PRT scientists to develop a common strategy for biosciences at the ALS. An immediate challenge the BioTA must address is preserving funding through the ALS-U Project and coming out stronger after the ALS-U dark period. The BioTA is seeking ways to take advantage of the ALS-U dark period to upgrade its resources and make use of the higher-brightness light provided by the upgraded ALS. The BioTA will work aggressively with the ALS to ensure every program has an upgrade plan and exits out of the ALS-U Project with new and improved capabilities.

Some of these activities have already begun. The Gemini macromolecular crystallography (MX) beamline, managed by the Berkeley Center for Structural Biology (BCSB), is funded to develop one, and likely two, branchlines with a view of what will be possible with the upgraded ALS. Brighter beams will enable the collection of better data from smaller crystals. ALS-U high-field bends are somewhat softer but much brighter than ALS superbend magnets, and optics optimized for ALS-U could more tightly and efficiently focus the light at MX beamlines in Sectors 4, 8, and 12. Initial R&D to develop upgrade plans has begun. The Structurally Integrated BiologY for Life Sciences (SIBYLS) SAXS beamline staff are developing plans to upgrade their endstation and perhaps reduce the optimized experimental energy to better overlap with ALS-U optima. For larger spatial scale imaging, building laser-induced fluorescent-based capabilities to be deployed side-by-side with x-ray tomographies on the same samples will greatly enhance the x-ray tomography programs and provide information even during the ALS-U dark period. These latter activities are currently unfunded, and finding appropriate funding sources must begin.

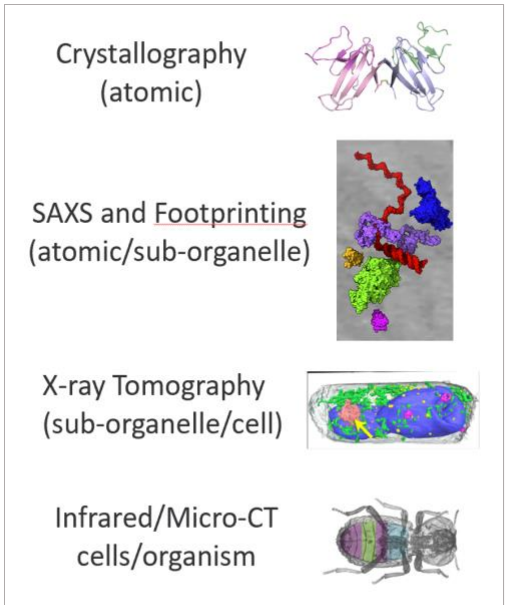

Fig. 5. Multiscale view of how synchrotron light provides insights into biology. Crystallography provides atomic details, x-ray footprinting delivers inter-macromolecular information, SAXS looks at the sub-organelle scale, x-ray tomography can characterize whole cells, IR delivers inter-cellular details, and micro-computed tomography (CT) offers organism-scale views.

The collective BioTA can help each of its members plan, fund, and execute an upgrade plan through integration into a multiscale view of biology (Fig. 5). Crystallography provides atomic details, x-ray footprinting delivers inter-macromolecular information, SAXS looks at the sub-organelle scale, x-ray tomography can characterize whole cells, IR delivers inter-cellular details, and micro-computed tomography (CT) offers organism-scale views. In addition, several of these techniques are capable of describing overlapping temporal mechanisms. To enhance this multiscale asset of biology at the ALS, the BioTA will seek projects that apply all techniques to a related system, connecting atomic- to organism-scale phenomena. Biofilms and plants are natural targets for cross-beamline applications and address climate and health areas.

To further enhance BioTA science, we will be looking to support programs at the Joint Genome Institute (JGI), the Joint BioEnergy Institute (JBEI), the Molecular Foundry, and the University of California (UC), Berkeley. These world-class institutions study important systems that the BioTA can uniquely inform. The BioTA will serve to broaden the application of each individual technique and extend studies to new scales for more impactful results.

2.1.6 Instrumentation and Computing

The Instrumentation and Computing TA comprises instrumentation experts; beamline scientists; computing, networking, and AI and ML experts; and partners who advise the ALS about instrumentation R&D opportunities. 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. The most important capabilities to be developed have been identified by the Instrumentation and Computing TA to be the following:

- Improve the quality of and access to beamline optics and diagnostics to meet the requirements set by the orders-of-magnitude gains in coherent power from the planned ALS source upgrade.
- Develop x-ray detectors for high-speed data acquisition rates, with adequate data transfer and data reduction capabilities.
- Develop in situ and operando sample environments, with an emphasis on multimodal experiments on multiple beamlines and in conjunction with facilities like the Molecular Foundry.
- Implement autonomous experiment capabilities to enable more complex procedures, efficiently use the very limited resource of beamline scientists, and enable remote operations to reduce the burden on users.
- Apply ML and AI techniques for efficient discovery and understanding from multimodal spectroscopy, tomography, and scattering experiments.
- Link theory with experiment at the beamline through the development of digital twins.
- Advance network, computing, and IT safety/security technology at beamlines to enable scientific goals through an agile strategy.

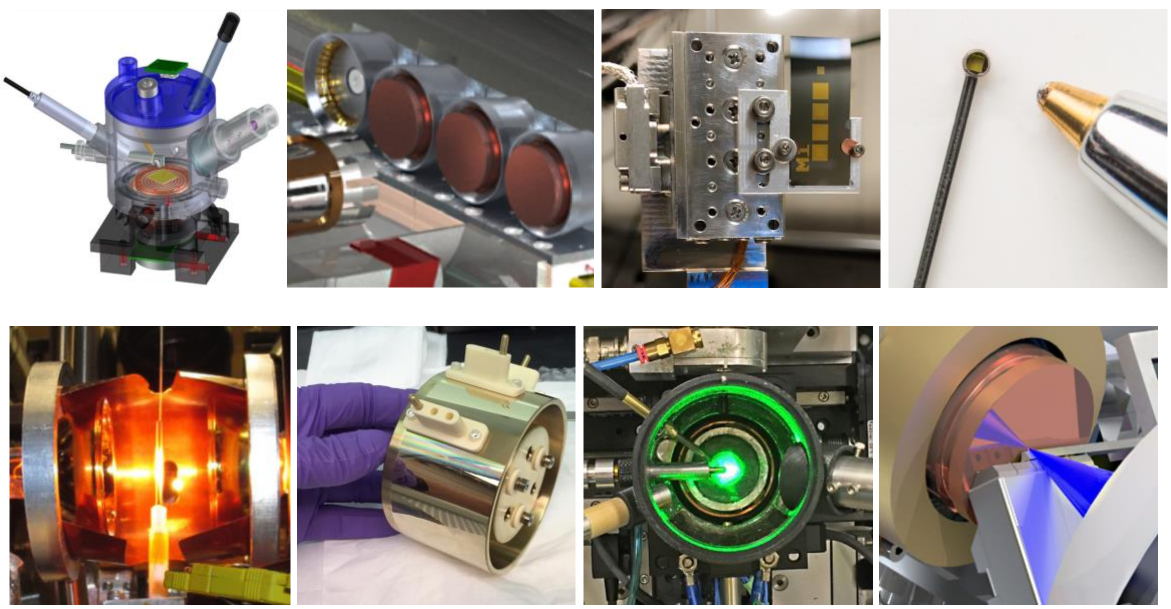

Fig. 6. Instrumentation developed at the ALS.

