Stanford Synchrotron Radiation Lightsource

Strategic Plan
2025-2029

Meeting the Scientific Challenges of the Future

May 2025

SLAC NATIONAL ACCELERATOR LABORATORY

Contents:

1 Executive Summary

The future will see a transformation in the ways that storage ring-based synchrotron radiation facilities impact user science. The construction of new or upgraded synchrotrons, based on multi-bend achromat designs, has led to greatly increased transverse X-ray coherence, enabling significant advances in X-ray science. At the same time, breakthroughs in automation of instrumentation, data collection, machine learning, simulation and analysis have the potential to boost the productivity of light sources and broaden their impact, and permit users to increasingly access their capabilities remotely. Finally, light sources will increasingly transition from being “photon factories” to centers of innovation that are critical to discovery and use-inspired research performed by their users. This plan sets forth SSRL’s role in this evolving landscape.

Many of the most critical scientific questions require moving beyond structure-function correlations to characterizing the structural evolution that dictates function. Progress in these directions places great emphasis on making the function of interest accessible to X-ray methods and tracking them in real time with the necessary temporal and spatial resolution. A greater focus on real-time observation of function will enable Stanford Synchrotron Radiation Lightsource (SSRL) to contribute significantly to the diverse scientific challenges facing society, as defined by our user community and prioritized by our scientific partners and sponsors, specifically in energy, quantum information, human health and critical minerals.

The strategic emphasis on real-time characterization of materials, chemical, and biological function with *in-situ* and *operando* methods aligns strongly with SLAC’s goal to be the premier X-ray and ultrafast science laboratory in the world. The strategy for achieving this objective is built on the bedrock of SLAC’s two complementary, world-class X-ray facilities, the Stanford Synchrotron Radiation Lightsource (SSRL) and the Linac Coherent Light Source (LCLS).

SSRL, as a Basic Energy Sciences (BES) Scientific User Facility, develops and amplifies SLAC’s core capabilities and leverages the proximity to the exceptional intellectual environment at Stanford University to address critical scientific challenges in support of the national interest and the Department of Energy (DOE) missions in energy, chemical, biological, and physical sciences. Our staff and the capabilities we steward support DOE’s goals of advancing energy addition and innovation.

The complementary user facilities at SLAC enable an emphasis on 1-to-1,000 picosecond-resolution (or longer) time-resolved X-ray capabilities at SSRL and on the shorter, sub-picosecond, time regime at LCLS. Together, SLAC’s light sources and their partnerships create a scientific environment that is unique among the BES supported Scientific User Facility light sources.

Throughout its history, SSRL has demonstrated a commitment to scientific discovery, innovation, renewal and exceptional user support. Continuing SSRL’s history of scientific excellence requires a sharp focus on the unique opportunities enabled by the strengths of SSRL and the SLAC-Stanford research environment. The scientific foci of SSRL’s Strategic Plan presented herein emphasize the following opportunities and goals:

- Develop new science programs and enhance existing areas to drive innovation in select strategic directions together with the user community, our funding agencies and partners.
- Implement new and upgrade existing SSRL beam lines to accentuate our strategic advantages and address grand challenge problems in energy, biosciences, and chemical and physical sciences and effectively couple to external partners from academic institutions, national laboratories, and industry.
- Focus SSRL’s accelerator development strategy on high-rate, short-pulse capabilities for time-resolved experiments that accentuate the synergy with LCLS and extend the current scientific strengths of SSRL.

- Meet and go beyond the expectations of our user community in providing new capabilities and the highest level of integrated scientific, technical, safety, and administrative user support. User satisfaction will continue to be the hallmark and signature of the SSRL experience.
- Expand SSRL's unique connections to Stanford University. This connection will continue to provide very important research and educational components designed to develop future leaders in all scientific and technical fields impacted by storage ring-based synchrotron radiation, in addition to creating an atmosphere that enhances the user community's experience.

SSRL's Strategic Plan will enable scientific advancement in the following major focal areas:

- Accelerate materials-by-design discovery and device optimization through studying materials at work under end-use conditions, integrate AI/ML with automated high-throughput experimentation, and enable rational process development for advanced manufacturing.
- Identify how the interplay among charge, orbital, spin, and lattice dynamics generates and impacts emergent behavior in quantum materials, and enables development of new materials.
- Pursue understanding of fundamental chemical function at electronic and atomic-levels, and under *in-situ*/*operando* conditions spanning molecular, thermal, electro-, photo-, bio-catalysis, and for bio-geological systems.
- Characterize complex biological systems via structural and functional studies at molecular and systems levels including biodynamics, bioengineering for drug discovery, the role of metals in human health and natural processes, through the application of multi-modal techniques integrated with theory and simulations.
- Expand state-of-the-art cryo-electron microscopy and cryo-electron tomography capabilities heretofore focused on biological studies to energy materials applications.

Each of these research areas has clearly defined strategic initiatives that ensure scientific impact and expansion of the community of researchers served by SSRL.

2 Stanford Synchrotron Radiation Lightsource

SSRL's SPEAR3 storage ring is operated at 3 GeV, with 7 nm-rad emittance and top-off injection at a current of 500 mA with a typical reliability of over 97%. An active accelerator research and development program is focused on continued performance and reliability improvements to the accelerator complex, including development of short pulse operation in the few ps range. SSRL has recently opened for operation three new undulator and one bending magnet beam lines for user research, with a complete refurbishment of a wiggler beam line underway. An ongoing program enables continuous upgrades to existing beam lines, including new optics and instrumentation to meet the needs of the user community. User science at SSRL spans a large range of areas including materials science, chemistry and catalysis, biogeochemical science, and structural molecular biology. In recent years, SSRL has focused on developing capabilities to support real-time measurements through the development of multimodal *in-situ* and *operando* measurements. SSRL has also developed a number of instruments which are fully automated and remotely accessible.

SSRL, being the premier hard X-ray source serving the Western U.S., currently operates 29 scattering, diffraction, spectroscopy, and imaging experimental stations, with capacity for further expansion. It is a highly productive scientific user facility with high user satisfaction, generating more than 600 peer-reviewed publications annually. Research conducted at SSRL continues to have major impacts in materials science, in chemistry and catalysis, and in biology.

As one of the DOE Office of Science's major scientific user facilities, SSRL focuses on the scientific opportunities and research priorities identified by the DOE Office of Science and other agencies, in particular the National Institutes of Health (NIH) and the National Science Foundation (NSF). SSRL works with a broad community of researchers to develop new capabilities, and to provide research infrastructure that enhances our users' scientific productivity while attracting and educating new user communities.

2.1 SSRL's Future in the Current Storage Ring Landscape

The current DOE investments in its U.S. light sources focus heavily on the development of low-emittance multi-bend achromat (MBA) lattice accelerators. These MBA X-ray sources provide high coherent brightness, enabling coherent X-ray imaging, scattering, and spectroscopy approaches such as nanoprobe imaging, X-ray photon correlation spectroscopy (XPCS), and X-ray standing wave spectroscopy (XSWS), which leverage this characteristic. This focus on forefront X-ray techniques, while important to realizing the ability to characterize novel physical, chemical, and biological phenomena, provides an opportunity to leverage the 3rd-generation accelerator at SSRL to develop bespoke capabilities which make a step-change in what is possible for characterizing temporal processes, via *in-situ* and *operando* measurements, to address key hypotheses driving next generation technologies for advanced manufacturing and efficient catalysis, integrating biological processes, and pursue biogeological natural processes, and responding to biomedical needs.

Scientific strategies

Time resolved X-ray methods combine photo-, electrical-, or chemical-triggers with the incisive power of X-ray scattering, diffraction, spectroscopy, and imaging to track in real time physical, chemical and structural changes.

The ability to follow physical and/or chemical phenomena spans a wide range of timescales, driven by the nature of the materials and relevant functional processes. SSRL's future capabilities will include optical pump X-ray probe measurements (psec) at our highest performing undulator beam lines, advanced spectroscopy and scattering applications at the msec-µsec scale with a consistent approach across the facility, and a range of approaches at longer timescales adapted to the systems under study and applied at any of the SSRL beam lines for such science needs.

The commitment to ultrafast (psec) based science rests on the further development of a SPEAR3 pseudo single bunch operations mode and at higher repetition rate than the current camshaft approach.

An overarching theme is the strategic focus to support real-time measurements through the development of multimodal *in-situ* and *operando* capabilities, across spatial and temporal scales in virtually all areas of SSRL science and beam lines. This includes tailored sample environments, integration of non-X-ray methods, specialized instruments, and multi-method data integration and analysis. A hallmark development will be to "bring the lab to the beam line" to expand *in-situ* and *operando* capabilities, for sample preparation, processing and testing, longitudinal studies with short repetitive X-ray measurements, and enabling seamless off- and on-line characterization.

The development of automation and remote-access capabilities will be expanded through increasingly sophisticated robotics and related instrumentation, controls and data acquisition software, and providing access to beam lines via remote-access mechanisms as appropriate for the science. This will enable enhancements of outreach, training, education and access to SSRL for new researchers and science communities.

As the complexity of both materials and experimental design spaces increase, artificial intelligence and machine learning will be developed to guide and intelligently select experimental parameters for *in-situ* and *operando* measurements. As the need for and application of AI/ML differs among techniques and applications, there will be a science-driven distributed development with a coordination strategy to apply this development. In a similar manner, data interpretation will be coupled to theoretical modeling and advanced analysis tools, developed in collaboration with external partners and expert user groups.

Scientific opportunities

SSRL will focus on the scientific opportunities and research priorities identified by the DOE Office of Science and other funding agencies, and work with researchers from academia, industry, and national laboratories to enhance accelerator stability and timing mode capabilities, develop new experimental and analytical techniques, design and construct state-of-the-art instruments, provide research infrastructure and support to enhance scientific productivity, and attract and educate new user communities. As the administrative home of the Stanford-SLAC CryoEM/ET facilities, the SSRL Directorate is committed to providing world-class bioimaging capabilities using both X-ray and EM methods, while also broadening the range of applications of cryoEM to critical DOE-relevant priorities in materials science and chemistry.

Partnership with scientific community

For the scientific foci discussed in this document, SSRL will build partnerships with the leaders and the community to *i*) identify the most important problems in the field, *ii*) guide the development of new experimental techniques, beam lines, instrumentation, research facilities, and data interpretation and simulation tools optimized for pursuing those problems, *iii)* leverage data infrastructure, AI and high-performance computing to accelerate scientific discovery and, *iv*) provide support to the community for efficient access, successful experiments, and high-impact scientific results.

Discovery to deployment

Discoveries from basic research often lead to technology developments that have significant economic impact, and the needs of industry and national security often inspire new basic research directions. National user facilities can catalyze collaborations among researchers from academia, industry, and national laboratories. Through redoubling our effort in outreach to industry and new users, SSRL will facilitate and strengthen such interactions and exchanges across the interface between basic and applied research.

Dedication to users' needs

SSRL continues to identify the steps a new user or user community follows to take an idea through to the successful conclusion of an experiment and improve each step of the user experimental cycle. This includes proactively reaching out to new scientific communities to build the needed tools and support for experimental design, data collection and data analysis, and to devise efficient and rapid access mechanisms. These improvements help ensure that SSRL focuses on the most pressing scientific questions and that users have what they need to make their time at SSRL productive.

Workforce development

Developing the next generation of leaders in science and technology enabled by advanced X-ray methods is a crucial goal of SSRL. This demands a commitment to nurturing scientific excellence at all levels of science and engineering. SSRL will engage STEM institutions to equip emerging leaders with the skills and confidence to push the boundaries of X-ray science, ensuring that the field continues to thrive and evolve to the benefit of the Nation. SSRL's internal workforce pipeline and career strategy will foster a dynamic environment that provides the strongest support and resources for professional growth and development

The Chapters that follow provide background, overview, and a more detailed current and future perspective of SSRL's scientific programs in the main areas of materials energy science, chemistry, catalysis, interfacial and geological science, structural molecular biology science, computing, data methods and infrastructure, accelerator science, instrumentation development, and for user research administration and workforce development.

3 Science at SSRL

3.1 Materials Science

Discovering and designing new materials with tailored performance characteristics, which may be amenable to manufacturing at scale, and which can be implemented in technology much faster than the current state of the art is crucial to addressing a broad range of economic and societal needs. Materials Science research at SSRL cross-cuts a broad range of end-use application areas including electrochemical energy storage, hydrogen production and storage, fuel and chemicals synthesis, microelectronics, quantum information, drug delivery, bio-integrated devices, and advanced manufacturing. This broad range of end-use application areas is unified through three key themes: developing fundamental understanding of synthesis and processing, understanding materials at work under intended end-use conditions, and accelerating materials discovery and optimization through integration of artificial intelligence/ machine learning (AI/ML) with automated high throughput experimentation (aHTE).

"Materials by Design" is a grand challenge goal in materials science. Achieving it requires understanding how a material forms, how it evolves during subsequent device processing or manufacturing steps, and how it dynamically responds to operating conditions. Further, these relationships must be understood across a range of spatial and temporal scales, and in a myriad of environments. SSRL is increasingly focused on integrating characterization capabilities with materials and device design pipelines, which has led to significant developments for *in-situ* and *operando* capabilities to support both synthesis science, and rationalizing materials and device performance.

The increased complexity of both *in-situ*/*operando* experiments and associated materials design spaces have motivated the development of AI/ML methods which use X-ray characterization as a primary feedback tool for real time discovery and optimization of materials with targeted properties. Integration of *in-situ* characterization of materials formation processes, *operando* characterization of performance, and AI/ML to steer experiments in real time is enabling a novel use of synchrotron X-rays as a proactive tool for materials development, moving beyond forensic characterization approaches.

SSRL's Materials Science programs will continue to develop and deploy a comprehensive set of tools and methods that enable accelerated materials discovery and optimization. This will be enabled through a RD&D focus on:

- Bringing the lab to the beam line to expand *in-situ* and *operando* capabilities.
- Developing multimodal approaches for characterization across spatial and temporal scales.
- Developing and deploying AI/ML to enable smart automated measurements, and design of experiments.

The SSRL Materials Science program will develop synergistic interactions and collaborations with other programs at SLAC, Stanford and other partner institutions to accomplish these RD&D objectives. Such collaborations have proven to be instrumental in developing world-leading capabilities. This includes the joint SLAC-Stanford Institutes, in particular the Stanford Institute for Materials and Energy Sciences (SIMES), the SUNCAT Center for Interface Science and Catalysis, and the SLAC-Stanford Battery Center.

- Collaboration with SIMES has led to development of *in-situ* synthesis and analysis of novel quantum materials at BL5, and *in-situ* cryogenic characterization of superconducting materials under mechanical strain at BL17-2.
- The SUNCAT-SSRL collaboration has led to new applications of X-ray scattering methods to understand catalyst materials evolution and degradation mechanisms.
- Collaborations with the SLAC-Stanford Battery Center have resulted in the development of world-leading multi-modal *operando* characterization of battery materials in relevant device structures.

This history of close collaboration between local scientific teams will continue and has been a hallmark of SSRL's approach to science and central to the development of technical capabilities beneficial to the general user community.

SSRL will broaden its impact through strategic partnerships with a number of entities in sustainable energy materials research, including EERE consortia such as HyMARC and the Bio-Optimized Technologies to keep Thermoplastics out of Landfills and the Environment (BOTTLE) consortium, Energy Frontier Research Centers, such as the Synthetic Control Across Length-Scales for Advancing Rechargeables (SCALAR), Stanford's Precourt Institute for Energy, and emerging opportunities with the new Stanford Doerr School.

The SSRL Materials Science division will also focus on developing deeper collaborations with other SLAC user facilities, such as LCLS and the Stanford-SLAC Cryo-EM facilities, to develop integrated multi-modal characterization approaches which enable deeper understanding than the sum of their individual parts.

Finally, we will carry on SSRL's long tradition of educating and training the next generation of materials scientists and engineers through introductory workshops for new synchrotron users, one-on-one mentoring for undergraduate and graduate students, and integrating materials into university courses, including with Stanford University.

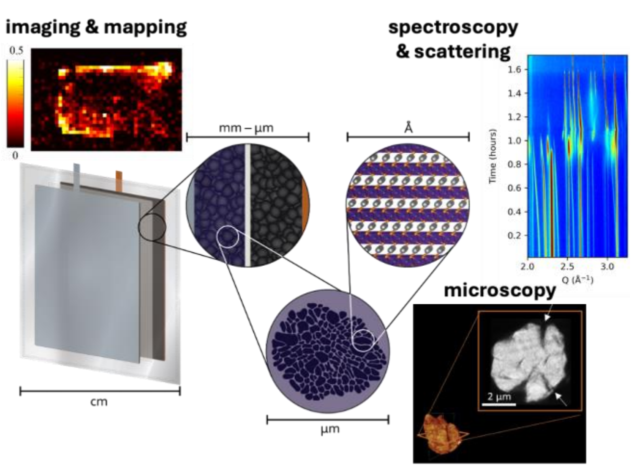
The following sections focus on the scientific challenges in the major materials science research directions at SSRL, which are aligned with broader SLAC strategic initiatives in sustainability, microelectronics and quantum information.

3.1.1 Energy Materials Research

Innovation in the energy ecosystem requires an enormous amount of materials research and development across sectors in energy generation and storage, separations and purifications, fuels and chemicals production, buildings, transportation, materials beneficiation, and manufacturing. SSRL's strategic focus on Energy Materials Research strives to meet this need through the development of capabilities to enable understanding of the fundamental physical and chemical processes which govern material formation and evolution in use to address key technology roadblocks for industry translation. We will enhance our focus on developing characterization capabilities of materials for energy generation and storage, hydrogen production, storage and transport, fuels and chemicals, separations, carbon capture and management, material circularity, and transformative manufacturing approaches.

Cross-cutting the specific research and development required in each of these technology areas are the need to i) develop integrated multi-modal characterization, ii) integrate lab-like capabilities at the beam line, and iii) integrate machine learning, artificial intelligence and robotic automation.

Enabling Multimodal Measurements. We will continue to develop multi-modal approaches for characterization of energy materials and devices across all pertinent time and length scales which govern their formation, performance, and lifetime. This will include the standardization of sample environments where possible such that they are compatible across beam lines, and techniques. This will follow the model previously employed to support battery research in which a novel pouch cell holder was developed that enabled realistic *operando* testing to occur at imaging, spectroscopy, and scattering beam lines.



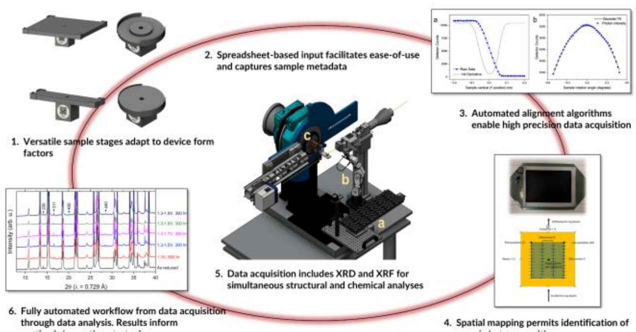
Integrated multimodal capability to characterize hierarchical structural evolution of batteries under operation. Standardization of pouch cell holder has enabled widespread adoption of this approach into the general user program, making a once heroic measurement accessible across multiple beam lines and X-ray techniques. Figures adapted from Paul, et al. Energy Environ. Sci. ***14****, 4979 (2021), Preefer et al. J. Phys. Chem. C* ***126****, 21196 (2022), unpublished work by Z. Liang et al. and Yan et al. Cell Rep. Phys. Sci.* ***3****, 100694 (2022).*

This approach enabled characterization of the hierarchical structural evolution of battery materials under operation as shown in the figure. We will endeavor to expand this approach to standardization of sample environments in the application areas of separations, fuels and chemicals, materials circularity and transformative manufacturing. We will also continue to deploy new microscopy approaches such as laminography, which broaden our characterization toolset in order to probe planar device structures such as battery pouch cells and enable microscopy on samples and devices which were previously incompatible with tomography. Lastly, we will continue to develop simultaneous multimodal capabilities to enable integrated imaging, spectroscopy, and scattering approaches with non X-ray characterization tools such as optical, IR and impedance spectroscopy.

Integrating Lab-Like Capabilities. SSRL has long focused on the development of *in-situ* capabilities which mimic lab and industrial processes for making materials and devices, as well *operando* capabilities for testing devices under realistic conditions. Our future focus will be on increasing accessibility for user-developed *in-situ* and *operando* capabilities through standardization of sample positioning systems, and connection points to beam lines. We will continue to develop sample processing and testing capabilities, such as reactors, thin film deposition and post processing, additive manufacturing, and electrochemical cells which will be deployed into the general user program. Lastly, we will begin piloting off-line testing of devices as part of the user programs focused on energy storage, hydrogen generation, and catalysts and chemicals production. Off-line testing is designed to enable users to perform long term durability studies on-site with access to X-ray characterization tools as indicated by changes in performance of devices. This supports a paradigm shift in which users condition samples at SSRL, and are able to characterize samples on-demand, as enabled by increasingly automated measurement capabilities.

AI for X-ray User Science. As the complexity of both materials design spaces and experimental design spaces increase, artificial intelligence and machine learning will be required to guide design of materials, and to intelligently select experimental parameters for *in-situ* and *operando* measurements. SSRL has developed and demonstrated approaches which utilize data driven discovery, guided by artificial intelligences to accelerate the discovery of high performing materials. This has required the development of automated ML for data interpretation, active learning algorithms for the design of experiments and guided materials optimization, and ML algorithms to automate instrument control. More recently, we have invested in deploying robotic sample handling capabilities to increase sample throughput at the beam lines and to support remote mail-in user programs. Moving forward we will focus on integrating these capabilities to move from *automated* measurements to *autonomous* measurements for both *ex-situ* samples and *in-situ*/*operando* experiments.

The integration of robotics, ML approaches for data interpretation, reinforcement learning for instrument control, and active learning for sample selection will enable fully autonomous user programs, such as those illustrated in the figure, and ultimately will enable digital twins of beam line instruments for virtual experiments and training.



Integrated processes of the autonomous flat-plate XRD program for accelerated characterization of material performance and durability. The high throughput of sample manipulation, data acquisition, and analysis significantly reduces measurement latency, and generates opportunities to derive large data sets on which ML models can be trained to optimize instrument control and sample selection/manipulation. In this paradigm, a large number of SOECs are operated in parallel with varying conditions and structural evolution determined from XRD inform on early term structural degradation leading to late-stage cell failure.

Further, the integration of autonomous data interpretation, and active learning for design of experiments will increase productivity during complex *in-situ*/*operando* measurements in which many degrees of freedom exist. Lastly, we will continue to collaborate on the development of leading-edge machine learning architectures, such as transformers and diffusion models, to develop new approaches which leverage large data sets to predict measurement conditions and sample responses in new materials domains.

In addition to the focus on cross-cutting capabilities described above we will also focus on increasing the breadth of science we support in the general user program in each of the application areas previously identified. The growth areas within each science program related to Energy Materials Research are described briefly below.

Energy Generation. We will expand our current user program to include the characterization of photovoltaic (PV) manufacturing processes, and the development of metrology tools which can support reshoring of domestic PV production. We will also target expansion of the portfolio to include the characterization of materials under extreme environments to support the development of new materials for nuclear power generation. This will be synergistic with efforts that will be growing at LCLS, with the upgrade of the LCLS Matter in Extreme Conditions (MEC) beam line.

Energy Storage. We will lead the development of novel approaches for *operando* characterization of materials for electrochemical energy storage. This will include the development of a new laminography capability, as well as mixed contrast ghost imaging capabilities which will be deployed as an upgrade to the current full field X-ray microscope at BL6-2c.

In addition to these capability developments, we will also develop µs time resolved scattering, and continuous scanning capabilities at BL17-2 to grow a user base focused on new electrode materials, and solid-state batteries for extreme fast charging. Lastly, we will expand beyond *operando* characterization to include a user portfolio focused on the synthesis of materials for batteries, and the scale-up of these manufacturing processes.

Hydrogen Production, Storage, and Transport. SSRL is currently developing world class characterization capabilities designed to address material- and operation-based barriers to widespread adoption of a hydrogen economy. For both hydrogen production and storage, we will develop capabilities which enable characterization of mechanisms governing material performance and durability. We will further grow these capabilities through increased automation of both measurement and data interpretation to enable high enough throughput measurements of devices cycled *ex-situ* to derive statistical models to predict process-structure-property relationships. We will expand this portfolio to include the characterization of materials for hydrogen transport.

Fuels and Chemicals. Leveraging the world class *operando* characterization of heterogeneous catalyst using EXAFS which currently exists at SSRL, we will build a user program which utilizes the combination of X-ray microscopy and scattering to characterize catalyst durability. This program will focus on building new experimental methods, jointly across the Materials Science and Chemistry and Catalysis divisions, and accelerated aging protocols which enable prediction of long-term catalyst performance. It will support discovery efforts identifying new catalytic processes for the wide-ranging feedstocks, which will require fundamental understanding of both catalyst performance and durability.

Desalination and Separations. Processes and materials for advanced separations are critically dependent on kinetic and thermodynamic parameters that vary depending on both the feedstock and environmental factors. Developing the design rules to create tailored and efficient separations necessitates a fundamental understanding of how both equilibrium and non-equilibrium properties drive chemistry in rich microenvironments with multiple, interacting species. We will develop end-to-end capabilities to characterize both membrane formation processes and structural response under operation. This holistic approach requires multimodal characterization with emphasis on developing a mechanistic understanding of nucleation and fouling along with detailed understanding of the non-equilibrium environments and their effect on the separation process.

Material Circularity. Circularity is emerging as a new material performance property. Material re-use has been demonstrated to have beneficial societal and economic impacts, and to provide much needed domestic supply chains for critical minerals. We will develop forefront X-ray methods for characterizing deconstruction processes for materials including commodity plastics, battery materials, semiconductors, and rare-earth magnets. This will include further development and deployment of reactors to support *in-situ* measurements, as well as expansion beyond scattering and spectroscopy capabilities to leverage X-ray imaging to support research on process scale-up.

3.1.2 Microelectronics

The demands of 21st century data-driven and artificial intelligence computing far exceed today's microelectronics capabilities. Currently microelectronics are built-up as separate logic, memory, and sensor chips. For data-intensive computation this causes up to 90% of operating energy to be wasted during data transmission between logic and memory. Vertical integration can shrink connections between logic and memory. However, 3D integration requires new materials which must be processable with strict thermal budget constraints.

At SSRL, X-rays are used to study microelectronic materials beyond silicon, such as ferroelectric hafnia-zirconia alloys for non-volatile memories, and new thermal processing approaches to enable 3D heterogeneous integration. The X-rays from the new high-brightness scattering BL17-2 can probe structural and chemical properties of nanometrically thin films revealing structural phases and their transformation during both formation and electric field cycling, providing key insight into both formation and degradation and failure mechanisms.

SSRL has had a long-standing user program characterizing materials for microelectronics. This program has focused on understanding process-structure relationships for semiconductors, ferroelectric, ferromagnetic, multiferroic, and insulating materials with an increasing focus on monitoring materials formation processes *in-situ*, and device performance in *operando* environments. Scientifically the research and development of capabilities to further grow this user program will focus on enabling rational process development for energy-efficient microelectronics and is motivated by the following four key scientific questions.

- How does structural and chemical heterogeneity emerge during growth and give rise to novel functionality in ME materials?
- How does this heterogeneity evolve in the buried layers of complex structures with the stacking of layers and under operating conditions?
- How do we correlate effects of heterogeneity to the relevant device physics?
- How can we exploit control of heterogeneity to control device physics?

The continued development of capabilities to support the microelectronics user community will leverage the new micro-focused scattering BL17-2. The high beam line flux density enables the time resolution needed to capture fast material transformations, and the micrometer focus enables characterization of materials at device-relevant scales. The characterization of atomic structural heterogeneity will be complimented by electronic characterization via photoemission spectroscopy, as well as resonant soft X-ray scattering.

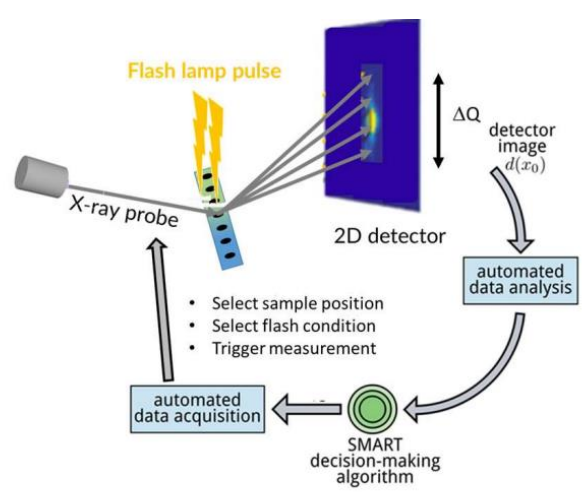
These developments are organized according to the same cross-cutting topics and are described further below.

Integrating Lab-Like Capabilities. SSRL has previously commissioned *in-situ* processing chambers supporting atomic layer deposition, sputtering, molecular beam epitaxy, flash annealing, rapid thermal processing, and roll-to-roll printing. We will focus on increasing ease of use for existing tooling, as well as new processing capabilities at the beam line.

This will include both expanding deposition processing (e.g., chemical vapor deposition), as well as etching processes with the ultimate goal of developing the underlying synthesis science to support the development of new microelectronic chip architectures.

Enabling Multimodal Measurements. We will develop a holistic characterization approach which integrates microscopy and spectroscopy of samples prepared *in-situ* at other beam lines. This will enable samples to not only move between beam lines, but also between facilities to support corollary measurements of samples using cryoEM, and imaging at LCLS. Two technical developments will be required to support this effort. First, the development of vacuum sample suitcases for sample transfer between facilities and beam lines. Second, where possible sample processing chambers will be designed such that they are compatible with multiple non-vacuum beam lines.

AI for X-ray Microelectronics User Science. *In-situ* measurements, the focus of this program, will require further development of both autonomous data interpretation and ML-informed design of experiment. Here we will leverage the development of autonomous scattering interpretation algorithms made to support autonomous remote mail-in experiments. These algorithms will be retrained to enable real-time interpretation of scattering data taken during processing. Secondly, the process optimization dimensionality will increase substantially, as methods like flash annealing are used to support 3D integration of memory and logic. We will continue to develop active learning algorithms to guide design of experiment in complex design spaces. An example of near future developments is shown in the figure.



Schematic illustration of closed-loop AI-enabled optimization of flash lamp annealing post-processing of materials for memory. The fully autonomous optimization of materials structural parameters, using X-ray scattering as the metrology tool will enable orders of magnitude improvement in both beam line efficiency, and process optimization.

3.1.3 New and Planned Capabilities

The science directions and opportunities described above will motivate continued development of capabilities within the division which will include revitalization of existing instruments, as well as the development of new beam lines.

We will revitalize our transmission X-ray full field microscope instrument at BL6-2c through an in-house design/rebuild to a new instrument. The goal is to maintain the existing capabilities for XANES imaging and nanotomography, large working distances to support *in-situ* sample environments, and ghost imaging and to expand these capabilities to include variable FoV, extended usable energy range up to 15 keV to access a larger range of absorption edges, and increased penetration depth.

We will implement AI-guided autonomous scattering capabilities for powder X-ray diffraction and wide-angle X-ray scattering at BL2-1, as well as for small angle X-ray scattering at BL1-5. These capabilities will increase throughput of *ex-situ* measurements, and support remote mail-in programs with the goal of simultaneously increasing the number of users we can support, and reducing barriers to accessing synchrotron X-ray user facilities.

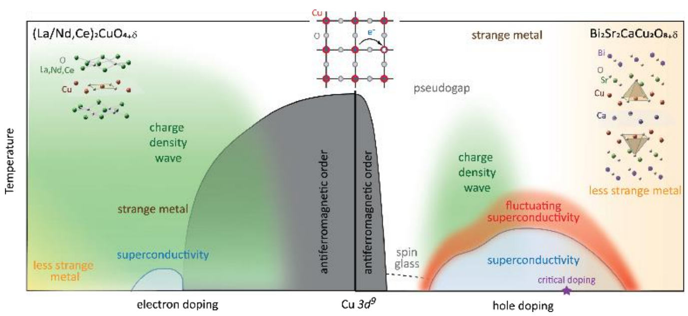
We will expand on the existing capabilities at BL17-2. The addition of specifically designed secondary optics will improve the focus to better than 1 µm x 1 µm, with flux greater than 10^{12} ph/s. A small angle X-ray scattering capability will be commissioned at the beam line to enable *in-situ* and *operando* characterization of multiscale structural evolution.

Optical pump capabilities will be commissioned to support a time-resolved optical pump, X-ray probe program that will take advantage of the pseudo single bunch capability of the SPEAR3 accelerator designed to reduce background signal and dose arising from non-probe X-ray bunches. Collectively these improvements will support science programs in all three strategically targeted areas: sustainability, microelectronics and quantum information.

Lastly, as part of the SSRL Beam Line Renewal Initiative, two new hard X-ray beam lines have been proposed, motivated by science topics in quantum information and microelectronics, with details provided in Section 5.2.3. A microfocus beam line with simultaneous spectroscopy and scattering capabilities would be developed to support a user program characterizing processing related to rationalizing heterogeneity in microelectronic devices. This beam line would represent an evolution in the approach of bringing the laboratory to the beam line and include a physical laboratory space adjacent to the beam line with microelectronic materials processing capabilities that could be utilized both off-line, and in-line with X-ray characterization. A second hard X-ray photoemission (HAXPES) beam line would be developed to support electronic characterization of buried interfaces as a complement to the *in-situ* characterization of structural evolution during processing at the microfocus beam line.