Beamline optics and Instrumentation. 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.

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

To preserve the diffraction-limited quality of the photon beam provided by the upgrade of the storage ring, we need to continue to improve our capabilities for the measurement and manufacturing of aspherical mirrors (diabloids), high-resolution grants, and diffraction optics such as zone plates.

Ex situ optical metrology. X-ray optics (mirrors and gratings) metrology is a foundational technology that has enabled the creation of optical elements in x-ray optical systems of diffraction-limited quality. Ex situ metrology enables investigation of contributions to optical performance from different spurious effects, such as surface figure and finish, vibration, and mechanical and temporal stability. Advances in mirror quality follow improvements in metrology, which occur through innovative instrumentation and fastidious attention to systematic errors via precise calibration and data reconstruction. Despite significant advances, metrology is challenged to exceed absolute accuracy levels much below 50 nrad in the slope domain and below 1 nm in the height domain. More investment in ex situ metrology is required, also to advance the optic accessibility via significant improvement of fabrication and performance optimization processes.

X-ray detectors. High-speed, efficient, and single-photon-sensitive detectors are central to ALS capabilities. Commercial availability of such detectors for the soft x-ray range has improved over the last decade, but it still lags well behind community needs and the capabilities of hard x-ray detectors. We will work with the ALS Detectors Program and other staff scientists to aid the development of the VeryFastCCD (a full-column parallel CCD sensor with 5 kHz frame rate) and also point detectors with picosecond time resolution for studying GHz dynamics in materials. Furthermore, we will explore options for making a pool of commercial detectors for general use or as contingency in case of detector failure.

In situ and operando sample environments. Operando multimodal sample environments are of utmost importance for collaboration-driven science at the ALS. Specifically, we need to develop in situ, multimodal probes to interrogate materials when they are evolving or out of equilibrium.

Many complex materials require the use of multiple techniques. To investigate the intricacies of perovskite solar cells, for example, it is important to be able to perform x-ray scattering, IR, and photoluminescence experiments in situ during the spin-coating process. The dynamics of novel devices for quantum information science (QIS) or energy storage, for example, occur on a hierarchy of length scales that cannot be captured just by integrative transport measurements. New tools are required that directly probe the order and dynamics of charge carriers in such devices at the crucial length scales, in their natural habitat, with current flowing and wires attached. Making such sample-modification environments available with multimodal approaches will drastically increase the impact of existing ALS beamlines.

Furthermore, 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.

Experiment automation. Increasing automation will enable a cohort of new possibilities for experiments at the ALS:

- The ability to run experiments remotely.
- A drastic increase in scientific output capacity due to the ability to run experiments more efficiently and without human intervention necessary at each step.
- Advanced planning of experiments, leading to a more efficient use of beamtime.
- The ability to take advantage of AI/ML to drive autonomous experiments.
- The ability to reliably capture metadata about experiments, leading to more “FAIR” data (findable, accessible, interoperable, reusable).
- Better reproducibility and reliability of experiments based on thorough characterization (calibration) of the setup and data deconvolution based on the calibration.
- Reduction in human error during experiments (especially relevant for experimental campaigns that often require long, overnight hours).

For all these reasons, increasing automation is a key priority. Significant work is required to build robust automated systems, both in hardware and user-friendly software. Hardware includes robotics and computer-controlled motors, actuators, and experimental tools, along with sensors and cameras that work together reliably. Software includes systems that allow end-to-end tracking of samples (including samples shipped to and carried onsite), sample changing, alignment, and comprehensive recording of beamline and instrumentation parameters.

Rather than leaving the design and deployment of automation to each beamline scientist, our strategy will be dedicating specialists to developing hardware and software systems that can be adapted and deployed across beamlines. This work should leverage the development that has been done at several beamlines and will also coordinate with work being done at other facilities. Similar developments are also vital for increasing the efficacy of ex situ characterization, tuning, and performance optimization of the beamline optics and optical systems under development.

Community-focused machine learning and artificial intelligence for the ALS.

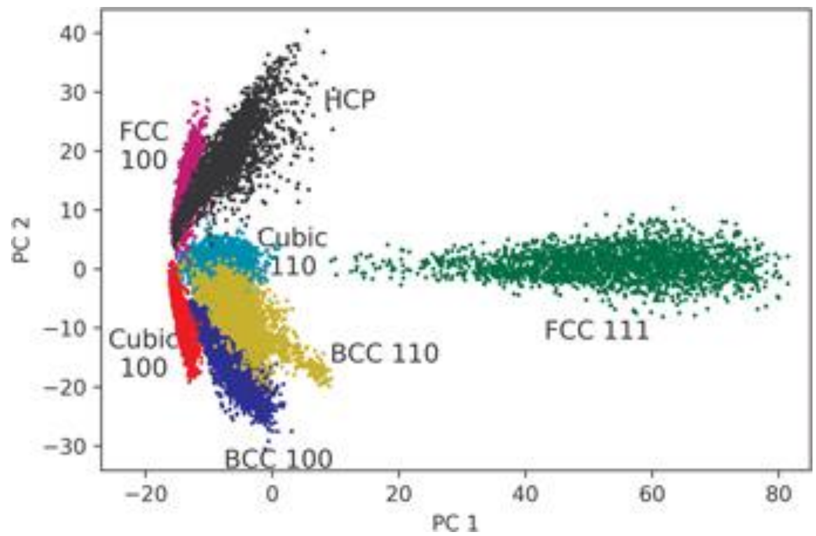

Fig. 7. Convolutional Neural Networks classification of nanoparticle orientation in a thin film learned by grazing-incidence SAXS (GISAXS) patterns. The network was trained on thin films with a success rate of 94% [S. Liu et al., *MRS Communications* 9, 586 (2019)].

There is tremendous potential in using AI and ML techniques for coordinating complex experiments and data analysis. AI/ML can aid in building reproducible science, optimize the use of experimental facilities, increase transparency, and widen the pool of available knowledge, allowing us to find and illuminate intricate scientific relationships inherent in the collected data. Advances in scientific machine learning offer an opportunity to leverage the commonalities, scientific insights, and collected experience of the larger scientific user facility community. Taking advantage of this community will enable an integrated view that maps the broader scientific context and delivers an aggregate view of the strengths and weaknesses of the field as a whole. The ALS focuses on developing community-driven AI/ML tools to aid user-facility scientists and users. Realizing the benefits of cross-facility AI/ML efforts requires enhancements to beamline data-acquisition systems, metadata databases, and data-storage systems. Acquisition systems that can integrate with software frameworks that are common to data science will help bring AI to the beamline directly. Feeding metadata databases with beamline information as it is captured will allow users take advantage of AI and ML tools during analysis.