3.1.4 Quantum Materials

Quantum materials exhibit a fundamental and intricate interplay among their charge, orbital, spin, and lattice dynamics. Strong correlation and spin-orbit coupling are key factors for creating a fascinating variety of phenomena. Examples of extreme and remarkable emerging properties include high-temperature superconductivity, topological phases of matter, and correlation-driven metal-to-insulator transitions. A hallmark of quantum materials is the remarkable adjustability of such emergent phenomena through the manipulation of each degree of freedom and their interplay, realized by carrier doping, pressure, magnetic field, etc. As a result, quantum materials often exhibit complex electronic phase diagrams.



Schematic temperature-doping phase diagram of electron- and hole-doped cuprate superconductors. Rev. Mod. Phys. 93, 025006 (2021).

The emergent phenomena in quantum materials present exciting opportunities to understand their profound physics and, ideally, to control the transport of energy and information. As better-controlled model systems become available, a sophisticated understanding of the universality of these diverse materials will lead to great revelations influencing science beyond their specific properties. There is no doubt that surprising discoveries will be made that dramatically advance our understanding of these materials, such as the recent discovery of high temperature superconductivity in nickelates under high pressure.

Just as these new materials have emerged, the advancement of state-of-the-art X-ray instrumentation has played a pivotal role in delving into the intriguing characteristics of quantum materials over recent decades. Within this realm, SSRL has excelled, enabling the deployment of cutting-edge experimental techniques such as ARPES and RSXS capabilities at its soft X-ray beam lines.

Angle-resolved Photoemission Spectroscopy (ARPES). As demonstrated by its impact on the understanding of high-T_c superconductors and topological materials, high-resolution ARPES has proven to be the most direct and powerful experimental probe of electronic structure – information that forms the foundation for a comprehensive understanding of complex quantum materials. With the extremely high angular and energy resolution now achievable, ARPES can probe electronic structure with unprecedented precision and sophistication.

Historically, SSRL has had a strong foundation in photo-emission spectroscopy. Over the last few years, this has been further strengthened with a new state-of-the-art undulator branch line 5-2 dedicated to high-resolution ARPES. This addition completely modernizes and greatly expands the capabilities of the original branch line 5-4 with full polarization control, extended photon energy range, and a significant improvement in flux and beam spot size. The recent upgrade of the electron analyzer to the new-generation DA30-L with electron deflectors, coupled with the micro-focusing beam spot available on BL5-2, has significantly improved data quality and data acquisition efficiency, thereby transformed this beam line into a highly oversubscribed premier micro-ARPES facility. Spatially-resolved high-resolution measurements provide opportunities to understand more complicated electronic structure, such as magnetic-domain-dependence of skyrmion phases.

We are developing complementary laser-based ARPES with ultra-high energy resolution and microbeam focus at the existing BL5-4 end station. The addition of a laser as the complementary light source will allow simultaneous operation of both end stations on BL5-2 and BL5-4, hence substantially increase the total available beamtime at BL5. The setup aims to achieve the highest total energy resolution of < 1 meV and micro beam spot size of ~1 × 1 μm^2 with a 6 eV CW laser. Enhanced high-precision ARPES measurement capability of fine electronic structure with smaller energy scales would further deepen the understanding of the mechanism of high-temperature superconductivity. Measurements of smaller samples such as exfoliated 2D materials also becomes possible with the microbeam spot size, expanding the scope of research at BL5. In addition, we plan to achieve smaller beam spot sizes at branch lines 5-2 and 5-4, by upgrading the beam line refocusing optics, which is also aligned with the future development of a new soft X-ray beam line for quantum information science.

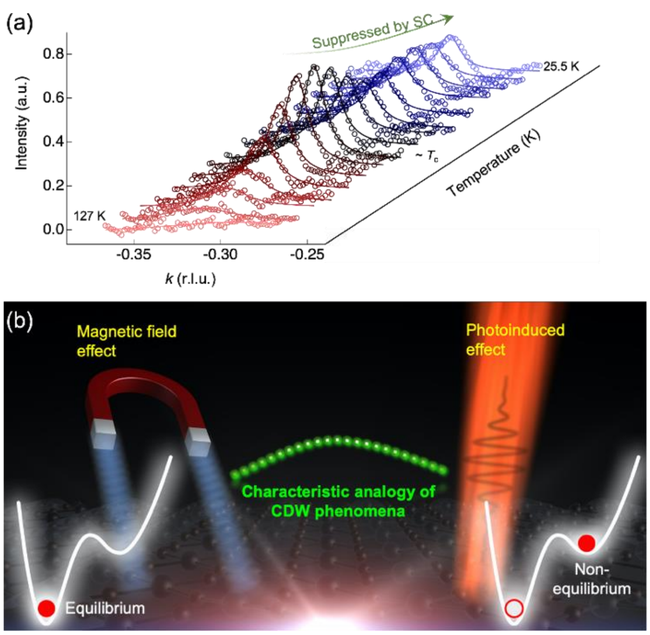
With data collection highly automated, the ARPES experiments at BL5 are moving toward more automated data analysis, to enhance beamtime efficiency and to attract non-expert users. Furthermore, ARPES-measured band dispersions are routinely compared with band structure calculations. Direct connection between the rapid development of ARPES experiments and theoretical simulations has been shown to be a strength and will be further enhanced. Close collaborations with the Theory Institute for Materials and Energy Spectroscopies (TIMES) have been established to realize the full potential of such a connection.

Integrated Materials Fabrication Capabilities. A unique capability at BL5-2 is that the ARPES endstation is *in-situ* connected to thin-film growth facilities: An oxide Molecular Beam Epitaxy (MBE) chamber and a chalcogenide MBE chamber, which has enabled us to establish a joint synthesis-characterization platform to investigate the electronic structures of epitaxial quantum materials with tailored properties and unprecedented accuracy. The past decade has witnessed revolutionary advances in the growth of novel materials and precise atomic control of thin films now happens on a routine basis. Such control enables researchers to better understand how structure, and the precise control of structure, affects physical properties. The recent success in the synthesis and systematic doping-dependent study of one-dimensional cuprates is an example demonstrating the new frontier in quantum material research by coupling sophisticated thin film growth techniques with modern ARPES techniques.

In addition to the *in-situ* MBE thin film growth capabilities, we have been developing on-site fabrication of exfoliated thin flake 2D materials and their heterostructures, using a glove box system located in one of SSRL's laboratories and a vacuum suitcase port. Furthermore, a microscope with a reentrant viewport is installed on the BL5-2 end station measurement chamber for *in-situ* exfoliation/characterization of thin flakes.

Interface Scattering. In addition to charge, spin and orbital degrees of freedom, the atomic structure of strongly correlated electron materials is of considerable importance, as it dictates emergent electronic properties. This is especially important for hetero-interfaces in metal oxides, such as $LaAlO_3/SrTiO_3$, where the precise atomic arrangements determine if the interface is doped n- or p-type. The quantum materials strategy will build on SSRL's strength in materials scattering to develop a program in hetero-interface structure determination on the new BL17-2, closely coupled to SSRL's RSXS spectroscopy program at BL13-3.

Resonant Soft X-ray Scattering (RSXS). Understanding the intricate interplay among different degrees of freedom in quantum materials is important to characterize the rich variety of ordering phenomena in their novel ground states. Resonant soft X-ray scattering is a powerful method for probing the spin, charge, orbit and lattice ordering that underpins many emergent properties of quantum materials. A good example is the study of charge-density-wave (CDW) phenomena in high-T_C cuprates, where RSXS has played a critical role.



Resonant soft X-ray scattering provides a sensitive probe of charge and spin order in strongly correlated electron systems. (a) CDW as a function of temperature in YBCO, measured by resonant soft X-ray scattering, showing the suppression below T_c [Sci. Adv. ***8****, eabk0832 (2022)]. (b) Illustration of exploring CDW phenomena under both equilibrium and non-equilibrium states.*

SSRL has developed an RSXS endstation at BL13-3, which is now open for general user operations. Furthermore, the RSXS experimental approach at SSRL synergizes well with non-equilibrium studies conducted at X-ray Free Electron Lasers (XFELs), such as LCLS, enhancing the overall understanding of quantum materials.

More recently, we have pioneered the development of a new in-vacuum scattering capability for RSXS experiments. Utilizing a manipulator-based low-temperature diffractometer, we successfully achieved a record-low base temperature of around 11 K while preserving wide angular motions. This presents a significant improvement over the typical base temperature of 25 K for the previous, traditional goniometer-based diffractometer. These advancements are expected to open substantial opportunities in quantum materials research in the coming years.

To further enhance the quantum materials program at SSRL through RSXS experiments, we plan to develop a pulse magnet system capable of reaching up to 50 Tesla and integrate it with the scattering capability. This development will be particularly impactful for studying quantum materials, especially in strongly correlated electron systems like high-T_c superconductors where the magnetic field serves as a critical tuning parameter for revealing the intricate interplay among different orders.

Expanding the capabilities of instrumentation through RSXS developments has involved significant parallel investments in software advancements. Efforts to improve data collection efficiency and, particularly, real-time in-line analysis remain critical priorities. These advancements aim to seamlessly bridge the connection between real and reciprocal space, offering a more comprehensive picture of quantum material properties. This ongoing progress will also benefit non-expert users by naturally broadening the horizon for intuitive data interpretation and lowering the barrier for researchers less experienced in experimental techniques.

A New Soft X-ray Beam Line for Quantum Information Science (QIS). As part of the SSRL Beam Line Renewal Initiative, a new undulator-based soft X-ray beam line with two branch lines – one for soft X-ray ARPES and the other for RSXS – was defined for future funding. This beam line would address two science drivers pertinent to the QIS applications: 1) probing electronic states across the interface; 2) exploring new quantum materials for future QIS applications. The proposed beam line would have strong synergy with existing BL5-2, BL5-4, and BL13-3, significantly enhancing the ARPES and RSXS capabilities at SSRL. Combined with the HAXPES/PEEM endstation proposed for a separate undulator beam line for microelectronics applications, it would strengthen the quantum materials program at SSRL with a comprehensive suite of modern ARPES facilities covering a wide photon energy range from VUV to soft X-ray to hard X-ray, enabling a deeper understanding of electronic structure.

3.2 Chemistry, Catalysis and Interface Sciences

Catalysis plays a vital role in the world economy and human prosperity, underpinning for example fuels production and chemical and materials synthesis. It plays a significant role in fertilizer production to support the earth's burgeoning population, and in lower the cost and improving the selectivity of chemical manufacturing. Catalyst characterization, particularly under working conditions, is central to the SSRL Strategic Plan, and the atomic resolution and specificity of X-ray methods naturally address key questions in catalysis research.

SSRL's chemistry, catalysis and interface science program will expand its existing specialized spectroscopy and imaging capabilities, in close collaboration with the user community, to develop primarily molecular-level characterization techniques of catalysts under *in-situ* reaction conditions – whether the catalysis be molecular, thermal, electro-, photo- or bio-catalysis. The focus will be on enabling the understanding of fundamental electronic and structural properties, and course of chemical reactions, on relevant scales of space, time and energy. This includes the continued development of optical pump X-ray probe methods to investigate photocatalytic reactions.

In the coming years, the emphasis will be on select topics, such as photo- and electro-catalytic reactions, reactions related to producing hydrogen from solar water splitting, and hydrocarbons from captured carbon dioxide, together with transformative breakthroughs in petroleum-based catalysis. Special emphasis will be given to the following developments:

- Integrating analysis of chemical reactivity and catalysis, where investigations of molecular, nano-, biological, geological, and catalyst materials enable a comprehensive view of homogeneous, heterogeneous, biological, and natural systems.
- *In-situ*, real-time characterization tools, based on hard, tender, soft X-ray absorption (XAS) and emission (XES) spectroscopies, inelastic scattering-based methods (RIXS), µXRF imaging with XANES and EXAFS capabilities, over multiple time and length scales.
- Developing modulation excitation spectroscopy methods and tools for enhanced detection and temporal sensitivity in reactivity studies.
- Expanding the time domain to milliseconds via continuous and quick-scanning capabilities and modulation spectroscopy, and to picoseconds via laser-pump X-ray probe techniques, bridging to LCLS/LCLS-II for research in the ultrashort time domain.
- Integrating non-synchrotron-based characterization and analytical tools, such as mass spectrometry, laser Raman spectroscopy, Fourier-transform infrared spectroscopy and UV-vis spectroscopy with the synchrotron techniques and facilities.
- Updating capabilities for grazing incidence spectroscopy and scattering methods for near-interfacial studies.
- Coupling experimental techniques closely with theory, modeling, and new analysis methods.
- Developing robotics, automation and software for remote-access and eventually fully automated data acquisition, and data handling.

We will commission and bring to the user community the new X-ray spectroscopy BL10-2b for catalysis research, which will include a full suite of *operando* catalytic reactors with the necessary infrastructure at the beam line, off-line catalyst treatments and testing of *operando* cells. The BES Chemical Sciences funded Co-ACCESS program will continue to provide specialized support for the catalysis community.

We will develop multi-modal approaches for biogeochemical research with particular emphasis on soils, sediments, colloids, nutrients and contaminants.

We will expand on, and create new, partnerships with institutions and industry in energy and catalysis research. This will include new and continuing collaborations with other national laboratories, DOE Energy Innovation Hubs like the Liquid Sunlight Alliance (LiSA), Energy Frontier Research Centers, DOE applied programs, industrial consortia, and Stanford University Institutes, Centers and Departments.

We will continue our long-standing tradition of educating and training the next generation scientific workforce through workshops, summer schools, web-based experimental simulation and remote-access tools, video tutorials, and mentoring of undergraduate and graduate students, and postdoctoral scholars.

The following sections focus on the scientific opportunities in the Chemistry and Catalysis Division, new beam lines and methods/instrumentation developments, which are aligned with SLAC's strategic initiatives in sustainability and energy research.

3.2.1 Energy, Fuels and Chemicals

The adoption of new energy systems relies in part on our ability to design and implement scalable catalytic processes that efficiently convert abundant feedstocks (such as water, CO_2 or biomass) into energy, fuels, and chemicals. The SSRL Chemistry and Catalysis Division mission is centered on deepening our understanding of catalytic processes at the atomic level. We focus on exploring how synergies among active sites (or site ensembles) and interactions among these sites and their support or ligand environments drive tailored, predictive reactivity. Understanding these synergies is crucial as they dictate how intermediates bind to catalytic sites and influence the subsequent steps that determine the efficiency and selectivity of the entire process. Enhancing selectivity is particularly important, as it minimizes waste and, in turn, improves the efficiency of chemical processes.

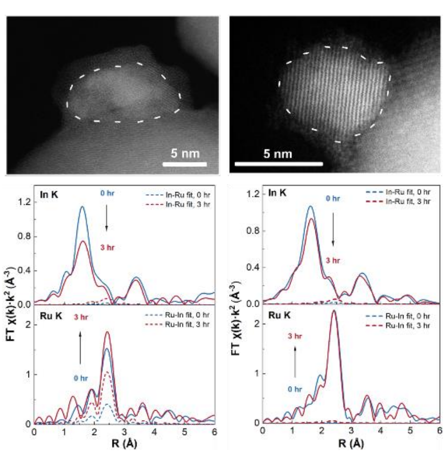
Developing methods to experimentally capture these interfacial processes is central to advancing the field of catalysis. These experimental insights are indispensable for refining theoretical models, pushing the boundaries of predictive understanding in catalysis.

Investigating Fundamental Catalytic Conversions. SSRL supports research into the fundamental processes that govern catalytic conversions, using materials from well-defined systems such as single-atom/uniform active catalysts and molecular catalysts inspired by enzymatic and biomimetic motifs. These well-defined materials provide an ideal platform for studying the active sites in catalytic reactions, allowing researchers to probe the electronic and structural properties of catalysts with high precision.

SSRL has developed a comprehensive suite of conventional and advanced X-ray spectroscopy techniques across multiple beam lines, which are applied under *operando* conditions to study catalysts from concentrated to dilute (few ppm) systems. These capabilities are crucial for investigating catalytic systems under realistic conditions, providing insights that might otherwise be inaccessible.

A significant element of SSRL's catalysis research is supported through the Consortium for Operando and Advanced Characterization via Electronic Spectroscopy and Structure (Co-ACCESS), part of the Stanford-SLAC SUNCAT Center for Interface Science and Catalysis. Co-ACCESS has established itself as a major resource, aiding user groups worldwide in applying synchrotron characterization methods to their catalysis research. It has focused on fully exploiting SSRL beam line capabilities. The upcoming catalysis-dedicated BL10-2b, will allow for both expansion of SSRL's catalysis program, and new areas to be further explored, especially the quick-scanning time domain (see below). Co-ACCESS will also continue to develop new data analysis tools (e.g. CatXAS), experiment planning tools (e.g. CatMass), *in-situ*/*operando* reaction cells optimized for various catalysis forms, and a combined *in-situ* XAS/FTIR capability.