Digital twin. A digital twin (DT) is defined as an in silico simulation of an in situ and operando experiment that can simulate outcomes, investigate failure modes, or rapidly prototype and test protocols at ALS beamlines. Our goal will be to expand the integration of theoretical and experimental exploration into DT of systems of interest, for example, chemical processes at solid/gas, solid/liquid, and solid/solid interfaces, or in studies of the role of defects on correlated states of superconductors, topological states, or quantum coherence. The DT will provide robust feedback between material and chemical synthesis, experiment, and theory driven by AI/ML. This effort will advance our ability to probe and understand emergent phases and dynamics that arise across fields when there are many configurational degrees of freedom and when competing interactions with comparable length and energy scales are involved. These innovations can significantly accelerate new scientific discoveries beyond what we would traditionally accomplish by comparing experiments to established theoretical insights and numerical simulations.

Computing. The beamline information technology (IT) infrastructure needs to be updated to support changes in the way science is performed at the ALS. Currently, the IT system is very open and many IT decisions are left up to the beamline scientists. This poses some problems. Control systems should not be exposed to the internet at large. Data-management tools developed for one beamline are fairly network dependent and cannot easily be applied to other beamlines. Remote work will become more popular and requires better security planning. Multi-beamline and multi-facility measurements are currently hampered by decentralized storage of experimental data and metadata. The ALS is studying how new infrastructure at beamlines could meet these challenges before and after ALS-U.

2.2 ALS Upgrade and long-range accelerator planning

ALS-U is an ongoing major upgrade of the ALS that will endow the light source 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 CD-0 status, the first milestone in making ALS-U a reality. In December 2019 the project received CD-3a approval (long-lead procurement), and in April 2021 it achieved the CD-2 milestone (approved performance baseline). Most recently, the project received approval to start construction (CD-3) in November 2022.

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 the booster- and storage-ring radio frequency (rf) systems, the accelerator control systems, the timing system, most of the magnet power supplies, and the linac high-power modulators, were already replaced with present state-of-the-art technologies, and upgrades of additional major systems, such as the replacement of the linac rf controls and other main systems, 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 instrumentation and an ML-based application for improving the stability of the performance of the ALS accelerators.

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.
- The annual User Meeting is organized by the UEC and includes topical workshops and tutorials planned collaboratively by our staff and users. 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. The User Meeting is currently held as a virtual meeting via video conferencing.
- In addition to the regularly held User Meeting, we also convene special ad hoc workshops and town halls. The ALS Thrust Areas organize Innovation Forums for members of our community that are designed to lead to new collaborations, educate the community about new capabilities, and inform the ALS science and instrumentation strategy.
- Approved Programs (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 beamtime 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
- Access a secure portal to use beamline computers remotely
- Link to LBNL human resources and foreign-visit and software applications to efficiently meet DOE requirements

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. A federated identity management system has been implemented that allows users and staff to access ALSHub either using their existing LBNL, ORCiD, or InCommon ID. The ALS currently undertakes a rolling program of assessment and, if necessary, upgrades 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 five years, it is anticipated that the ALS will do the following:

- 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 such as ORCiD and DOIs, to add metadata to scientific data collected at the ALS. This will be necessary to enable streamlined mechanisms of data analysis and storage. APIs to give staff targeted and secure access to User Office database information have already been developed.

2.3.2 Strategic planning

Fig. 8. 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 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.

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 ALS Science Council, an ALS internal review board, advises ALS management about prioritizing resources, for example for beamline and endstation projects, administers the selection process for the ALS fellowship programs (see section 2.3.5) and identifies speakers for the ALS Colloquium, a regularly occurring set of seminars featuring a diverse group of high-profile speakers.

The ALS SAC is composed of national and international experts from many disciplines and meets at least twice per year to provide high-level advice to LBNL and ALS management. The ALS strategic plan and resulting 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, including current and potential users, DOE, other synchrotron facilities, and the general public. 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 these audiences, and also plays a critical role in user communications and internal staff communications.

The ALS's primary distribution channels for news and updates include the ALS website and a monthly newsletter, ALSNews, which has over 5,000 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 uses in combination with multimedia to better reach a breadth of audiences, including the general public and younger demographics. The ALS also offers online forums to apprise users of critical news and opportunities involving ALS-U and receive feedback.

The Communications Group continues to build out features on its public-facing website that make the content more accessible and to highlight capabilities and pathways for collaboration with our scientists. The group is now working with Photon Science staff to launch program websites that will complement the public-facing site by offering more detailed technical information about beamline offerings and techniques geared towards users. In addition, brief fact sheets on beamline techniques will be developed and posted to the website and printed for distribution around the ALS facility and at in-person and virtual conferences.

Another focus of the Communications Group 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. The Communications Group maintains an intranet site that is accessible to anyone with a Lab login. The intranet comprises both dynamic and static content—an archive of timely email updates and event announcements as well as resources the staff need, including safety information, administrative guidelines, and document repositories. The recently instituted ALS all-to-all (all-staff) meetings serve as a central forum for internal communications. The Communications Group produces a summary of the main points as a text-based complement to video recordings of the meetings.

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 and Protocol 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. The Communications Group also provides tours and high-level overviews of the

ALS to visitors invited by the Lab's K–12 and Workforce Development and Education offices, educating students and exposing the next generation of potential scientists to synchrotron career options. When appropriate, the Communications Group also connects these visitors with ALS staff, who provide a more specialized perspective on the facility. The Communications Group also offers internal tours, to allow LBNL staff members to become more familiar with the research done at our facility. In light of the pandemic, a virtual tour was developed as part of the Protocol Office's virtual LBNL public tour, reaching a global audience over video, and is likely to remain part of the ALS's outreach portfolio. The Communications Group also recently revamped an educational poster on how the ALS works and is expanding on the content by developing a web-based tutorial.

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. As well, it will become increasingly important over the next few years for the Communications Group to recommend and support communications to users and staff around the logistical impacts of the ALS-U Project, including key project updates and impacts to user and other ALS operations. A multi-pronged strategy encompassing the ALS website and intranet, newsletters and other email distributions, virtual town halls, and in-person and other virtual meetings is being implemented.

The Communications Group also works with ALS scientists to ensure that they have the outreach resources they need to 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 IDEA framework encompasses several task forces and an IDEA Committee (Fig. 9). 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, two at-large representatives elected annually by ALS staff, and an early career representative elected annually by ALS postdocs and students comprise the IDEA Committee, which coordinates task force activities and makes recommendations on policy changes to the ALS leadership. The IDEA framework is flexible, allowing task forces to sunset or be created to address new priorities.

The IDEA Committee and its task forces are working 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. Over the past few years, the ALS IDEA Committee and task forces have:

Fig. 9. IDEA task force structure.