Investigating Extended Catalytic Systems. While single-atom, uniform active and molecular catalysts offer precise insights into catalytic mechanisms, nanoparticles and other extended catalytic systems often exhibit unique catalytic behaviors that are influenced by factors such as particle size, shape, and the nature of the support material.



The heterogeneous catalyst Ru/In_2O_3-ZrO_2 was studied using operando EXAFS at the In and Ru K edges and the structures correlated with ethanol production during CO_2 hydrogenation to ethanol. The Ru nanoparticles were found fully encapsulated by In_2O_3 and alloyed with In after prolonged reaction (left images), while partially encapsulated and un-alloyed under engineered conditions (right images). Angew. Chem. Int. Ed. ***63,*** *e202406761 (2024).*

These properties can lead to differences in catalytic activity, selectivity, and stability, which are critical for optimizing reactions at an industrial scale. For instance, in nanoparticle catalysts, the coordination environment and electronic structure can vary across the surface, creating regions of differing reactivity. Understanding these variations is key to designing catalysts that maximize efficiency and minimize unwanted side reactions.

SSRL's suite of conventional and advanced X-ray spectroscopy techniques plays a vital role in characterizing these catalysts. By monitoring their structural evolution and stability in real-time, researchers gain insights into how these materials behave under working conditions. This includes understanding how nanoparticles interact with reactants and how their properties change over time.

Integrating Catalysts into Functional Devices. SSRL is spearheading efforts for the characterization of electrolyzers, particularly for hydrogen production and CO_2 conversion reactions. As a core partner of the CO_2 Reduction and Upgrading for e-Fuels (CO2RUe) DOE BETO consortium, SSRL contributes significantly to the development and scaling of these technologies by overcoming the technical barriers to making CO_2 electrolysis commercially viable. SSRL efforts are focused on optimizing key parameters of electrolyzer operation, energy efficiency, and the overall durability of these devices during prolonged operation under harsh conditions, such as high current densities and varying temperatures.

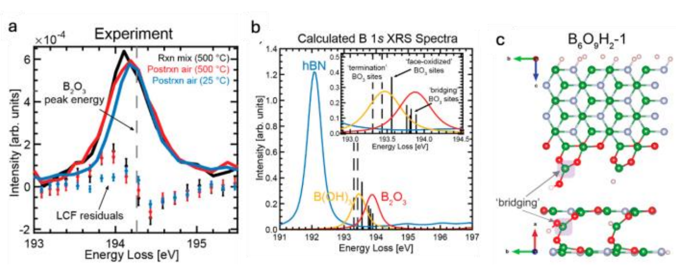
SSRL will facilitate advanced durability studies by providing unique X-ray tools that allow researchers to observe and analyze how electrolyzer components evolve over time. This includes monitoring the gradual degradation of catalytic materials and identifying the factors that contribute to loss of efficiency and eventual device failure. These applied research areas are of significant interest to the energy technology industry, and SSRL will engage with industrial partners to help translate experimental findings into scalable solutions underlying future energy technologies.

Developments in Advanced Spectroscopy. SSRL's advanced X-ray spectroscopy techniques, such as partial fluorescence yield XAS, particularly high-energy-resolution fluorescence detection XANES (HERFD-XANES), has provided unprecedented information on the electronic structure of active catalysts. By monitoring their structural evolution and stability in real-time, researchers can gain insights into how these materials behave under working conditions. This includes understanding how nanoparticles interact with reactants and how their properties change over time, thus informing the design of more durable catalysts.

Given the demands of the catalysis community, SSRL plans to develop and implement new HERFD spectrometers around the facility, including at BL10-2b. Furthermore, developing and supporting grazing incidence (GI) methods and facilities, particularly for electrochemical interfaces, remain a priority. SSRL will focus on expanding critical instrumentation and expertise in GI spectroscopy, scattering, and diffraction measurements of chemically active surfaces and solid-liquid interfaces under conditions including thermo-, electro-, and photochemical.

Expanding Time Domain Capabilities. The time domain in catalysis is particularly critical because the structure of active sites evolves over time—from microseconds to weeks—impacting catalytic activity, selectivity, and durability. Catalytic reactions often involve multiple intermediate steps, which play a crucial role in determining the overall efficiency and selectivity of the process. Kinetic models show that intermediates can exist across a broad range of timescales, from tens of microseconds to seconds. Therefore, the ability to sensitively follow these processes is invaluable for designing next-generation, tailored catalysts. SSRL's capabilities will support long-term experiments focused on catalyst deactivation, continuous scanning XAS (min-sec), quick scanning XAS (msec), modulation excitation spectroscopy (msec-sec), energy-dispersive X-ray emission spectroscopy (msec-µsec), and optical pump X-ray probe measurements (psec). These studies provide critical insights into the temporal evolution of active sites, enabling the design of more robust and effective catalysts. Synergistic studies between SSRL and LCLS will provide complementarity of time scales between SSRL BL15-2 and LCLS XCS/XPP instruments to the fs and nsec.

Coupling to Theory and Simulations. A detailed interpretation of experimental spectra, and the understanding of catalytic processes, can be elevated through coupling with appropriate theoretical modeling and advanced analysis tools. SSRL collaborates with the FEFF project, the TIMES program in collaboration with SIMES and LCLS, as well as with the OCEAN developers (NIST), and other relevant groups to apply these insights to XAS, XES, XRS, and RIXS spectroscopies. The routine usage of these codes is facilitated by our systematic access to supercomputing facilities like NERSC and SLAC's S3DF.



Operando boron 1s XRS spectra of species on hexagonal boron nitride during oxidative dehydrogenation of propane(left). High precision calculations (OCEAN code - center) reveal surface oxyfunctionalization transformations of BN sheets via bridging sites (right) J. Am. Chem. Soc. ***145****, 25686 (2023)*

3.2.2 Harvesting Solar Energy

Efficient harvesting and converting solar energy into chemical energy is a fundamental challenge and opportunity in the pursuit of future, distributed energy solutions. Photocatalysis, which harnesses light to drive chemical reactions, offers a promising pathway for directly utilizing sunlight to produce fuels, degrade pollutants in water sources, and synthesize valuable chemicals. The ability to harness sunlight for chemical transformations addresses the need for greater energy production with the potential for reduced pollution. Photocatalytic processes, such as water splitting to produce hydrogen or CO_2 reduction to generate fuels, have the potential to revolutionize the energy landscape. However, the efficiency of these processes is often constrained by the dynamics of charge carriers—electrons and holes generated through photoabsorption in semiconductors and molecular chromophores. Understanding how these charges are generated, separated, and ultimately utilized in catalytic reactions is crucial for unlocking the full potential of photocatalysis.

The SSRL Chemistry and Catalysis Division is at the forefront of advancing photocatalysis. Our research underpins initiatives like the LiSA Solar Hub, dedicated to harnessing sunlight to produce CO_2 upscaling products, and BES research projects focused on the photocatalytic production of hydrogen and ammonia. State-of-the-art X-ray spectroscopy techniques are applied to explore the fundamental and sequential processes involved in photocatalysis capturing the dynamics of charge carriers and catalytic activity at the atomic and molecular level.

New laser pump X-ray probe time-resolved spectroscopy capability developments have unlocked our ability to observe these processes from picoseconds to longer time domains. This enables not only correlating the structure and reactivity properties to function at a fundamental level but also to probe the charge carriers' dynamics. At the same time, our *operando* spectroscopy tools enable following the evolution of durability and decomposition mechanisms over realistic time frames, critical for the long-term viability of such emerging technologies.

The Division will continue to drive innovation in solar energy research by further optimizing the performance and availability of its X-ray tools. We will expand our capabilities by broadly implementing modulation excitation X-ray spectroscopy, to detect subtle spectral changes when synchronizing the X-ray detection with pulsed illumination of complete, multiphase photocatalytic systems, and introduce the new methods to the user community. This approach will provide deeper insights into the active phase and stability of photocatalysts, ultimately guiding the development of more robust and efficient systems. Central to our vision is the quest for efficient, earth-abundant molecular chromophores that can be attached near tailored biomimetic catalytic sites that drive targeted photocatalytic chemical conversions.

In the future, AI-driven predictions and advanced synthetic chemistry capabilities will be important drivers of this research and development program. These efforts, combined with continued technology development that allow for the detection of transiently formed species in complex photocatalytic environments are essential for realizing the full potential of solar energy conversion and paving the way for scalable energy solutions.

3.2.3 New and Planned Capabilities

The new SSRL BL10-2b will be a world-class, catalysis-centric, multi-modal, quick-scanning XAS beam line. The new optics include a Rh-coated collimating mirror that features a new cooling design that "sculpts" the heat transfer across the mirror surface minimizing thermal distortion effects, a toroidal focusing mirror and a quick-scanning double-crystal monochromator with an XAS collection speed of 10 Hz (1,500 eV scan range/ oscillation).

The end station will be equipped with advanced detection systems, including a 24-element Ge solid-state detector with Xspress electronics. The integration of dedicated *in-situ*/*operando* infrastructure will allow researchers to obtain seamless correlations between XAS and process conditions. The hutch will feature dual sample stages to facilitate simultaneous experiments, along with a sophisticated gas handling system that enables complex flow patterns and precise monitoring of catalytic materials, complemented by product detection through mass spectrometry and micro-gas chromatography.

We will enhance high-resolution spectroscopic capabilities across various beam lines. This includes developing and deploying user-friendly, robotic-based X-ray emission spectrometers for HERFD. We will implement modulation excitation spectroscopy capabilities by integrating advanced synchronized data acquisition systems at selected beam lines, broadening the scope of experiments that can be conducted at SSRL. We plan to expand our tender high-resolution X-ray spectroscopy program by optimizing and adopting a high-throughput X-ray emission instrument developed based on SSRL concepts for use at LCLS-II, ensuring that we remain at the forefront of X-ray spectroscopy innovation.

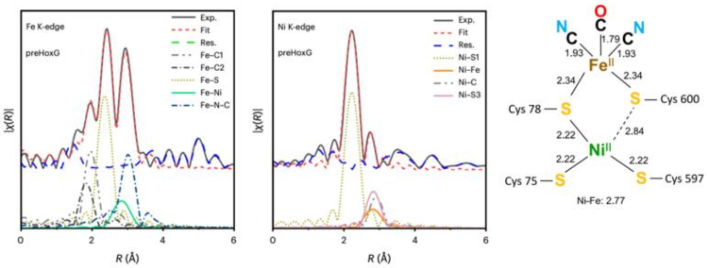
3.2.4 Enzyme and Bio-Inspired Catalysts for New Energy Sources

A key challenge in designing and developing new energy sources is the scarcity of suitable and inexpensive catalytic systems based on relatively abundant and economically viable first-row transition metals. Fortunately, Nature elegantly and efficiently utilizes these elements in complex metalloenzyme catalysis ranging from ammonia synthesis, production of potent fuels such as hydrogen and methane, functionalization of carbon dioxide, and the water-splitting reaction, with a high degree of precision under ambient, physiological conditions.

To harness the principles of biological catalysis and develop biohybrid or bioinspired technologies, a fundamental molecular understanding of metalloenzyme catalysis has to be developed, starting with atomic-resolution local geometric structure of the metal-based active site and extending to its detailed electronic structure in both its resting and transient intermediate states. The physico-chemical parameters emerging from such fundamental understanding of the metal active sites and their impressive catalytic activity can then be translated to industrial catalyst design to invigorate the principles of novel, efficient catalysts.

SSRL is playing a major national role in enabling detailed characterization of the structural and electronic properties of metalloenzymes related to bioenergy and associated biomimetic model systems. A novel multi-edge, HERFD and standard XAS approach spanning metal K- and L- and ligand K-edges is applied to biological systems, allowing for a holistic experimental definition of the electronic and geometric structure of the catalytic active site.

For a subset of biological systems amenable to in-vacuum measurements, researchers can conduct soft-to-hard X-ray spectroscopy experiments on sensitive biological systems – a unique strength of SSRL. This methodology is augmented with Kβ and V2C XES, and 1s2p RIXS measurements, which provide complementary spin state information and reveal specific bonding signatures that have direct implications to the performance of the biocatalytic systems.



The Fourier Transformed Fe K-edge (left) and Ni K-edge (middle) EXAFS of one of the maturation intermediate (preHoxG) of Ni-Fe hydrogenase formed during the sequential assembly mechanism of the $NiFe(CN)_2(CO)$ center in [NiFe]-hydrogenase which are biotechnologically relevant enzymes catalyzing the reversible splitting of H_2 into $2e^-$ and $2H^+$ under ambient conditions. The final structural model deduced from EXAFS analysis (right) Nat. Chem. Biol. ***19****, 498 (2023)*

Specialized beam lines and instrumentation will continue to enable hard and tender X-ray absorption spectroscopy of the active sites in metalloenzymes, biomimetic model systems, and homogeneous catalysis systems with bioenergy applications, including enhancements to multi-element Ge and Si energy discriminating detector systems, advanced electronics for signal processing, flexible cryostat systems – maintaining SSRL at the forefront of biological spectroscopy.

In addition, instrumentation and methodologies developed in the Chemistry and Catalysis Division for materials systems will be expanded to biological and biomimetic applications. Developments made for time-resolved and *operando* spectroscopy will be adapted for application to X-ray sensitive biological systems, such as the tender X-ray spectrometer for ligand Kβ XES, adding to the robust number of interrogation techniques available for biological systems. New sample delivery methodologies will be optimized for the conservation of biological samples consumed during these measurements.

SSRL will continue to drive research focused on geometric and electronic structure elucidation and structure-function correlation of metals centers in, and inspired by, biology. Some of the planned developments for biocatalysis are described below.

Automation and Remote Access. The concentration-limited nature of biological samples typically requires longer acquisition time. This makes them well-suited for the development of complete automation and operator-less experimental protocols. SSRL will develop robotics, automation and software to create an end-to-end pipeline for sample tracking, delivery and measurement on several of its hard X-ray spectroscopy facilities supporting biological XAS with a future goal of enabling full-remote measurements for enhanced user access and operational flexibility and efficiency.

Time Resolution. SSRL's BL15-2 adds the new dimension of static and time resolved spectroscopy capabilities for biological systems that are activated by light or by binding of small molecules. These include enzymatic systems such as nitrogenase, hydrogenase and photosystem II. These systems are particularly attractive for energy applications especially as a component of biohybrid solutions that use the enzymes, suitable mutants or model complexes that functionally mimic the active sites to perform the most energy demanding or complex catalytic steps. Furthermore, when coupled with genetic manipulations and/or chemical and photo-stimulation, transient reaction intermediates can be formed, trapped and interrogated using HERFD techniques. These studies will be coupled with similar measurements at LCLS at the fastest time domains.

Dynamics. For the investigation of chemical dynamics in the 1-300 ms time domain, microfluidic sample delivery technology developed at Stanford, which allows for smooth and precise liquid delivery will be coupled with XES measurements. These will build on recent combined HERFD-XAS and Kβ XES methods applied to model complexes that mimic the dilute, sensitive nature of biological samples demonstrating the ability to interrogate the electronic structure of very short-lived intermediates.

Simulations. Development of an integrated theoretical approach for spectral simulations of XAS/XES spectroscopic data, involving the specifics of biological environments, will be coupled to analysis and modeling of experimental data, through in-house research coupled with collaborations with groups that develop associated theory and codes. SSRL will leverage SLAC's S3DF facility to host its bioXAS scientific computing resource.

External and Internal Drivers. SSRL will continue to collaborate with DOE consortia targeting biological systems for catalysis, such as X-ray spectroscopy applications within the BOTTLE consortium whose focus is to determine the role of bio-inspired and biological catalysts in plastics degradation and upcycling. The X-ray measurements will be combined as appropriate with *in-situ* methods, such as electrochemistry and photoexcitation, as described in Section 3.2.1.

Furthermore, the biological spectroscopy program will continue BES Chemical Sciences-Physical Biosciences funded research, which focuses on the assembly of energy transduction systems and the regulation of energy-related chemical reactions within cells, including the structure/function of energy-relevant protein active sites for designing efficient bioinspired catalysts. Examples include the metalloenzyme carbon monoxide dehydrogenase (CODH), which is part of the multistep CO_2 capture and functionalization anaerobic pathway.

3.2.5 Planned Capabilities for BioXAS

As part of the SSRL Beam Line Renewal Initiative, an undulator-based spectroscopy and μXRF imaging beam line facility has been proposed for biological and biogeochemical applications (Section 5.2.3). The development of this future facility will be a focus for the bioXAS program at SSRL, and will feature many new developments in automation, robotics, fast scanning and high-throughput measurements.

3.2.6 Geochemistry and Biogeochemistry for Subsurface and Ecosystem Science

Chemical processes in soils and the subsurface are driven by reactions occurring at the molecular scale at interfaces between water, minerals, and biological surfaces, and in complex natural mesoscale systems in which dimensions range from 100 nm to kilometers. Full understanding of these natural systems often requires consideration of both bio- and geo- components and how they interact. There is emerging awareness of the need to understand the molecular-scale basis of these processes.

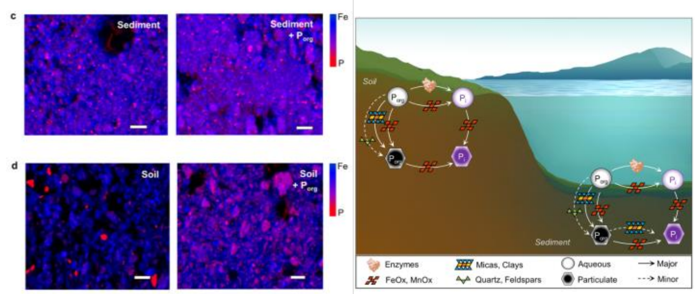
SSRL will respond to these needs through scientific leadership and continued enhancement of experimental synchrotron techniques, to provide information about bonding environments and electronic structure under *in-situ* conditions over a continuum of length and temporal scales, and to serve the needs of the national and international geo- and biogeochemistry communities. X-ray absorption spectroscopy and µXRF imaging continue to drive scientific frontiers. New and evolving research thrusts bring specialized analysis requirements. Strategic capability needs that will guide the development of beam line resources over the next few years include foci in the following sub-areas:

Redox Dynamics in Soil Microsites. Soils and sediments are critical filters and strong modifiers of groundwater and surface water quality, and atmospheric composition. Redox dynamics at small spatial (molecular to cm) and short temporal (minutes to days) scales are increasingly recognized as contributing to environmental outcomes at watershed scales. SSRL has developed the capability to image redox-sensitive element speciation at the micro-scale across large spatial domains in soil and sediment cores to detect and quantify microsites across a wide variety of soil environments, enabling advanced modeling of the contribution of microsites to the global carbon cycle and, for example, contaminant mobility.

Colloid Transporters. SSRL is developing a pipeline approach for studying colloids, i.e. small, suspended particles that move with water, but are not dissolved and therefore have different dynamics. As colloids are underestimated carriers of carbon, nutrients, and contaminants, there is a strong need for characterizing them to understand and predict their role in natural environments. The approach will include field sampling and bench-top experiments, field-flow fractionation of colloids based on physical characteristics, and XAS and microscopic (e.g., cryoEM) analyses of their composition.

Multi-modal Imaging Platform. The SSRL µXRF imaging program has developed an integrated setup for simultaneous UV-visible, XAS and µXRF imaging data collection, as well as sequential collection of spatially-resolved FTIR microscopy data.

The integration of these multimodal datasets enables complementary information on materials (such as organic compounds) that typically do not have strong hard X-ray signatures. In the future, SSRL will grow this multi-modal imaging platform through collaborations with university and national laboratory partners for mass spectrometry imaging (EMSL) and synchrotron IR (ALS), development of integrated software analysis packages, and expansion to additional imaging modalities, i.e. fluorescence bioreporter imaging, fluorescence lifetime imaging, and Raman spectroscopy, targeting DOE's biological and environmental sciences research mission.



*µXRF imaging data (left) (SSRL BL2-3) showing that phosphate incubation of soil and sediment was primarily associated with Fe oxy(hydr)oxide minerals, as determined by Fe K-edge XANES spectroscopy highlighting the role of Fe-based minerals in abiotic catalysis. (right) Proposed role of soil and sediment minerals in the geochemical cycling of organic phosphorus. Nat. Commun.**15**, 5930 (2024)*

SEES Science. SSRL is partnering with the NSF Synchrotron Earth and Environmental Science program (NSF SEES) to advance research and education in synchrotron-based Earth and environmental science. The future goal of this multi-year effort is to better understand our planet from the atmosphere to the core, and to train the next generation of scientists. SEES leverages facilities across all DOE funded synchrotrons in the U.S.

HERFD µXRF imaging. Trafficked nuclear materials pose a world-wide threat, and it is of high importance to determine the origin of illicit materials. Subtle molecular clues can indicate specific nuclear fuel cycle chemical processes during fabrication and types of further chemical processing. SSRL has developed a HERFD µXRF imaging spectrometer which enables quantification of actinide redox and chemical states with high chemical contrast at the L and M edges, and at the micro-scale (NNSA funding). The technique enables the additional characterization of micro-scale variability and can provide complimentary information to particle morphology and isotopic compositions. Use of the instrumentation and methodology will in the future be expanded to the general geological and biogeochemistry user communities.

3.3 Structural Molecular Biology

The goals of understanding biological structure and function and applying this knowledge to address a wide range of issues is a large, worldwide multidisciplinary effort. It engages academic, national laboratory and corporate researchers whose goals range from innovative fundamental discovery-based science to applied uses, such as more effective approaches involving biotechnology, the acceleration of drug discovery, and enhanced approaches for bioenergy and bioremediation.

Within this context, the SSRL Structural Molecular Biology (SMB) program (funded by the Department of Energy, Office of Biological and Environmental Research, the National Institutes of Health, National Institute of General Medical Sciences, and non-federal partners), is focused on enabling scientists to rapidly obtain and utilize structural information on biomolecular and bioinspired systems at the micron-to-atomic length scale to understand function (and malfunction) in biological processes. The SMB program has pioneered and will continue to lead development of new and enhanced approaches for investigating the links between biomolecular structure and function, and making these methods widely and rapidly available to the biomedical, bioenergy, chemical and biogeo-chemical research communities.

The focus of the SMB program is on integration of macromolecular X-ray crystallography (MC), biological small/wide angle X-ray scattering/diffraction (SAXS/WAXS), µ-X-ray fluorescence (µXRF) imaging, and X-ray absorption (XAS) and emission spectroscopy (XES) to study the most challenging and wide-ranging biological systems – leveraging the powerful capabilities of the SSRL synchrotron (SPEAR3) and state-of-the-art beam line instrumentation and methodologies.

There is further synergy with the LCLS X-ray free electron laser and the SLAC-Stanford cryo-electron microscopy (cryoEM) and cryo-electron tomography (cryoET) facilities and various advanced light, electron and X-ray bioimaging programs across SLAC/SSRL. Collectively, these techniques provide a remarkably rich and broad window on structure and function across a wide range of biologically relevant length and time scales, creating the foundation to extend results at the atomic and molecular level to understanding complex macromolecular interactions, and to studies of organelle, cell and tissue organization and function. Towards this, SMB program scientists are leading the science case for a proposed beam line related to the SSRL Beam Line Renewal Initiative, i.e. an undulator based spectroscopy and µXRF imaging beam line facility for the investigation of biological and biogeochemical problems.

The SMB program will continue to strengthen partnerships with *i)* Stanford University Institutes and Centers, including ChEM-H, Bio-X, and IMA, expanding on existing joint programs for MC beam line development and science, *ii)* with industry on high throughput drug discovery developments, and *iii)* private institutions on emerging scientific topics. Partnerships with the new Stanford Doerr School are also being vigorously pursued with its departments involved in biogeochemical sciences.

The SMB program will continue to engage with other user facilities and where relevant, lead multi-user-facility arrangements in areas that provide user access to complementary techniques, such as with the Environmental Molecular Science Laboratory (EMSL) and the Joint Genome Institute (JGI), and in coordinated outreach programs within BER-funded facilities and research groups. This includes targeted outreach to potential new SMB users at universities and the BER Bioenergy Research Centers, and collaborations with large-scale Science Focused Areas involved in understanding complex plant-rhizosphere and soil-microbial interactions at the national labs.

3.3.1 Bioengineering and Human Health

Macromolecular Crystallography (MC) will increasingly focus on understanding the complex biological machinery that enables and drives the biology and chemistry in cells, and on harnessing this knowledge to accelerate developments in biotechnology, medicine and bioenergy. This is particularly facilitated by the internationally competitive, microfocus undulator beam line (BL12-1) commissioned in 2020, and by a variety of related methodological and technical developments. Together, these can rapidly provide crucial information that advances the understanding of complex biochemical processes. This focus is also enabled through synergistic implementation of some of these developments at the Macromolecular Femtosecond Crystallography (MFX) station at LCLS and coupled developments with SLAC's cryoEM/cryoET capabilities.

More specifically, our aims involve: *i)* structural studies of macromolecular assemblies, membrane proteins and metallo-enzymes, *ii)* accessing the biodynamics of these systems through advanced multi-temperature and time-resolved approaches, and *iii)* new automated and AI-assisted workflows supporting increasingly challenging bioengineering goals, including accelerated structure-based therapeutics developments.

With advances in crystallization, sample delivery, instrumentation including robotics and remote-access, data analysis and computational methodologies and X-ray beam properties, a significant number of new and challenging structures can be determined by SSRL's large user community, providing details essential for understanding a range of cellular functions regulated by these complex systems and leading to practical benefits such as the acceleration of structure-based drug design. For example, research in structural virology will offer essential insights in an expedient manner that can help drive the development of pharmaceuticals and other interventions.

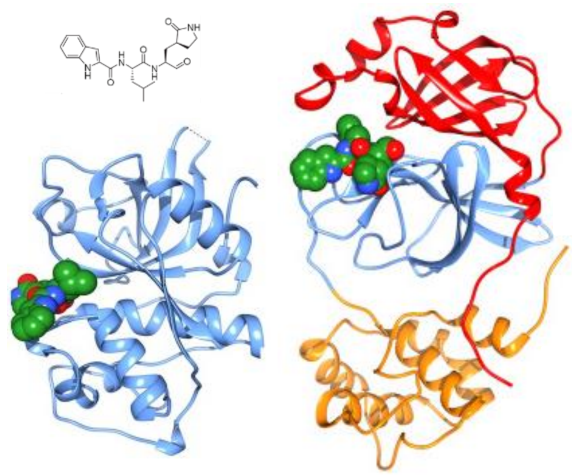
Further, as aging cells display features that are not present in healthy cells, they may be targeted through drug-related therapies as an approach to extending both the duration and quality of life. Such new drug-related therapies will tackle age-related pathologies, including cancer, cardiovascular diseases, neurodegeneration, chronic pulmonary diseases, and diabetes — the leading causes of death in the US.

Through a DOE BRaVE-funded initiative, our developments will enhance US biopreparedness by providing advanced AI tools and advanced workflows that address bottlenecks in structure-based drug development. This initiative will also bring high-throughput methods for drug discovery to a wider research community. We leverage extensive advancements at SSRL, supported initially by the NIH Protein Structure Initiative, to accelerate fragment-based drug discovery. We expect these tools will expand collaborations with industry, Stanford and other universities and research institutes.

With continued R&D, structure determination of metalloenzymes in medically relevant intermediate states will become routine, enabling users to investigate transiently formed, trace metal-bound species which provide direct insights into the mechanisms of biochemical processes linked to human health and disease. In this context, new approaches will be developed to detect *in situ* formed transient species and mitigate radiation damage in high-valent metal intermediates and oxygen-sensitive enzymes.

The methodological and technological developments, summarized below, will enable the science outlined above, as well as enabling a growing array of related studies by SSRL's user community. These developments build on the highly automated, reliable and fully remote-accessible MC beam lines at SSRL, as well as on automated data collection, reduction and analysis software supported by high-capacity, high-performance computing facilities. Specific emphasis going forward will be on the following areas:

- Development of next generation time-resolved methods at undulator micro-focus BL12-1 through the implementation of state-of-the-art experimental capabilities that include µs to ms pulsed, high-intensity, broad bandwidth X-rays synchronized with its EIGER-2XE-16M detector, a high-speed X-ray chopper, and a high-speed microcrystal goniometer.
- Development of innovative methodologies to tackle challenging projects that explore the link between biological structure and function, including investigation of high-valent intermediate states of metalloenzymes and the study of large multi-component complexes. These experiments will require developing methods for *i)* collecting X-ray diffraction data free from radiation-induced artifacts, *ii)* utilization of small, radiation-sensitive crystals, and *iii)* implementation of controlled sample environments across multiple temperatures.
- Synergistic developments on the LCLS MFX station with emphasis on supporting customized experimental instrumentation and new software for data reduction and analysis of femtosecond and broad X-ray bandwidth data – with the goal of providing an effective gateway between the SSRL BL12-1 and the LCLS MFX station for the SMB research community across SSRL and LCLS.
- Development of novel automated workflows for accelerating structure-based drug design efforts. The focus will be on fragment-based screening and the integration of molecular dynamics and modeling approaches and structure-based informed feedback. Emphasis will be placed on discovering new drugs for serious illnesses and in combating the escalating challenge of drug resistance.
- Harnessing the powerful synergy between high-throughput structural biology and advances in machine-learning, we will develop predictive models that expand automation in data collection and real-time structural analysis, enabling rapid, reliable insights into protein-ligand interactions and dynamic enzymatic processes. At the same time, the structural data we generate—particularly from time-resolved studies and compound-bound protein complexes—will serve as critical training sets to develop next-generation AI/ML models. The compounded benefits of this cycle between high-throughput experiments and machine learning analysis will accelerate progress in enzyme engineering, predictive analytics, and therapeutic innovation.



Co-crystal structures of two SARS proteases critical to virus replication: CTSL (left) and SARS-CoV-2 M^{pro} (right) complexed with the active form of olgotrelvir (represented as green-red-blue spheres). The strong drug inhibitor resides in an active site cleft in both complexes and forms similar covalent bonds to a cysteine sulfur as well as forming hydrogen bonds with surrounding residues. Med. ***5***, *1 (2024).*

3.3.2 Biological Structure and Dynamics in Solution

The native aqueous solution environment plays a crucial role in enabling and maintaining biological function. Studying the structure of biological macromolecular systems in solution as non-crystalline or partially ordered arrays of biomolecules is thus vital for understanding their biological mechanism and function. Unlike crystalline structures, which are primarily rigid and well-ordered, non-crystalline systems in solution are dynamic, can exist in various conformational states and allow for the functionally important structural flexibility of such biological systems and assemblies. These systems often include proteins, nucleic acids, lipids, and complex assemblies that do not easily form crystals.

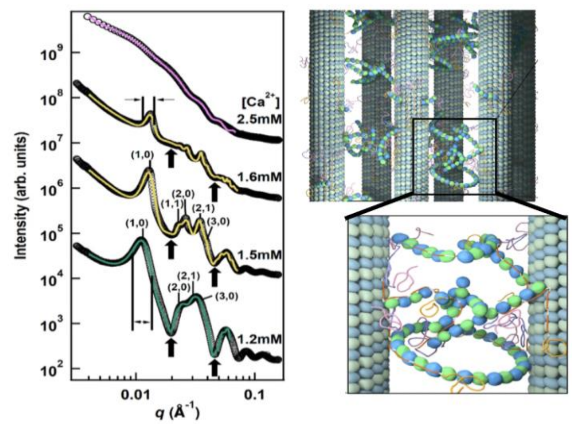
Biological small/wide-angle X-ray scattering and diffraction (BioSAXS/WAXS, hereafter simply BioSAXS) is one of the primary tools to study the solution structure of non-crystalline partially ordered biological macromolecular systems. The studies can be performed under near physiological conditions and require only small amounts of material. These conditions are also well-suited for time resolved measurements, e.g. measuring the kinetics of conformational changes, or the identification of reaction intermediates in a biologically relevant environment and on biologically relevant time scales.

The SSRL biological BioSAXS BL4-2 features state-of-the-art experimental facilities for solution scattering, lipid membrane and fiber diffraction at moderately high to very small scattering angles. Advanced robotic sample handling provides capabilities for robust on-site and remote high-throughput experimentation with small sample volumes. *In-situ* chromatography coupled solution SAXS (with optional in-line MALS and DLS detection) and millisecond time-resolved SAXS data collection modes are supported. Real-time data processing enables data analysis during the experiments to drive the scientific and experimental strategy. Non-X-ray offline characterization tools include dynamic light scattering instrumentation, providing at times critical sample characterization information.

Prime examples of scientific applications of BioSAXS are the maturation process of virus particles or protein folding, disordered biomolecules such as the amyloid precursor proteins as well as the solution states of protein families related to the human and bacterial microbiomes, systems for drug delivery, and mechanistic insights into biological processes through understanding of conformational flexibility differences in solution and crystal forms. Future developments will focus on the further integration and simultaneous use of non-X-ray-based characterization tools and methods, such as refractive index, UV/Vis absorption, and static and dynamic light scattering, and taking full advantage of recent advances in protein structure prediction (e.g. AlphaFold) to guide and complement the SAXS analysis as well as coupling this to cryoEM developments and applications.