- Led a community process to refresh the ALS's mission statement and identify a set of core values;
- Administered three annual ALS climate survey and identified areas of success and areas that need improvement;
- Publicized harassment and discrimination reporting policies and contact information;
- Developed guidelines for LBNL Spot Awards, which acknowledge and reward outstanding individual and/or team workplace contributions that occur on a day-to-day basis;
- Introduced improvements to the performance review process;
- Broadened the impact of ALS-developed best practice guidelines for recruitment and hiring processes by developing Energy Sciences Area-wide guidelines in collaboration with the Molecular Foundry;
- Established a mentorship program in collaboration with the Energy Sciences Area to establish a culture of support for staff through one-on-one mentor–mentee relationships;
- Initiated monthly discussions of IDEA principles at the weekly all-staff "all-to-all" meeting; and
- Developed a work-life balance statement that articulates our current values and helps guide supervisor and employee discussions and decision-making processes at the ALS.

Future priorities include continuing to institutionalize the ALS core values and to assess and refine improvements that have been implemented. Some specific goals for the next year include publicizing Lab-wide career development and promotion resources and programming and identifying ALS-specific areas that need improvement; recommending and implementing improvements to gender equity; tailoring the hiring guide for operations and postdoctoral hires; developing mechanisms and guidelines for internal and external award nominations; and establishing a formal mechanism for employee–supervisor work-life balance discussions.

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 annually. The 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 the user community in strong collaborations.

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

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.

Accelerator and 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. The lead floor operator position assists the operations supervisor in accomplishing these tasks. The radiation safety program at ALS is overseen by the lead radiation physicist, who works in conjunction with floor operators, review committee chairs, and technical groups to protect people from harmful effects of exposure to ionizing radiation. A second radiation physicist position has been added to assist with ALS and ALS-U work, and a shielding policy for ALS-U has been developed to inform the designs for new shielding for the upgrade. The ALS recently updated the Unreviewed Safety Issue procedure and is routinely screening issues to ensure the operating envelope defined in the Safety Assessment Document and Accelerator Safety Envelope is not exceeded.

The ALS Safety Configuration Control (ASCC) software application was initially designed to track beamline statuses, key-enables, safety inspections, radiation surveys, and work authorizations. The software has expanded to include various schedules, ALS procedures, and reviews and is under continued development to manage annual tests and the beamline review process. Additional training on ASCC is currently in development. The system was recognized as a noteworthy practice during the FY22 Triennial Accelerator Safety Review.

Annual Beamline Safety Day. A full evaluation of hazards at the beamlines is scheduled annually, 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. Issues that require correction or improvement are assigned and tracked with software. During the COVID-19 pandemic, much of the Safety Day activities were moved to a week-long safety effort to reduce crowding at the beamlines and to accommodate staff schedules during restrictions on employee headcount at the Laboratory. This practice is continuing, in order to accommodate schedules and ensure adequate time for evaluation of safety and related systems. The ALS Safety Group has recently begun safety walkthroughs of technical spaces along with corresponding staff members, with the goal of evaluating each lab and shop semiannually.

Training and communication. The ALS training program continues to grow with new courses. The required safety course for badge access, ALS1001, was overhauled to provide broad content, more interaction, and to target the various audiences who enter the ALS facility, including users, vendors, and emergency staff. New hutch access training has been rolled out that includes interactive, online training and specific on-the-job training for each hutch. The ALS radiation safety course, ALS 5005, is in the middle of a major update that includes lessons learned.

A new Division Safety Committee was formed in FY22 to have broad representation from ALS and ALS-U managers with the mission to solicit and distribute timely concerns, issues, best practices, and lessons learned with all ALS and ALS-U staff. Committee members also are encouraged to provide input into division self-assessments and participate to ensure institutional assurance deliverables are met.

A safety minute has been incorporated into the weekly all-staff “all-to-all” meetings, and various staff members have presented safety topics to enhance awareness and promote a health and safety culture.

Continued user support. The ESAF, which is the online ISM evaluation form for users, is used to coordinate the work of all users, including users of beamlines supported by PRTs, to achieve floor-wide user coverage. Ongoing improvements have been made in the ESAF to enhance early communication between users and ALS safety staff. Online training is being 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 has been 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
ALS injector upgrade Phases 1 and II (includes an upgrade of the low-level rf (LLRF) controls for the electron gun, linac, and booster, an upgrade of the sub-harmonic bunchers' rf amplifiers to solid-state technology, and an injector timing upgrade)	AIP	FY25	Phase I to be initiated in FY23
Equipment protection system (EPS) upgrade	EQU	Sector 5 in FY23; remainder TBD	Sector 5 is funded and underway. Other sectors remain to be completed and are dependent on funding and resource availability.
Radiation safety system (RSS) upgrade	EQU	TBD	Prototype system initiated in Sector 3. Other sectors remain to be completed and are dependent on funding and resource availability.
Online radiation-shielding configuration control Phase I, II and III	OPS	FY23	Phase I and II completed; Phase III funded and initiated
Storage ring utilities upgrade	AIP	FY23	Five work packages completed; one still in progress

AIP: accelerator improvement project; EQU: equipment project; OPS: operations project

A number of projects in this category will be completed or initiated during the next five years. Strategic attention and priority are 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:

ALS injector upgrade Phases I and II. After the successful replacement of the legacy linac modulations, the upgrade of the ALS injector subsystems will continue in two phases. In Phase I new rf amplifiers based on state-of-the-art solid-state technology will replace the legacy tube-based amplifiers of the 125 MHz and 500 MHz linac sub-harmonic bunches. Phase I also includes the start of the upgrade to digital technology of the legacy LLRF controls for the linac sub-harmonic bunchers, the linac accelerating sections, and the booster. These upgrades will be completed in Phase II, together with the upgrades of the electron gun controls and the injector timing. The ALS injector upgrades will improve reliability but also significantly improve the overall performance and stability of the system.

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 relay-based 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 was initiated in FY22 and will continue in the years to come, with the completion date dependent on workforce and funds 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 logic. 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 has been initiated by the development of a prototype system for Beamline 3.3.1. Other sectors remain to be completed, and the continuation of the project is dependent on funding and resource availability.

Online radiation shielding configuration control. ALS beamlines use a complex and custom set of radiation shielding arrangements that require careful configuration control to avoid undesired personnel radiation exposure. The previous control system was based on a number of physical forms that needed to be filled out and linked together depending on the particular beamline at which the radiation shielding operation was being performed. Phase I of this project, completed and in operation, moved the whole shielding configuration control system to a computer-based online application, effectively mitigating the risk of human errors while performing these critical operations. Phase II, also completed and in operation, extended the configuration control to areas other than shielding, and Phase III, funded and initiated, includes the support and management of the activities related to the Accelerator Review Committee and of the Beamline Review Committee, which control the safe execution and operation compatibility of accelerator and beamline projects.

Storage ring utilities upgrade. A number of utility systems and rights-of-way are being upgraded and/or relocated to accommodate ALS-U. Issues of physical interference, capacity, and capability are being addressed.