Specific scientific and technological developments for the BioSAXS facilities at SSRL will focus on:

- Increasing the angular range of the instrument to routinely enable simultaneous SAXS/WAXS measurements with a continuous q-range to increase the structural resolution of the solution measurement and take advantage of new, emerging modelling approaches.
- Significantly advancing the instrument capability for remotely accessible data collection of high-quality time-resolved SAXS data from biological samples using microfluidic and stopped-flow approaches.
- Increasing the capabilities for remote experimentation by expanding the robotic sample manipulation to enable elaborate changes of sample conditions such as filtration and buffer exchange.
- Expanding the real-time data processing and analysis pipelines and increasing their flexibility to enable new experiment-specific workflows and data quality assessments as well as the inclusion of complementary characterization data.
- Developing and implementing standard workflows for SAXS data analysis that take full advantage of available complementary sample characterization data as well as recent advances of in-silico structure prediction.



SAXS data infer that tubulin oligomers and the microtubulin associated protein, tau, form a viscoelastic intervening network that cross-bridges microtubules (MTs) into bundles. The bundling occurs due to coded assembly where tau's MT binding repeats link together αβ-tubulin oligomers in the intervening network (IN) and near the MT surface to tubulin in the MT lattice (right top, and enlarged at bottom). The complexes of tubulin oligomers and tau within the IN, as well as those bound to MTs not in bundles, may represent an important site of enzymatic modification of tau leading to aberrant tau behavior causing tau fibrils in tauopathies. Nat. Commun. ***15****, 2362 (2024).*

3.3.3 Role of Metals in Human Health and Bioenergy

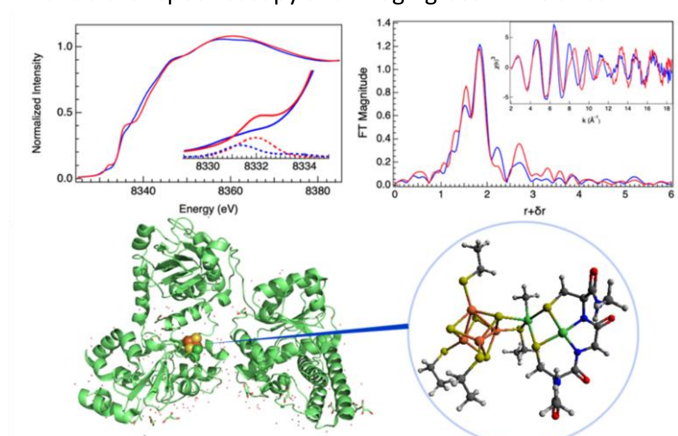
Metal ion transformations and homeostasis are vital to life and natural processes. For human health, intricate and codependent cellular processes exist that are tightly coupled with metal regulation for electron transfer, oxygen transport/insertion, molecular signaling and transformations. Their dysregulation directly manifests in neurological disorders, cardiovascular diseases, cancer, cytotoxicity and DNA damage. Beyond health, biology has many examples of flexible, self-repairing, and adaptive molecular-to-organism scale systems that can generate, store, and transform energy. Synthetic approaches involving biometallocenters and biohybrid catalysts can create entirely new functions to transform the technological landscape of energy and environmental conservation systems.

In addition to molecular/cellular processes, metal ions and ligands play critical roles in heterogeneous soil, microbial and rhizosphere processes and integrally participate in plant-soil-microbe interactions. Understanding their complex transformations can increase or restore bioenergy plant ecosystem productivity, and improve plant responses to a wide range of environmental perturbations. In these heterogenous and multicomponent interactions, metal ions and ligands display their remarkable ability to achieve an impressive range of redox and chemical states, which have the promise of guiding scientists to find cures for diseases and to develop transformative technologies.

The SSRL SMB BioXAS and imaging program has developed dedicated facilities with optimized beam lines and specialized instrumentation and analysis capabilities for enabling biological, biomedical, and bioenergy research that enable researchers study metal ions and ligands in their native, unperturbed (solution and stain-free) and biochemically redox-poised forms or as transient intermediates using sec-msec characterization modalities. Towards this, a suite of spectroscopic capabilities, including standard and high-resolution (HERFD) X-ray absorption (XAS), extended X-ray absorption fine structure (EXAFS), emission (XES) and resonant inelastic scattering (RIXS) spectroscopies, are implemented spanning tender to hard X-ray energy regimes. Spatially-resolved information about metal distribution and speciation in materials of biological and medical relevance, ranging in length-scale from the cellular-to-tissue and larger can be achieved using our μXRF facilities. By providing detailed atomic-level local electronic and geometric information that is highly complementary to the structural information obtained by MC or SAXS, the SMB program's capabilities enable unprecedented understanding of biological transformations through direct study of the chemistry of the active metal sites.

Future R&D and methodological developments on the BioXAS and imaging facilities will focus on expanding remote access and high-throughput measurements, improving detection limits and sampling modalities and integrating software approaches for measurement and analysis, including:

- Expansion of BL7-3 for full remote access experimentation featuring robotics for sample transfer and automation for uninterrupted measurements on dilute biological samples, significantly enhancing user access and measurement flexibility.
- Growing the biological user program on the microfocus undulator BL15-2; pushing the forefront of biological XES/RIXS/HERFD-XAS applications to increasingly dilute systems for static and dynamic measurements, including experiments in the ns-ms time domain at SSRL and, with coupling to LCLS experiments, into the fs time domain.
- Developing new instrumentation with implementation of partial fluorescence yield analyzer detection approaches and robotics enabled spectrometers for enhanced precision and adaptability, improved S/N ratio and experimental throughput.
- Integration of multimodal imaging and spectroscopy tools, which provide complementary and holistic information on metals and ligands, starting with electron paramagnetic resonance, IR, optical fluorescence and soft X-ray μXRF capabilities.
- Developing instrumentation for imaging of biological specimens, extending to XAS tomography. Software developments will create a holistic platform to integrate, co-register and analyze multi-laboratory data such as synchrotron IR, mass-spectroscopy imaging and various optical modalities with X-ray data, revealing precise understanding of metal-organic matter interactions.
- Driving innovations in plant sample growth, delivery and high throughput μXRF measurement for plant rhizosphere research at SSRL that allows for the systematic evaluation of plant-soil-microbial interaction on bioenergy crop growth and yield to support SLAC's broader effort in energy and biological sciences and future development of a new undulator spectroscopy and imaging beam line at SSRL.



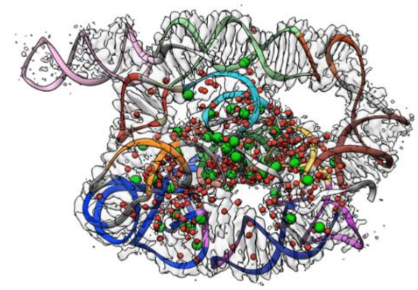
Ni K-edge XAS (top left), EXAFS and Fourier transforms (top right) of the trapped methylated intermediate of acetyl CoA synthase (bottom), which is a critical enzyme in the anaerobic Wood-Ljungdahl pathway of CO_2 fixation. These high-k Ni K-edge data reveal the geometry and electronic structure of the active site, the role of Ni in binding reduced CO_2 species, and the final step of C-C fusion and acetate formation. BioXAS program-supported scientific computing capabilities enabled detailed quantum chemical calculations on these intermediates to arrive at the role of protein residues and the covalently linked Fe-S cluster in tuning reactivity. J. Am. Chem. Soc. ***145****, 13696 (2023).*

3.3.4 Cryo-Electron Microscopy and Tomography (CryoEM/ET)

Using electrons, Cryo-Electron Microscopy (cryoEM) and Cryo-Electron Tomography (cryoET) techniques provide images of biological materials that are frozen in their native state, ranging from proteins and nucleic acids to very large biological assemblies and complexes, at resolutions that range from nanometer to the near atomic level. CryoEM uniquely captures dynamic ensembles of macromolecular structures as they occur in frozen solution through its ability to sort and average conformational sets. Image analysis can then separate these ensembles to produce high-resolution snapshots capturing their compositional and conformational variance and their dynamics.

CryoET is an emerging technique that can resolve subcellular structures inside the cell and tissue, with the capability to reach nanometer resolution for the entire sample and near atomic resolution for abundant molecular components *in situ* with post-tomographic data processing of those structures. Cryo-Fluorescence Light Microscopy (Cryo-FLM) and subsequent cryoET of frozen, hydrated cells can be used to label specific proteins and study cellular and molecular locations, functions and dynamics in the 3D context of cells and tissues at a higher resolution than any other imaging techniques. cryoET can be preceded by Focused Ion Beam Scanning Electron Microscopy (cryoFIB-SEM), to produce lamellae from vitrified cells that are thin enough for cryoET imaging.

CryoEM/ET facilities within the CryoEM & Bioimaging Division at SSRL are wide-ranging and currently include a suite of seven 100-300 kV electron microscopes, three cryoFIB-SEMs, and sample preparation and data analysis tools.



CryoEM structure of a ribozyme revealing a complex network of water and Mg^{2+} throughout the RNA. Nature (2025) doi.org/10.1038/s41586-025-08855-w.

Some of these are associated with two NIH funded national centers, the Stanford-SLAC CryoEM Center, and the Stanford-SLAC CryoET Specimen Preparation Center. There is synergy among the cryoEM program and the SSRL's SMB X-ray facilities in R&D, science and user access programs.

The suite of cryoEM/ET instruments are used for a wide range of biological and biomedical research by scientific staff, faculty and external users. Scientific applications include high resolution structural study of viruses and their interactions with receptors and antibodies, membrane-bound proteins including trans-porters and pumps, molecular machines involved in metabolic pathways, bacteria, free-living algae, plant tissues and cells under normal or environmentally stressed conditions.

There is a growing interest in extending these techniques to materials science applications at SSRL. A DOE-BES field work proposal project at SLAC and Stanford currently supports both cryoEM and -ET studies of beam sensitive electrochemical materials and methodological developments to facilitate cryo-genic microscopy studies of beam-sensitive materials. The SSRL Directorate is committed to growing the scientific and user support interface by SLAC's cryoEM facilities and the Lightsource.

4 Computing and Data Methods and Infrastructure

The computing, networking and data topology at SSRL was designed primarily to enable robust storage of user data, transfer that data back to the user home institution, and limited support to access scientific computing software and data processing tools on local servers hosted by SSRL. Over the last decade, several factors have increased both data rates and data complexity including the growing deployment of large area detectors, integration of multiple characterization modes within a single experiment, increased experimental throughput, and expanded *operando* and *in-situ* user programs. These trends are driving an evolution in how SSRL is approaching data stewardship and computing.

The increased throughput of *ex-situ* measurements, and increased complexity of *in-situ* and *operando* measurements both require maturation of data handling to enable real-time data visualization and interpretation to enable both humans and algorithms to make informed decisions actively during the course of a measurement and across a full experimental run.

SSRL has been at the forefront of developing machine learning algorithms and automated data analysis pipelines. Our focus on developing automated data interpretation algorithms will continue; however, the diversity of science at the facility makes it unlikely that SSRL will be able to tackle this challenge alone in a way that scales to all users. To complement our internal development efforts, we will also focus on continuing to build a strong network of collaborations with the global light source community, local industry ecosystem, and academic partnerships to enable both collaborative development as well as building awareness of new tools, developed elsewhere, which can be deployed at SSRL.

User experiments are already moving to increased automation. Beyond visualization, automated data analysis also enables artificial intelligence and machine learning algorithms to actively drive experiments and/or inform researchers about possible next measurements in complex multi-parametric experimental design.

Enabling Advanced Scientific Computing and Machine Learning

We will continue to collaboratively develop and deploy classic active learning algorithms, that can be run either autonomously or with human-in-the-loop, to drive decision making during measurements.

Large language models are beginning to fundamentally change the way scientists can incorporate prior scientific knowledge into experimental design. We will leverage the world leading expertise within the local University ecosystem to tailor large language models and multi-modal transformers to enable users to incorporate prior literature, data, and instrument configuration into agentic frameworks that can partner with scientists during their beamtimes.

The development and deployment of algorithmic tooling into the user experiment will require shifting how SSRL stewards data and connects users to computing resources. We will mature our approach to data stewardship, deploying modern data storage modalities such as relational databases that enable user data to be collated, and correlated across instruments, experiments, and beamtimes while also enabling facile data access. The compute resources required for algorithm training, autonomous data interpretation, and algorithm deployment will vary from that available locally at the beam line to what can only be provided by high performance computing centers. To provide these capabilities, we will build increased connectivity between local SSRL, SLAC, and DOE computing resources. Collectively, these approaches will enable SSRL to scale the integration of AI/ML and advanced computing broadly to our user program and move beyond demonstration.

5 Operational Innovation

5.1 Accelerator Improvement Plan

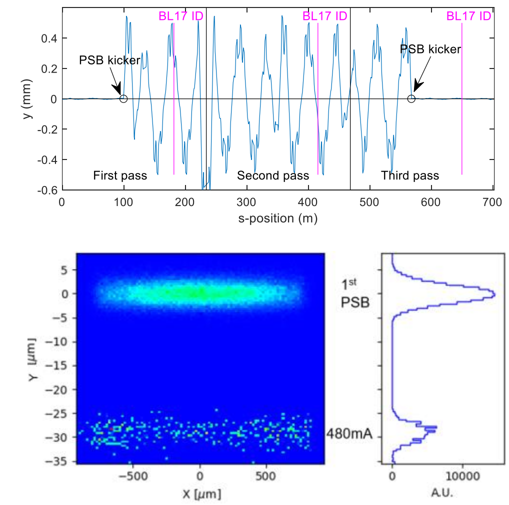
The SSRL accelerators form the foundation for the high level performance of the synchrotron radiation experimental stations at SSRL and the user science they produce. The reliability of the entire SSRL accelerator complex and the electron beam performance in SPEAR3, the 3-GeV storage ring for SSRL, are critical to the SSRL user experience and the overall science output. The SPEAR3 ring delivers a steady 500-mA beam for user programs in top-off mode. New accelerator operational modes are in development that will enable new science opportunities at the facility. The SSRL accelerator team is devoted to operating the accelerators at their optimal conditions and developing new capabilities to meet user needs. This is achieved through continuous improvement of the accelerator hardware, control software, and operational protocols. The team is also engaged in R&D toward future major upgrades of the facility, and other R&D work that will benefit the accelerator community at large in accelerator design, commissioning, and operation.

The next sections discuss the ongoing, short-term accelerator improvement work, major accelerator projects aimed at improving long-term operational reliability that have recently been enabled by the increase in SSRL base operations funding, and various accelerator related R&D activities at SSRL.

5.1.1 Short-term Accelerator Performance Improvements

Pseudo Single Bunch

There is an increased focus at SSRL on science programs that are based on time-resolved capabilities. SPEAR3 accelerator developments have evolved such that today SSRL can accommodate time-resolved experiments without impacting regular experiments by using a hybrid fill pattern which consists of a camshaft bunch separated from a few bunch trains. Currently, the camshaft bunch that serves timing experiments is on the same orbit as the regular bunches; hence synchrotron radiation from the latter causes sample damage and undesired background signals for timing users. By employing a high repetition-rate, fast kicker installed in the storage ring, the camshaft bunch can be placed on a different orbit than the regular bunches. This pseudo single bunch (PSB) mode of operation can greatly benefit timing experiments, while it remains largely transparent to regular users. The PSB can operate at the ring revolution frequency of 1.28 MHz or, if combined with a small change to the lattice, at reduced repetition rate as desired. The PSB mode requires a kicker and a pulser to drive the kicker. The pulser specification has been determined and the kicker design work is ongoing. The completion of the PSB project, currently planned for FY2026, will substantially enhance the timing experimental capabilities of SSRL. Associated beam line modifications are described in Section 5.2.1.



(Top) The PSB kicker puts the camshaft bunch on a different orbit to create a transverse separation between the timing and the regular beams and restores the orbit on the third pass. (Bottom) The photon beam separation at the focus point. The signal-to-noise ratio is increased to 1000:1.

31-Bunch Timing Mode Development

Some timing experiments prefer a higher repetition rate than 1.28 MHz as provided by the camshaft bunch. An alternative fill pattern of 500 mA in 31 uniformly distributed bunches would provide a repetition rate of 39.7 MHz and the desired high bunch current. This mode of operation would be transparent to non-timing users. However, because of the increased peak current, vacuum components would see substantially higher beam-induced heating. In experimental tests, the intermediate mode of 500 mA in 124 bunches has been demonstrated, albeit with a lower than desired bunch current. Heating issues for a device that is used to measure the beam current was found to be the limiting component from realizing the desired 31-bunch mode. R&D work is ongoing to determine the appropriate replacement of the device, and a future project will enable its implementation and initiation of this new mode of operation.