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	FY23–24	Funded and initiated.
Development of next-generation beam position monitors (BPMs)	OPS	FY23–24	Approved and initiated.
Machine-learning applications for the ALS accelerator	OPS	Continuous effort	

AIP: accelerator improvement project; OPS: operations project

Despite the increasing commitment of the ALS workforce to reliability-improvement activities in preparation for ALS-U, several accelerator projects targeting performance improvements of the present ALS to ultimately provide users with a better-quality photon beam are planned in the years preceding the ALS-U dark time.

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 FY23–24. The upgraded rf distribution will provide much higher operational flexibility and performance stability to both the current and upgraded ALS.

Development of next-generation beam position monitors (BPMs). The position stability of the electron beam in the storage ring directly affects the stability of the photon beam and the spatial resolution of the beamlines. The pursuit of higher and higher spatial resolutions requires an electron-beam stability beyond presently achieved performance. Higher-resolution beam position monitors (BPMs) for electrons are necessary for next-generation diffraction-limited storage rings such as the planned upgraded ALS. In such rings, the electron and photon beam sizes dramatically decrease, requiring the development of higher-resolution BPM electronics. A project for the development of prototype BPMs with a performance that matches the needs of the upgraded ALS has been approved and is underway. Completion and testing of such prototypes are expected in FY23–24.

Machine-learning applications for the ALS accelerator. ML techniques are finding applications in nearly every field of human activity, including particle accelerators. At the ALS, a new activity was initiated in FY19 to develop ML accelerator applications to control and improve the performance of the ALS. The project, funded by the DOE Accelerator and Detector Research program (ADRP) of the Basic Energy Sciences program, and the DOE Advanced Computing Science Research (ASCR) program, successfully developed a new scheme using deep-learning techniques to effectively compensate for beam-size variations induced by insertion devices. The second phase of this activity targeted the development of ML-assisted, multi-objective optimization using genetic algorithms (MOGA). Results showed that the synergetic use of ML and MOGA can reduce optimization times in complex multi-variable, multi-objective problems by approximately two orders of magnitude. Several other ideas for accelerator ML applications are being explored, and continuation funds are being pursued from BES.

3.2 Photon-science projects

3.2.1 Beamline instrumentation projects under construction or in commissioning

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

Source point	Project title	Target com-missioning	Partner and funding	Scope and notes
7.0.1.1	COSMIC scattering	Continuing	DOE midscale, ALS EQU	Half-length undulator and SXR beamline for XPCS studies of spontaneous fluctuations in spin, quantum, and topological materials
2.0	Gemini	Continuing	HHMI, LBNL/MBIB, LDRD	Two high-brightness microfocus macromolecular crystallography branchlines to support structural biology targeting automated data collection from micron-sized crystals.
6.0.1	AMBER	Continuing	PNNL, JCAP, JCESR, ALS EQU	Repurpose undulator; in situ/operando high-energy-resolution and high-throughput RIXS studies of catalysis, earth & environment, energy conversion and storage
5.3.1	Tender SAXS & FastXAS	Continuing	ALS EQU	Development of Tender capabilities in preparation for ALS-U, plus novel controls pilot
6.0.1	AMBER-2	Start 2023	ALS EQU	Second branch for high-throughput RIXS
6.0.2	QERLIN	Start 2023	Moore Foundation, ALS EQU	Repurpose undulator; soft x-ray RIXS beamline & double-dispersion design for high throughput & resolution; spin & quantum materials
4.0.3	MERLIN upgrade	Start 2023	ALS EQU	High-energy-resolution beamline for ARPES and spin-resolved ARPES

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 development.

COSMIC (now)*.* Since 1995, the ALS has led the world in developing soft x-ray (SXR) STXMs. 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. It is currently available to users. This branch achieves image resolutions below 5 nm, combining 3D tomographic reconstruction with full chemical contrast. The second, scattering branch and endstation probe spatial correlations in spin and quantum materials in the time domain using SXR XPCS and speckle metrology, and commissioning of the endstation is continuing.

Gemini beamline (now). The ALS macromolecular crystallography beamlines provide high-performance hard x-ray diffraction capabilities, keeping pace with the changing needs of the structural biology community with outstanding scientific productivity. Driven by an in-vacuum undulator, the new high-brightness protein crystallography facility in ALS Sector 2, called Gemini, was funded by HHMI and employs a fully automated data collection pipeline to maximize productivity. Using a diamond beam-splitter, the beamline can accommodate two branchlines operating simultaneously, in parallel. One will operate at a fixed wavelength, while the other allows the photon energy to be tuned for multi-wavelength anomalous dispersion measurements. Commissioning of the first branchline is nearly complete, and design has begun on the second branch.

AMBER and AMBER-2 (now and 2023). The AMBER beamline is optimized for advanced-materials preparation and for multimodal, high-energy-resolution and high-throughput, operando analysis of interfacial and chemical processes and energy systems. Enabled by the repurposing of Sector 6, AMBER improves ALS capabilities and increases capacity in this area, providing in situ sample preparation with RIXS and XAS spectroscopies. AMBER has been 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 Innovation Hubs. Work has started on a second branch (AMBER-2) for high-throughput operando RIXS.

Beamline 5.3.1 (now). Beamline 5.3.1 is being recommissioned to host two new endstations. The first is for SAXS measurements at tender x-ray energies. This branch will host the development of instrumentation for the ALS-U Tender beamline, including sample environments for operando measurements. The second endstation will be for fast XAS for ultra-high-throughput and time-dependent XAS measurements for materials discovery. Beamline 5.3.1 is also our testbed for instrumentation controls upgrades. Looking to future control systems with EPICS and Bluesky, we are developing and deploying new tools in collaboration with other DOE light sources. Advances include autonomous measurements, experiments augmented by machine-learning techniques, new user interfaces, and modern, real-time visualization.

QERLIN (2023). Angle-resolved photoemission spectroscopy (ARPES) measures the coupling of electrons and holes to low-energy excitations, yet it can be difficult to identify which excitations lead to particular emergent properties. It is therefore 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 momentum space. In this context, one of the highest ALS priorities is to complete the commissioning of QERLIN, a new SXR RIXS beamline in Sector 6. QERLIN is based on a novel high-throughput optical design that multiplexes the incident beam across the face of the sample and the scattered beam across a high-resolution pixelated detector. This approach will deliver a 100-fold increase in throughput with a resolving power above 20,000, probing an entire photon-energy in vs. photon-energy out map in parallel. Offline setup and commissioning of the endstation and spectrometer has started while beamline construction is being completed.

MERLIN upgrade (2023). The upgrade now in progress on Beamline 4.0.3 will significantly improve the energy resolution, flux, and stability in the near term and into the future. This work prepares MERLIN for the ALS-U era, with new ARPES methodologies that require high brightness, flux, and energy resolution, including ultrahigh-energy-resolution spectroscopy, spin-resolved ARPES, and momentum microscopy. The design and procurement of improved optics and a new monochromator was recently completed. Installation is planned for summer 2023, followed by fall 2023 commissioning.