SPEAR3 Orbit Stability Improvement

With fast orbit feedback (FOFB), the electron beam in a storage ring generally has high stability of beam position. However, the stability performance is still subject to limitations in beam position monitor (BPM) and corrector-to-beam response. Ground motion and thermal drift affect both BPM and beam line optics, further impacting photon beam stability, the ultimate performance metrics that matter to users. A coordinated effort is ongoing to identify the sources of photon beam performance drifts and to mitigate them. Potential paths for improvement include incorporating photon beam parameters in the electron beam orbit control, improving the orbit feedback algorithm, and developing better feedforward to compensate known sources of drifts.

5.1.2 Accelerator Reliability Improvements

Injector Control Software Upgrade

Work has commenced on upgrading the part of the SPEAR3 Injector control electronics and control software that rely on the VMS operating system.

The Injector employs CAMAC control electronics as it was widely used on accelerators in the early 1990's, the era in which the Injector was built, and the VMS operating system, a powerful system with real-time control capability, was chosen to run the Injector control software at that time. Channel access to the CAMAC controls was enabled with software that runs on VMS in a later upgrade. The system has run reliably for many years. However, CAMAC and VMS have become obsolete. Maintenance of such hardware and software has become increasingly difficult as expertise needed for the task becomes hard to find. The upgrade work currently underway is expected to be completed in two years. Replacing these legacy systems with modern ones will ensure reliable operation of the Injector for many years to come.

SPEAR3 Orbit System Upgrade

We are working on upgrading the SPEAR3 orbit control system, including BPM electronics, corrector power supplies, and fast-orbit-feedback (FOFB) control. The new system will be based on a modern design such as the one for the Advanced Light Source Upgrade (ALS-U) project. The upgrade will address reliability concerns with the current system and bring in many advanced features, substantially enhancing the orbit control performance. The upgraded system will take advantage of the vast technological advances in electronics in the last decade. New BPMs will have modern features such as turn-by-turn capability, which is very useful for beam diagnostics. There may also be gated sampling capability, enabling measuring the orbit of a fraction of the beam bunch train. The gated sampling feature would be of tremendous value for the timing experiments utilizing the PSB mode as it will allow independent orbit monitoring and control for the camshaft bunch.

SPEAR RF Solid State Amplifiers

The SPEAR3 RF system is based on technologies developed for the PEP-II collider. The strategy to rely on PEP-II RF technology has resulted in substantial savings in development and maintenance cost. However, with PEP-II decommissioned and the team of engineers and technicians supporting the technology gradually phasing out from SLAC, it is increasingly difficult to support operations of the SPEAR3 RF system. The system consists of high voltage power supplies (HVPS) and klystrons now unique at SLAC. Continued operation of this system into the future on the 10-15-year time scale will be very challenging. RF power sources based on solid state amplifiers (SSA) are a mature technology today and have been in use in a multitude of synchrotron light source facilities. Upgrading the SPEAR3 RF system by replacing the HVPS and klystron with SSA will provide an ideal solution to the challenge. SSRL is currently undertaking a planning process for this replacement with the goal to seek additional funding for its implementation.

5.1.3 Accelerator Research and Development

SSRL Upgrade Lattice Design Studies

With the completion of the emittance reduction AIP project in 2022, SPEAR3 operates with a 7-nm emittance at 3 GeV, a remarkable achievement for the limited footprint of the ring. However, compared to the sister laboratories (e.g., ALS-U and APS-U) that are going through major upgrades to rebuild the storage rings as multi-bend achromat (MBA) lattices, the photon beam brightness at SSRL will become much less competitive for brightness-limited experiments.

Achieving a long-term competitive position in the synchrotron light source community in photon beam brightness requires replacing SPEAR3 with a modern storage ring. Building upon the experience and technology advances at other synchrotron light source laboratories, SSRL has the opportunity to design and build a world-leading storage ring with unparalleled performance. Design studies for lattice upgrade options have made significant progress in the last few years. Work will continue to explore options that can yield substantial performance gains. Technological developments that can increase storage ring performance under financial constraints, e.g., in magnet and vacuum technologies, and with outstanding operational stability, will also be explored.

Advanced Operation Modes in Diffraction Limited Rings

One of the upgrade options for SSRL is to build an ultra-low emittance storage ring in the 2.2-km PEP-II tunnel. The PEP-II tunnel consists of six 120-m long straight sections, which opens up possibilities for advanced operation modes that could produce substantial performance enhancement compared to regular storage ring beams. For example, ring-based free electron lasers (FELs) could be possible via echo-enabled harmonic generation (EEHG), cavity-based X-ray FEL (CBXFEL), or other schemes. SSRL will continue to pursue this concept to assess the performance and to understand possible limitations of various options.

Beam-based Optimization Algorithm Development

Beam-based methods are critical for accelerator commissioning and operation as they help discover errors in the machines and find proper settings to compensate for the errors. The SSRL accelerator team has played a leading role in developing beam-based optimization algorithms and applying them to solve important real-life accelerator problems. For example, the robust conjugate direction search (RCDS) and the multi-generation Gaussian process optimizer (MG-GPO) are two methods developed at SSRL which have found applications in many other laboratories. A more recent innovation is the development of a method to compensate accelerator performance drifts. The team has also developed many beam-based correction methods, such as parallel beam-based alignment (PBBA) and linear optics correction and coupling correction with closed-orbit modulation (LOCOM). Work will continue in this area, in particular on three topics of great interest to the community: correction of nonlinear optics errors, efficient tuning of nonlinear beam dynamics, and development of safe tuning methods suitable for application during user operation. By combining expertise in beam dynamics, numerical simulation tools, and advanced data analysis techniques, such as machine learning methods, we expect to make further contributions over the next several years.

5.2 Beam Line Development and Technical Capabilities

SSRL has developed and substantially implemented a plan that will keep SSRL beam lines competitive and productive over the coming years by using key scientific objectives to direct the integrated development of new and upgraded beam lines with innovative hutch equipment and state-of-the-art detectors. This beam line build-out plan significantly increases both beam line capability and capacity. The light source currently features 24 operating beam lines equipped with 29 experimental stations: 9 independently operating bending magnet beam line stations on 5 bending magnet sources and 20 independently operating insertion device beam line stations on 11 insertion device sources (4 in-vacuum undulators, 2 elliptically polarizing undulators, 5 wigglers).

SSRL recently completed an ambitious program of developing new undulator beam lines as one key goal of the strategic development plan. The first of these new in vacuum undulator (IVU) beam lines, BL15-2, was developed to support advanced spectroscopy applications including time domain measurements and has recently commenced regularly scheduled user operations. IVU BL12-1 was developed as a micro-focus macromolecular crystallography beam line, which expands upon the successes of the companion BL12-2 IVU crystallography beam line. BL12-1 completed an accelerated commissioning program in 2020 and was immediately employed in COVID-related research. IVU BL17-2 was developed to serve the materials scattering research community requiring a higher brightness source than existing wiggler beam lines at SSRL. This beam line, which features SAXS, WAXS, and time domain research capabilities, commenced user operations in 2022.

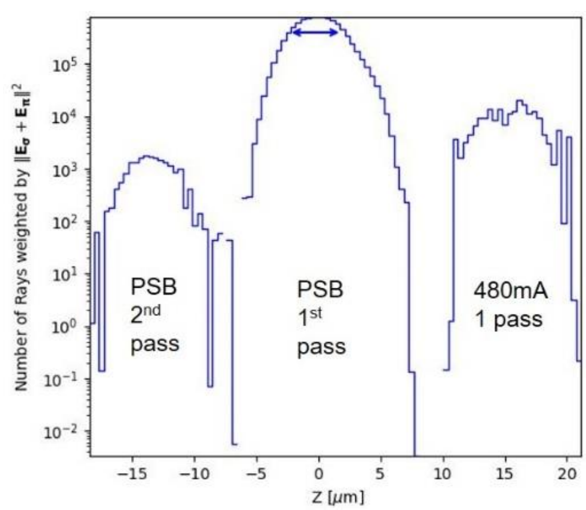
Future new beam line developments will be tied to a Major Item of Equipment (MIE) project proposed to DOE-BES. As discussed in Section 5.2.3, the proposed project scope includes the development of three new state-of-the-art beam lines. Projects to support this initiative will provide floor space and other conventional facilities infrastructure, such as associated laboratories.

5.2.1 Pseudo Single Bunch Timing Studies

As described in Section 5.1.1, SPEAR3 pseudo single bunch (PSB) fill patterns involve deflecting a camshaft electron bunch into a different vertical orbit than the remainder of the filled bunches in the ring. Consequently, the camshaft bunch photon emission cone occupies a different vertical phase space than the emission cone from the remaining filled bunches. Properly configured beam line optics can exploit these differences to isolate the X-rays emitted by the camshaft bunch while suppressing the X-rays from the remaining filled bunches. Using a combination of fixed vertical slits and the monochromator on BL17-2, for example, the simulated flux from a single turn of the 480-mA “normal” bunches is 0.02 that from a single turn of the 20-mA camshaft bunch.

The source position of the camshaft bunch is displaced in the vertical with respect to the remaining 480 mA; therefore, X-ray imaging optics will produce a focused beam spot for the camshaft photons that is displaced from the focus of the remaining 480 mA. This affords further isolation of the camshaft photons as a vertical slit at the focus can select only the photons emitted by the camshaft bunch.

For example, the figure below depicts a SHADOW simulation of the vertical focus of BL17-2 at 12 keV. In this simulation the beam line optics are configured to accept photons from the first pass of the PSB and suppress most of the photons from the remaining 480 mA of stored current whose bunches are displaced 140 µm, 54 µrad, and 125-655 ns from the PSB. The source demagnifying KB focus optics result in approximately a 15 µm vertical displacement of the camshaft photon focus from the focus of photons remaining from the 480-mA stored current. (The PSB executes two revolutions around the ring on different vertical trajectories before it is kicked back into the same trajectory as the 480-mA beam. Thus, the figure also shows a displaced X-ray focus from the second pass of the PSB which is displaced 122 µm, -83 µrad, and 780 ns with respect to the first pass of the PSB.) In this simulation introducing a 10 µm vertical slit centered on the first pass PSB beam spot essentially eliminates all photons other than those produced by the first pass of the PSB camshaft, resulting in a well-defined X-ray beam pulse without significant contamination of X-rays outside the desired time window. Consideration of the figure reveals that this means of isolating the PSB photons is very sensitive to the focus optics quality as extended tails of the undesired beam spots can contaminate the PSB photon focus.



SHADOW simulations of the BL17-2 KB mirror vertical focus at 12 keV with realistic mirror shape errors assuming a 20-mA pseudo single bunch (PSB) vertically displaced 140 µm and 54 µrad with respect to the remaining 480 mA stored current. The PSB executes two revolutions on different orbits before it is kicked back into the same trajectory as the 480-mA beam. In addition to the obvious spatial displacement of the foci, the first PSB pulse is separated 125-655 ns and 780 ns from the 480 mA pulses and the second PSB pulse, respectively. In the simulation, BL17-2 is configured to accept beam from the first PSB pass and suppress flux from the second PSB pass (displaced 122 µm and -83 µrad) and 480 mA stored current. A 10 µm slit centered on the first PSB peak effectively eliminates the second PSB and 480 mA flux. (Note the z axis is the vertical coordinate.)

While introducing a slit at the KB mirror system focus to isolate the photons from the camshaft PSB is effective, it requires the sample to be positioned downstream of the focus where the X-ray beam spot is both enlarged and beam structure is introduced owing to focusing optics residual shape errors. BL17-2 has been designed to allow retrofitting a second vertical focus mirror upstream of the KB focusing optics. This upstream mirror creates a demagnified source image on a slit configured to accept only the flux from first PSB in the same fashion as a slit at the KB focus depicted in the figure above.

The PSB X-rays transmitted through this selection slit propagate downstream and are refocused by the KB mirror system onto the sample thus avoiding focus spot degradation at the sample location. Current PSB plans envision operating BL17-2 with single stage vertical focusing while SSRL gains operational experience with the PSB operations mode starting in FY2026. Both BL15-2 and BL17-2 can be retrofitted with two-stage vertical focusing for improved PSB performance if operational experience and user demand warrants the upgrade.

5.2.2 Revitalization of Existing Beam Lines

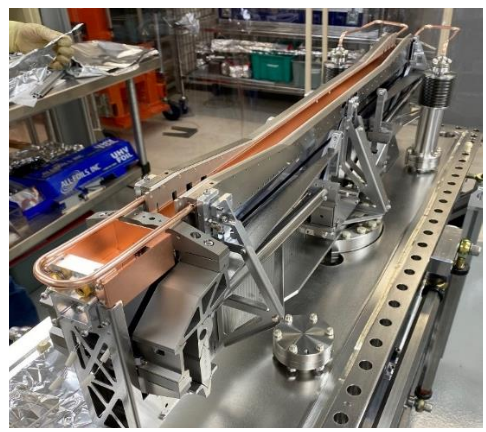
The goal of SSRL's long term beam line upgrade plan is to optimize each source and associated beam line optics for the intended application to meet new scientific and experimental requirements. This plan is manifest in a continuing program of beam line optics upgrades, repurposing and addition of bending magnet stations for targeted applications, and the repurposing of wiggler stations as experimental programs move to the new IVU beam lines.

For example, the materials scattering program relocation from BL7-2 to BL17-2 facilitated migrating the µXRF imaging program from BL10-2 to BL7-2. In turn this enabled relocation of the Co-ACCESS heterogeneous catalysis program from bend magnet BL2-2 to the BL10-2 wiggler end station. As part of this BL10-2 repurposing, the BL10-2 optics were upgraded in 2024 for improved spectroscopy performance. Specifically, the former optical layout consisting of a toroid focusing mirror upstream of the monochromator was replaced with the collimating mirror – monochromator – focusing mirror layout employed successfully on a number of SSRL spectroscopy beam lines. The new collimating mirror employs a novel design that uses a trough with liquid Gallium-Indium and a tuned-conduction heat exchanger that allows better shape error correction of the mirror (see figure). Moreover, the standard LN_2-cooled double crystal monochromator will be exchanged with a LN_2-cooled fast scanning monochromator capable of collecting spectra at 20 Hz. BL10-2b commissioning has begun in the FY2025 run.

Beyond beam performance improvements owing to these source and optics upgrades, the BL10-2 end station affords the Co-ACCESS program the physical space to establish a full featured, catalysis research infrastructure including catalysis-required gas handling, novel *in-situ* reaction cells, and auxiliary sample characterization capabilities such as described in Section 3.2.1.

With the completion of the IVU BL15-2, the suite of advanced spectroscopy instruments at BL6-2 were relocated to this new undulator station. The fraction of time on BL6-2 liberated by this change was then reapportioned to the TXM located in BL6-2c as well as tender X-ray energy XES and CT imaging programs in BL6-2a and b, respectively.

In addition to specific beam line shuffling to take better advantage of X-ray sources, a program to revitalize existing beam line hardware is underway. We developed new optics stands that substantially stabilize optics by placing them on granite air bearing positioning systems. The first field installation of this type of stand was installed to support the BL5-4 M_0 mirror system in the summer of 2024. We envision using granite air-bearing systems in all new beam line installations. In addition to the stabilization program, many optics are approaching end of life and exhibiting reduced performance, having been in the field for more than 20 years. An iterative program to upgrade the optics and mechanical movers of a series of mirror and monochromator systems is being accelerated with the very recent increase in the U.S. synchrotron user facilities' base operations budgets, and is envisioned to occur over the course of the next 5+ years.



Prototype collimating mirror that employs a Gallium-Indium trough and a tuned conduction heat exchanger. Incorporating this new design into older beam lines will greatly improve performance of beam lines on high-power wiggler sources.

In addition to beam line repurposing and optics upgrades such as listed above, SSRL invests in experimental end station instrumentation and detector upgrades to facilitate new research initiatives and greater productivity of existing programs as detailed in Chapter 3. New beam diagnostics systems are in development: a Talbot-based wavefront detector, an upgrade to the current mirror pointing system detector, and a "Diagon" detector designed to allow alignment of the SPEAR3 electron beam through the IVU sources. The Talbot detector is based on a model developed and used extensively at LCLS and is envisioned to permit routine and simplified KB mirror focusing. The current beryllium blade-based detector for mirror pointing control will be upgraded to a single blade system with a smaller footprint and less dependence on pitch alignment. We envision developing a new detector (the Diagon detector), which will allow selection of specific energies from IVUs to permit the optical analysis of photon beam position relative to the optimal beam position through the beam line. The electron beam through the IVU can then easily be vertically tuned to optimize the photon beam position through the beam line.