3.2.2 New ALS-U and ALS beamline projects

Table 4. ALS-U (blue) and ALS (gold) beamline (by location) and endstation (ES) 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 full-field imaging
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 nano-scale ARPES
4.0.2	Magnetic spectroscopy & microscopy	TBD	ALS	Reliability and brightness upgrade of beamline for spectroscopy, microscopy and resonant scattering
ES	Low-T SINS	TBD	ALS	Low-temperature and nanometer-resolved infrared spectroscopy setup for quantum materials research

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 several workshops organized by ALS-U and the ALS and by five crosscutting reviews in 2017–2018 that reviewed ALS beamlines. To maximize the scientific impact of the ALS upgrade, a synergistic 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-selection 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, and the ALS will build the endstations for these new beamlines. The project 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 Beamline 4.0.2, a beamline for magnetic spectroscopy and scattering that will be ready to utilize the 100 times greater brightness of the ALS after the upgrade, and is preparing for an enhanced low-temperature SINS endstation for the IR Program to directly address research needs in quantum materials.

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 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. The second branch will be optimized for coherence-requiring imaging techniques. XPCS experiments will achieve an improvement in time resolution of three to four orders of magnitude over the current ALS, while diffraction-imaging techniques promise measurements with up to 10-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 4.0.2 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 some mirror systems will be upgraded with brightness-preserving optics compatible with ALS-U. The ALS Photon Science Development team has developed a design package that will be executed when funding and resources have been identified.

Low-T SINS. The ALS is preparing 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. Cryogenic operations will allow this new endstation to directly address research needs in quantum materials.

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 novel soft x-ray detectors that enhance the facility's productivity and scientific reach. The program also helps to 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 on both branches of the COSMIC beamline at ALS. The next-generation VeryFastCCD has been tested on the COSMIC imaging beamline.

The *S*pectroCCD, a very-fine-pitch (5 x 45 μm^2) detector developed for 1D RIXS, and a 2D version, based on a back-illuminated CMOS sensor, has been recently deployed on the momentum-resolved RIXS (qRIXS) endstation for QERLIN. A higher dynamic range CMOS sensor was tested on the PEEM beamline. All of these developments benefit from our efforts in ultra-thin contacts and sensor processing.

Future soft x-ray detector advances will be needed to cope with the higher data rates provided by source and optics updates related 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.

These detector developments and adaptations are primarily supported by ALS operating funds. Workshops held every one to two years at ALS User Meetings and elsewhere collect community need and interest, driving our priorities.

3.4 X-ray optics and metrology

Optics for the new generation of high-coherent-flux beamlines have focusing capabilities that require a quality of mirror surface figures and grating patterns well beyond those of our current systems. Optical surfaces must be measured and controlled to fractions of a nanometer and tens of nanoradians, even under irradiation by intense beams, when cooled to cryogenic temperatures, and when subject to mechanical drift and vibration on the experimental floor.

3.4.1 Adaptive optics and wavefront sensing

Adaptive x-ray optics (AXOs) provide a way to optimize and control the x-ray wavefront, compensate for optical aberrations and misalignment, and shape the beam downstream. These flexible mirrors are central to the insertion-device beamline designs within the ALS-U project, and their fine-control is the subject of multi-lab research collaborations that include APS and UC Berkeley.

As feedback for AXOs, we have developed and tested a grating-based intermittent wavefront-sensing tool with picometer sensitivity levels that will be installed on new beamlines. The wavefront sensor was tested at soft x-ray wavelengths, on the COSMIC scattering branch, in 2021. Tests planned for 2023 will operate at tender x-ray and hard x-ray photon energies.

Relying on an array of piezo-bimorph actuators, shape control for adaptive mirrors is frustrated by creep, drift, and hysteresis. Working with scientists from UC Berkeley and APS, we have developed a control procedure based on machine learning that captures the dynamic behaviors and compensates for errors, promoting stability. We are continuing this work to be ready for operations of the upgraded ALS.

3.4.2 Soft x-ray and tender x-ray gratings

High-efficiency custom gratings are central to soft x-ray and tender x-ray monochromators, providing both focusing and dispersion for energy resolution. New applications and the increasing source brightness are driving us to pursue innovations in gratings that can achieve ultra-high resolution or high tender x-ray efficiency while preserving the wavefront quality for coherence-based experiments.

The new ALS QERLIN RIXS spectrometer is one such example requiring highly efficient x-ray gratings with a very high groove density. Nanometer-scale groove placement precision and a perfect, saw-tooth shape are necessary for high throughput. Yet the fabrication of such gratings is beyond the capabilities of traditional manufacturing. Leveraging the nanofabrication capabilities of LBNL's Molecular Foundry, we are developing in-house processes for creating advanced x-ray gratings. We have successfully demonstrated blazed gratings with groove density up to 6,000 lines/mm with diffraction efficiency close to theoretical predictions. Further improvement of diffraction efficiency via multilayer blazed grating development is underway.

Extending the operational energy range of grating monochromators into the 2–8 keV tender x-ray energy range is a recent trend in the field of synchrotron x-ray optics. These gratings require very shallow grooves, with low line density, and very low blaze angles. Such ultra-low aspect ratio structures are extremely challenging to make. We are developing processes for low blaze angle (LBA) gratings by iteratively reducing the groove depth of Si blazed gratings made by mature, in-house processes. Proof-of-principle experiments have shown blaze angles as small as 0.04°. Further R&D will improve the fabrication and extend the LBA process to full-size x-ray gratings.

Grating substrates significantly exceeding 6 inches in length, with groove placement accuracy below 10 nm, are exceedingly difficult to manufacture or procure, or they are beyond the capabilities of leading vendors. Furthermore, a worldwide supply-chain bottleneck has caused some delivery times to exceed two years for gratings that can be procured. With DOE funding, we are developing an in-house, prototype, laser-based grating-writing tool that overcomes many of the mechanical limitations of traditional grating ruling. With the substrate moving on an ultra-high-precision linear stage, our approach focuses a pulsed laser source to a narrow line, flashing exactly when the grating reaches the correct positions. The grating pattern is thus transferred into a photoresist coating for further processing. We are ultimately targeting 5–10 nm position accuracy across long grating substrates.

3.4.3 Cryogenically cooled, wavefront-preserving mirrors

The ability to cool x-ray mirrors, gratings, and crystals is essential to dissipate heat from optics under intense x-ray power loads. Now, with the advancing requirement of maintaining shape to nanometer tolerances under variable power loads, cryogenically cooled silicon optics have become an attractive solution and an active topic of collaborative research across the DOE light sources. What makes this so compelling is that silicon's coefficient of thermal expansion becomes zero at 125 K, meaning that for optics held near this temperature, beam-induced thermal distortions are negligible. All of the insertion-device beamlines in the ALS-U project will have cryogenically cooled mirrors as the first beamline elements to preserve the wavefront quality. In a DOE-funded cryo-mirror project, we are working closely with other light sources to study cooling methods and characterize any observable shape changes during the transition down to cryogenic temperatures.