There are several end station upgrades that are being implemented. At BL6-2, the TXM Xradia/Zeiss Microscope will be completely replaced with an in-house design. There will be significant improvements in sample rotation axis run-out to less than 100 nm, an automatic lens camera system, and the ability to tilt the rotation axis by 30 degrees for other types of experiments like laminography. At BL15-2, a new 30-crystal X-ray Raman spectrometer in the high Q position is now installed, which will complement the existing 40-crystal instrument (the two will be used simultaneously) in collecting primarily C, N, and O spectra, while providing new information of this higher momentum transfer interaction.

Fast-scanning monochromator designed for operando chemical catalysis science.

Improved X-ray beam flux and focal size have been achieved at a number of beam lines by incorporating new polycapillary and KB mirror microfocus systems. We will further improve on these results by developing an in-house KB microfocus system for dedicated use on the materials science BL17-2.

With the broader use of remote data collection necessitated by the COVID pandemic, SSRL continues to leverage the Structural Molecular Biology program's remote data collection experience by expanding implementation and utilization of sample handling robots and remote data collection software on chemistry/catalysis and material science beam lines. This investment anticipates that users will continue to exploit remote data collection capabilities in the future. Some of these developments are aimed at full automation to enhance the throughput in measurements, while software developments will enable rapid data treatment that eventually will contribute to driving users' experimental strategy through application of ML, as described in Chapter 3.

5.2.3 New Undulator Beam Line Developments

The 2021 BES Scientific User Facilities Quadrennial Review of SSRL included a recommendation that SSRL "Develop a plan to renew critical beam line infrastructure, focusing on use of existing resources and identifying options that require additional funding at the small project or major item of equipment level."

Pursuant to this recommendation and with BES encouragement, SSRL developed a SSRL Beam Line Renewal Initiative proposal encompassing six new or fully upgraded beam lines servicing five scientific disciplines. After BES independent review SSRL was encouraged to down select to a scope that would fit inside the $100M Major Item of Equipment (MIE) boundary conditions.

Examining the portfolio of facility research capabilities — and the science they are driving and enabling — at SSRL and within the portfolio of U.S. light sources, SSRL identified, prioritized and defined new experimental capabilities that would address critical gaps in the research that can currently be performed across the United States, and with international benchmarking. The scientific foci of these new proposed capabilities are in the areas of *i*) probing biological processes at the plant/soil/water nexus and *ii*) understanding how heterogeneity introduced during microelectronic materials growth and fabrication processes affect device operation. The new developments build upon the accelerator characteristics and performance of a 3rd generation low-emittance light source, with a focus on new beam lines and end stations that are designed to either perform real-time, dynamic characterization via *in-situ* and *operando* methods or provide long-term system interrogation via multimodal studies of evolving component interactions. Three new in vacuum undulator (IVU) beam lines are proposed to support these two thrust areas.

Plant/Soil/Water Science Beam Line - This proposed beam line will serve the bio-critical tender-to-hard X-ray energy range of 2.1–13.2 keV with a spatial resolution of ~500 nm to 2 µm. The IVU beam line will have the high flux necessary to chemically and structurally probe sub-mM concentrations from biologically relevant light and heavy elements. The ability to span important metal and ligand edges on the same beam line facility with microprobe spatial resolutions that complement the proposed nanoprobe capabilities at APS, ALS, and NSLS-II will be essential for the research community in connecting molecular and nano-scale structure and processes with meso- to ecosystem scale phenomena.

This beam line and associated laboratory facilities will address science drivers posed in Section 3.2.4 and fill the technological gap at SSRL and U.S.-DOE light sources by creating a µ-XRF facility dedicated to biological research that will allow sub-micron to 10s of micron investigation of chemical transformations on a single beam line facility. A second experimental station will provide high-throughput XAS and ultra-dilute sample EXAFS for in-depth structural characterization of biological, biogeochemical, and heterogeneous systems. Additionally, this facility would be integrated with a sample laboratory that allows for long-term plant growth, manipulation, and secondary characterization, enabling a new paradigm for user operations.

The microelectronics science drivers discussed in Section 3.1.2 will be supported through the development of two new beam lines.

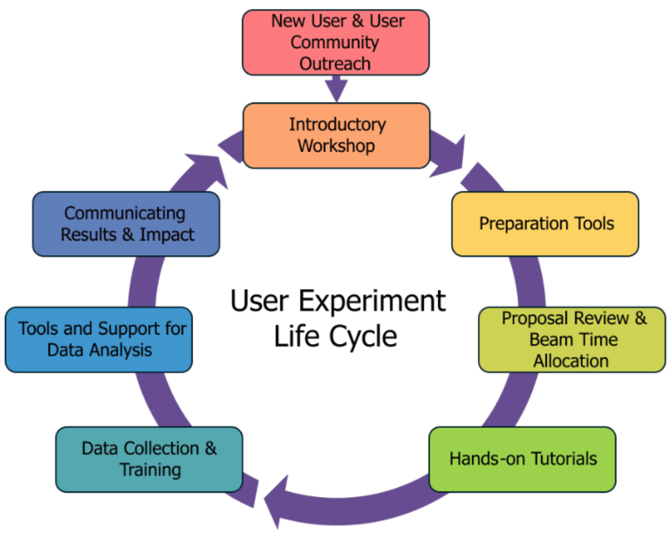
Multi-tool X-ray Scattering and Spectroscopy Microelectronics Beam Line – This IVU beam line will operate in the 4-12 keV energy range with ~20 x 1 μm^2 focus down to ~1 x 1 μm^2 while retaining a generous 300-mm working distance to facilitate integration with several *in-situ* growth, processing, and *operando* chambers to study emerging material heterogeneity during materials synthesis and fabrication. Achromatic focusing will be employed to facilitate both scattering- and spectroscopy-based studies.

HAXPES/PEEM Microelectronics Beam Line – A second IVU beam line serving the 4-12 keV energy regime will be developed for HAXPES/PEEM. Similar to the Multi-tool beam line, a generous 500-mm working distance will be maintained for integration with a commercial HAXPES/PEEM instrument capable of sub-micron spatial resolution. A variable focus ranging from ~25 x 3 μm^2 down to 5 x 3 μm^2 will be provided by achromatic reflective optics and a dual Si(111) and Si(311) capable double crystal monochromator will ensure adequate energy resolution.

These two new beam lines with integrated processing and *operando* capabilities will be unique and transformative scientific assets of the DOE national laboratory complex. As described in Section 3.1.2, they will serve a vitally important user community seeking to enable materials and process discovery and new device concepts for unparalleled performance and enabling new modes of computation, communication, and sensing. Outcomes of these fundamental advancements will also impact DOE science by helping to transform computing technologies derived from these basic science studies (e.g., high performance memory, logic and materials or integration strategies enabling new computing paradigms) including DOE's high-performance computing infrastructure and that of large-scale experimental facilities, which have rapidly growing edge computing requirements.

6 Outreach, User Support and Education

Building on SSRL's well-established roots within the synchrotron research community, a strong connection to Stanford University and close connections to technological developments in Silicon Valley, SSRL supports the users' research life cycle from beginning-to-end to ensure that they get the best science from their time at the facility. The SSRL approach to supporting the user community is illustrated in the User Experiment Life Cycle scheme below and described in the sections that follow.



Reaching Out to New Scientific Communities

SSRL has remained at the forefront over the facility's 50-year history by continually enhancing the synchrotron source, developing new methods, beam lines and instrumentation, and bringing in new ideas from its users and scientific staff. The facility has successfully fostered new scientific communities in areas including structural molecular biology, hard X-ray scattering, photoemission spectroscopy, imaging, environmental science, and catalysis, while networking with established and emerging scientific research centers. Guided by a strategic plan that includes accelerator capability enhancements, including new modes for timing studies, new and upgraded beam lines for emerging science, and development and implementation of novel instruments, sample environments and software, we strive to continue the growth and the support of our existing and new user communities.

Outreach to introduce SSRL's new capabilities to existing and new users will continue to be a focus, and will contribute in important ways to SSRL's future scientific impact.

Providing Introductory Workshops to Potential New Facility Users

After reaching out to new user communities, SSRL staff members follow up by offering introductory workshops in selected areas of science and techniques. A large number of these workshops are held during the SSRL/LCLS Annual Users' Meeting which attracts hundreds of participants. The workshops are organized by staff scientists in collaboration with the SSRL Users Organization and typically include instruction by nationally and internationally recognized scientists in the targeted areas of science and/or methodology.

Providing Tools for Experiment Design

SSRL provides multiple online resources to help users best design their experiments. The Structural Molecular Biology Division at SSRL has pioneered remote access systems that integrate an interactive interface with both real and simulated beam lines and data acquisition. SSRL is rapidly expanding similar tools and other web-based visualization and simulation platforms across its other facility beam lines to enable design of high-throughput and other experiments. Wide-spread implementation of these developments in the next few years is planned but their pace will depend on the specific beam lines, techniques, research areas, and pilot testing phases.

Reviewing Proposals and Allocating Beam Time

To ensure the facilities are leveraged for the most productive and important research, beam time proposals are peer-reviewed and rated based on scientific merit and impact. Proposals directed to the SSRL facility focus on answering a scientific question or questions. Accordingly, a proposal can include several techniques, energy ranges, and beam lines. While most proposals are valid for 1-2 years, to enable timely and current research, SSRL also provides several rapid-access proposal mechanisms. Moreover, SSRL has a mechanism through a letter of intent to provide a short amount of beam time for users to test the feasibility of new experiments.

In the coming years, driven by the evolution of science directions and the needs of the user community, SSRL will continually review the proposal system and alternative scheduling modes to accommodate changes, such as those required to enhance remote access, rapid access, and mail-in programs, or long-term experiments that require frequent short access periods. The goal is to allow for more flexible and efficient access to the scientific tools at the beam lines while maintaining high scientific standards.

Running Hands-on Tutorials

To ensure effective usage of beam time, collection of high-quality data, and successful publications, new and returning researchers are invited to take part in SSRL's many tutorial sessions. These include hands-on training at summer schools, short courses, and workshops that focus on synchrotron techniques, one-on-one tutorials, and how-to materials shared via web-based tools including short video clips.

Assisting with Experimental Set Up and Data Collection

SSRL has nurtured a culture of pride among its staff in providing expert service and support. Facility staff members provide resources to help the scientific users make the most of their beam time, including:

- Specialized, state-of-the-art beam lines, instrumentation, and capabilities.
- Technical support from experienced facility scientists, engineers, and support staff.
- Ancillary laboratory equipment including wet laboratories, glove boxes, anaerobic chambers, laboratory instrumentation, chemicals and other materials.
- Assistance with sample preparation.
- Remote access where applicable, allowing users to collect and process data from their home institution, using specialized access mechanisms and software, and enabled by beam line automation.
- SSRL-specific safety training courses in addition to those required for general facility access.
- Amenities for users, including an on-site guest house, exercise facility, and a central check-in and orientation location for all SLAC users.

In the next five years, SSRL intends to increase staff to further help researchers optimize beam time use and data analysis.

Providing Tools and Support for Data Analysis

To enhance the productivity of users, the SSRL scientific staff has developed and/or imported from the international community several open-source data analysis software packages that are made available for users during their experiments, and for download to their home institutions. Training on how to use the software is provided during experiments and, for some, during workshops and summer schools. The availability of analysis software at the beam line enables rapid analysis to optimize experiments in real time and to promote completion of experimental sessions with high-quality data.

Assisting with Communicating Results

More than 600 papers are published annually as a result of research using SSRL, totaling over 18,000 publications since the facility began operation in 1974. SSRL staff members make a concerted effort to communicate these results to the public, including the local community, and other scientists through public lectures, press releases, science articles, social media and websites.

Industry Research – Engagement and Facilitation

To reach industrial researchers, SSRL networks and collaborates with firms ranging from local start-ups to large multi-national companies to pursue opportunities in energy research, biotechnology, and information technology. Most industrial users connect to the facility via outreach in their respective technical fields. For example, SSRL sees industrial use through partnerships and collaborators on research funded through STTR, SBIR and EERE grants or through comparable funding models. Consortia that include industrial members represent another entry point for specific fields of research such as batteries and other energy-related topics. A significant number of industrial users come from the Biopharma industry to use SSRL's macromolecular crystallography beam lines.

SSRL accommodates proprietary research by users who have scientific projects for which they wish to maintain confidentiality of proposal, data and results for a certain period of time (as needed for patent or other reasons) following established processes.

Regardless of the entry point to the facility, all industrial users benefit from SSRL's user support and training opportunities as well as various access mechanisms that allow faster turn-around if required.

7 Workforce Development

Developing the next generation of leaders in the science and technology enabled by advanced X-ray methods is an important and crucial goal of SSRL and SLAC, which is necessary to advance synchrotron science and drive future innovations. This endeavor demands a commitment of nurturing scientific excellence at all levels of scientific and engineering education and training. It requires an approach to identify, recruit, and retain top talent in a competitive environment. A culture of excellence is essential for developing technologies that support the varied needs of the scientific community and for advancing the mission of the Department of Energy and other SSRL funding agencies and partners. By providing access to resources, mentorship, and opportunities, we equip emerging leaders with the skills and confidence to push the boundaries of X-ray science, ensuring that the field continues to thrive and evolve in a way that benefits the nation.

SSRL's strategy to create a world-class scientific and technical workforce is synergistic with our outreach strategy for engaging and growing new user communities, based on building awareness and reducing barriers to engage with SSRL. SSRL's user base includes a large cohort of early career individuals who reside at the entry point to our country's scientific and technical workforce pipelines.

Expanding the User Base to New STEM Communities

To broaden the awareness of SSRL, we will reach out to institutions providing strong STEM education, primarily at the undergraduate level, through seminars, webinars, social media and other approaches to disseminate the science and technology available, and the training opportunities that exist and to be developed. While primarily focusing on California and Bay Area institutions, we will expand to other states' universities and institutions across the nation.

Once engaged, we will develop the existing and emerging scientific work force through our own training and education programs.

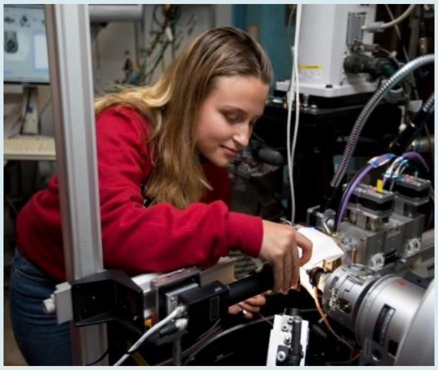
SSRL will expand our online training portal. We will create specific workshops to engage new PIs to help them identify how SSRL can positively impact their research portfolios and students and take some of these workshops "on-the-road". Additionally, we will expand our remote-access and mail-in experimental programs for a wide range of techniques to provide greater accessibility and remove travel barriers for new users, including undergraduate researchers.

Enhancing SSRL's Workforce Development

SSRL is committed to developing our current and future workforce by providing early career scientists with opportunities to disseminate their work through various programs and encouraging participation in conferences and workshops. SSRL staff play a leading role in SLAC's strategic initiatives in X-ray and ultrafast science, accelerator R&D, quantum information, microelectronics, bioscience and human health, and we will leverage these initiatives to facilitate networking and strategic development. Moreover, Stanford's leadership training programs and cross-training opportunities at other light sources are integral parts of our workforce development plan.

SSRL's scientific staff are encouraged and supported to write proposals to seek additional funding for their own research and to support growth opportunities for the Lightsource. Currently, staff are participating as PIs, co-PIs, or team members in several consortia and multi-institution research projects supported by a varied distribution of funding sources. SSRL will continue to encourage staff to submit proposals to relevant FOA's, etc., as they are announced. SSRL will also continue its strong efforts in enabling staff to propose and pursue SLAC LDRD projects, as well as to mentor junior staff members so that they become competitive for Early Career Awards.

In summary, SSRL's workforce pipeline and career development strategy is crucial for fostering a dynamic environment that not only attracts young and un-tapped talent but also provides the necessary support and resources for professional growth and development. By focusing on staff scientific development, barrier reduction, and professional networking opportunities, we are paving the way for a more robust and innovative future for SSRL.



Throughout the research lifecycle, SSRL actively participates in building a pipeline of future scientists and engineers. For example, more than 60% of the experiments at SSRL are conducted by undergraduate students, graduate students, or postdoctoral scholars. Their hands-on experience helps students learn to formulate new scientific ideas, prepare successful research proposals, plan and conduct experiments, and analyze and interpret data. It also clearly shows the next generation the potential of synchrotron research to enable faster, more novel, and more precise measurements leading to scientific discoveries.

In addition to offering young researchers the opportunity to participate in experiments at SSRL, the facility actively engages in SLAC's various internship programs. These programs allow young scientists and engineers to work closely with SSRL staff, exposing them to career opportunities at user facilities firsthand.

In the coming years, SSRL will enhance our efforts to educate future generations of scientists through increased targeted outreach to universities and colleges with a focus on STEM education.

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