3.4.4 Development of new mirror shapes

Recent advances in mirror metrology and fabrication enable optimized mirror shapes that fully exploit the ALS's high and increasing brightness with ALS-U. When the source is large, optical aberrations from cylindrical, spherical, or toroidal mirrors are tolerable. We have developed and are testing new, optimized mirror shapes to preserve the high brightness of the beam and the x-ray wavefront. The diaboloid is one such hybrid shape that combines a collimating parabolic tangential profile with a focusing sagittal elliptical profile. In protein crystallography beamlines, diaboloidal mirrors may lead to a thirty-fold increase in brightness at the sample. We are investigating ways to produce and measure these special mirrors.

3.4.5 Optical metrology

Before new mirrors are installed, careful ex situ testing and quality assurance tests must be performed at levels reaching the state of the art. We apply a host of visible-light metrology techniques that are under continual development at the ALS.

The ALS's dedicated X-Ray Optics Laboratory (XROL) is a cleanroom facility close to the ALS floor that houses a number of measurement systems. The newly commissioned Optical Surface Measuring System is capable of multi-trace (2D) surface-slope profiling with a proven tangential slope measurement accuracy of 30 nrad (ms for flat optics, and for significantly curved optics (radius ≥ 15 m), around 600 nrad rms. For next-generation optics, we need an absolute slope accuracy of 50 nrad (that would correspond to approximately 20 nrad rms) and a height accuracy of below 0.5 nm in many cases. In close collaboration with optics teams from other DOE BES facilities and colleagues around the world, we are developing new methods that should take us to these goals within a few years.

Significant effort is being dedicated to R&D on a new long trace profiler called "LTP-2020," capable of surface-slope metrology with an accuracy below 50 nrad (absolute) with both x-ray mirrors and also variable-line-space diffraction gratings.

We are developing tools and techniques for stitching interferometry, a real-space, surface-imaging and shape-measurement technique pioneered by leading groups in Japan. We view stitching as especially important for the characterization of monochromator gratings for high energy resolution (e.g., RIXS), and for tender x-ray applications.

3.5 Data management and computing

The Light Source Data and Computing Steering Committee (LSDCSC), composed of members from the five BES light sources, has evaluated and quantified 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 LSDCSC estimated that, collectively, these facilities will produce up to 1 exabyte (quintillion bytes) of data per year and will require a peek on-demand computing resources of 1 exaflop (quadrillion floating-point operations per second). The ALS alone is estimated to require much less than this—a mere 210 petabytes (quadrillion bytes) per year and 30 petaFLOPS during peak, numbers that even by themselves will require serious effort to achieve.

The LSDCSC 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 cross-facility 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, web-based graphical user interfaces for analysis, advanced data transfer solutions to large storage and compute facilities and soon seamlessly coupled with integrated ML 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, SciCAT, will allow users to view or download results during or after their beamtime. The web portal also allows users to seamlessly move their data into the Jupyter environment for further processing.

Table 5. List of data management, analysis, and workflow 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 using web solutions	The ALS is going to develop a fully web-based graphical user interface as an integrated platform for synchrotron data acquisition, management, visualization, and analysis. The program plans to: a) enable parameterized analysis using metadata from databases such as SciCAT, b) enable exploratory analysis using interactive visualization tools, and c) support workflow-driven data processing and machine-learning solutions powered by Dask/plotly and typescript/react.
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 web 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. The ALS is using a software called SciCAT, which is developed by multiple synchrotrons across Europe.
RAC	RAC is a new tool that enables secure remote access to ALS beamline computers via a portal that is embedded in ALSHub. The Computing Program is planning to expose the web-based beamline graphical user interfaces in the RAC as well.
Jupyter hub environments	The ALS is currently developing a solution to connect jupyterhub directly to SciCAT with the single click of a button. On top of Jupyter, several graphical user interfaces have been developed.

3.5.2 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.

The ALS is developing a collaborative ML platform for scientific discovery in collaboration with other BES light sources and nanoscience centers and participates in projects funded by the 2020 DOE call for "Data, Artificial Intelligence, and Machine Learning at DOE Scientific User Facilities (MLExchange)." Led by the ALS, a set of tools is being developed to make ML architectures and models available to users and facility scientists. One of the milestones is to develop a user-friendly interface to manually or automatically label data that can then be fed into ML models to speed up data analysis and materials characterization. A layout of the MLExchange architecture can be seen in Fig. 10.

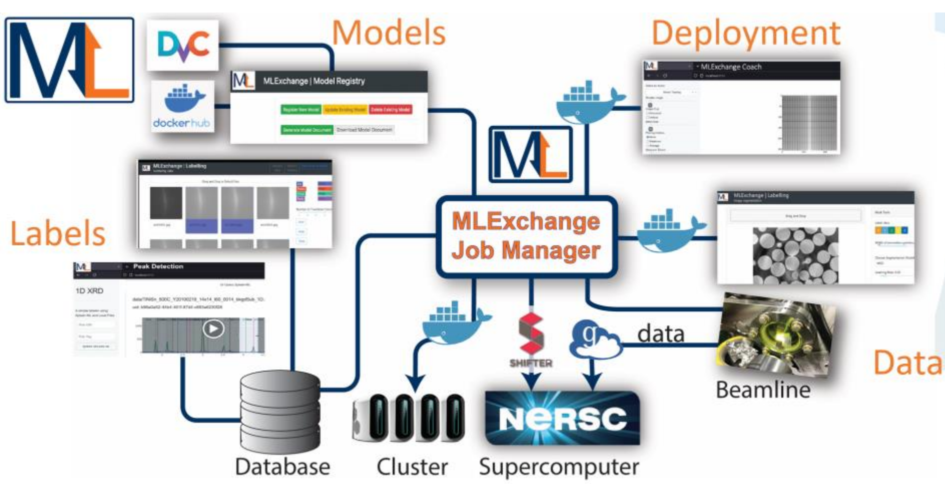

Fig. 10. Infrastructure diagram of the MLExchange framework.

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

Tools	Description
Electron beam size stabilization	The ALS has developed 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.
ML platform for scientific discovery	Research and develop the construction of new mechanisms for data labeling and to automatically extract features.
MLExchange: Label Maker	MLExchange has developed flexible tools to label scientific images. The application consists of three individual web applications: a) Label Maker, a visual application to create labels, view scientific data, and label data using a supervised approach, b) Data Clinic, an unsupervised solution to accelerate data labeling and develop labels easily in Label Maker, and c) ML Coach, a convolutional neural network (CNN) solution to classify labeled data.

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 the coming five to ten years, significantly enhancing our capabilities in synchrotron science. Proposed instrumentation upgrades have been endorsed by ALS crosscutting reviews and workshops, and they 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. Projects will be prioritized and executed 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	Bending-magnet beamline optimized for soft-x-ray ambient-pressure photoemission spectroscopy, upgrading or replacing 9.3.2
11.0.2	11.0.2 upgrade	Upgrade of beamline to go into the tender x-ray regime for operando APXPS/Scattering/RIXS interfacial science
4.3.1	SAXS/WAXS	High-throughput SAXS/WAXS beamline at an ALS-U high-field port
Endstation	SPIN-MM	Low-temperature, high-resolution ARPES and momentum microscopy instrument at BL 4.0.3
Endstation	Q-STXM	STXM endstation optimized for high-field, low-temperature magnetic microscopy at BL 4.0.2
Endstation	Tender STXM	Tender nanoprobe endstation with a spatial resolution of a few nm to enable operando multimodal microscopy at ALS-U BL 8
Endstation	Tender Scattering	Scattering endstation to study spatio-temperal behavior/XPCS of soft matter/bio/energy materials at ALS-U BL 8
Endstation	Coherent Scattering	Coherent scattering endstation (XPCS) for quantum materials at ALS-U BL 10 (FLEXON branch 1)
Endstation	Novel Imaging	Novel imaging endstation using coherent light for quantum materials at ALS-U BL 10 (FLEXON branch 2)

Beamline 9.3.2 APXPS replacement. Despite aging optics, Beamline 9.3.2 serves a growing community using x-ray photoelectron spectroscopy at ambient pressures to study surface catalytic reactions and electrochemistry. This work is a priority of the Chemical Transformations TA. The beamline needs major upgrades, including a new M1 mirror tank and optic, and a replacement port at either 9.3.2 or 9.1.1. Plans are being developed for a possible start after the ALS-U dark time and are being coordinated with the ALS-U project where needed to preserve the beamline's source point.

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

Beamline 7.3.3 relocation. The SAXS/WAXS/GISAXS facilities at 7.3.3 support one of the most productive user communities at the ALS and their work is closely allied with numerous collaborating teams at LBNL. However, this beam port is not currently slated to remain operational after ALS-U. The ALS is therefore seeking to relocate the experimental systems from an ALS warm-bend magnet to an ALS-U high-field bending magnet, significantly increasing the performance and enabling high-throughput experiments for the soft-matter, bio, energy, and functional materials community. A preliminary optical design is complete for source point 4.3.1. As the ALS-U dark time approaches, there is urgency to find a solution that minimizes downtime.

Ultralow-temperature spin-momentum microscopy. The QMRD TA has prioritized the development of new endstations for electronic structure measurements at temperatures below 1 K in combination with efficient spin detection. One endstation 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.

Q-STXM endstation. To serve the magnetism, spintronics, and quantum materials communities, this low-temperature, high-field STXM would be optimized for studies of the electronic, chemical, and magnetic properties of spin systems exhibiting nanoscale phases. This endstation is a priority of the QMRD and the CMI TAs. An LDRD proposal has funded successful exploratory work.

Coherent tender x-ray endstations for ALS-U. New tender x-ray endstations will access the Na, Ca, P, S, Si, and Ti absorption edges, important for both biology and earth sciences, and higher photon energies will allow the use of thicker samples. The ALS seeks to develop two endstations that will be located at a beamline employing a full-length insertion device optimized for coherent, tender x-rays. Leveraging the dramatic improvements in coherent flux, one endstation will employ a nanoprobe operating in a STXM/ptychography-mode for nanometer-scale spatial imaging, while the second will probe spatio-temporal dynamics using XPCS.

Coherent soft x-ray endstations for ALS-U. Accessing spatial resolutions and time scales far beyond current capabilities is a high scientific priority for the QMRD TA. Two new endstations are planned on a full-length insertion-device beamline. One focuses on spatio-temporal dynamics using XPCS, while the other employs novel scattering geometries and detection schemes for ultrahigh-spatial-resolution imaging of novel electronic and ordered phases.

5 List of abbreviations

ADRP	Accelerator and Detector Research Program
AI	artificial intelligence
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
ASCC	ALS Safety Configuration Control
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
CMI	Complex Materials and Interfaces
CMOS	complementary metal-oxide semiconductor
COMPRES	Consortium for Materials Properties Research in Earth Sciences
COSMIC	COherent Scattering and MICroscopy
CT	computed tomography
CXRO	Center for X-Ray Optics
DEI	diversity, equity, and inclusion
DFT	density functional theory
DLTP	Developmental Long Trace Profiler
DOE	Department of Energy
DT	digital twin
DWG	Data Working Group
EPICS	Experimental Physics and Industrial Control System
EPS	equipment protection system
ES	endstation
ESAF	Experiment Safety Assessment Form

FAIR	findable, accessible, interoperable, reusable
FAST	fast x-ray absorption spectroscopy in transmission
FLEXON	FLuctuation and EXcitation of Orders in the Nanoscale
FLOPS	floating-point operations per second
GISAXS	grazing-incidence small-angle x-ray scattering
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
IT	information technology
JBEI	Joint BioEnergy Institute
JCAP	Joint Center for Artificial Photosynthesis
JCESR	Joint Center for Energy Storage Research
JGI	Joint Genome Institute
LBA	low blaze angle
LBNL	Lawrence Berkeley National Laboratory
LCLS	Linac Coherent Light Source
LDRD	Laboratory Directed Research and Development
LLRF	low-level rf
LSDCSC	Light Source Data and Computing Steering Committee
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
MOGA	multi-objective optimization using genetic algorithms
mRIXS	mapping of resonant inelastic x-ray scattering
MSI	microstitching interferometry
MX	macromolecular crystallography
NASA	National Aeronautics and Space Administration
NAWI	National Alliance for Water Innovation
NERSC	National Energy Research Scientific Computing Center
NLK	nonlinear kicker
NN	neural network
NSF	National Science Foundation
NSLS-II	National Synchrotron Light Source II
OPS	operations project

OSMS	Optical Surface Measuring System
pBPM	photon beam-position monitor
PEEM	photoemission electron microscopy
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
QIS	quantum information science
qRIXS	momentum-resolved resonant inelastic x-ray scattering
R&D	research and development
RADSI	relative-angle determinable stitching interferometry
REXS	resonant elastic x-ray scattering
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
SIBYLS	Structurally Integrated BiologY for the Life Sciences
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
TReXS	tender resonant x-ray scattering
UC	University of California
UEC	Users' Executive Committee
UHV	ultrahigh vacuum
USGS	United States Geological Survey
VUV	vacuum ultraviolet
WAXS	wide-angle x-ray scattering
XAS	x-ray absorption spectroscopy
XFEL	European X-Ray Free-Electron Laser Facility
XMCD	x-ray magnetic circular dichroism

XMLD	x-ray magnetic linear dichroism
XPCS	x-ray photon correlation spectroscopy
XPS	x-ray photoelectron spectroscopy
XRD	x-ray diffraction
XRF	x-ray fluorescence
XROL	X-Ray Optics Laboratory