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1 Executive Summary

One of SLAC's mission objectives is to be the premier photon science laboratory in the world. The cornerstone of the strategy is 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 BES Scientific User Facility builds upon and utilizes SLAC's core capabilities and leverages the proximity to the exceptional intellectual environment at Stanford University to enable forefront science and support DOE missions in energy, environmental and biological sciences. SSRL's program can be characterized as a set of four interrelated themes: to Innovate, to Discover, to Serve and to Train. We Innovate in accelerator R&D, x-ray instrumentation and new x-ray methodologies; we Discover through enabling and performing high impact, cutting-edge science using SSRL in areas particularly relevant to our Nation's energy security and human health, and through partnerships with university, other national laboratory and industry scientists; we Serve a growing x-ray science user community, providing outstanding user support; and we Train the next generation of our Nation's scientific workforce using workshop, remote access, hands-on and classroom approaches, and one-on-one mentoring of undergraduate and graduate students, and postdoctoral scholars. Bridging these themes are common enabling factors that include strong interactions and collaborations with Stanford and regional universities, and our foundational capabilities in accelerators, instrumentation, data acquisition and analysis. SSRL strongly couples to and enables research in SLAC's Materials Sciences and Chemical Sciences Divisions, and continues to exploit the synergy with LCLS in science and technical developments.

Throughout its long history, SSRL has been a facility where innovations have driven scientific discovery and renewal of its capabilities. This focus continues to enable world-class science by selecting important problems that make the best use of SSRL's source properties. Specifically:

- The accelerator development program will keep SPEAR3 at the forefront through improved source emittance and short-pulse operation.
- New SSRL beam lines will be implemented within a strategy to address grand challenge problems in energy, biosystems, and the environment, as well as to effectively couple to external partners from industry, national laboratories, and academic institutions.
- Within SLAC, the synergistic coupling to the LCLS, in both science areas and as DOE BES national user facilities, will enhance the research capabilities and ability to offer users effective scientific complementarity, commonality in user services, and support.
- SSRL's unique connection to Stanford University will continue to provide a very important research and educational component to develop future leaders in the field, in addition to creating an atmosphere that enhances the user community's experience.
- The outstanding support experienced by users at SSRL is consistently reflected in the “excellent” scores received in the end-of-run summaries and external reviews, and continues to be the hallmark and signature of the SSRL experience. It is SSRL's goal to meet and go beyond the expectations of our user community in providing new capabilities and the highest level of scientific, technical, safety, and administrative user support.

The sections below 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 environmental science, structural molecular biology science, accelerator science, and instrumentation development.

2 Synchrotron Radiation – A Unique Tool

Over the last four decades, the unique properties of synchrotron radiation and the continued improvement of synchrotron light sources have enabled the development of a wide range of powerful experimental tools. These tools have transformed structural biology, materials science, and geosciences research, among other fields, and led to not only scientific discoveries, but also technology breakthroughs. Notably, Nobel prizes have been awarded to seven scientists who used synchrotron light sources for their research. New applications are continuously opened up as the broader scientific community becomes aware of the power of the synchrotron radiation methods.

Today, there are more than 50 synchrotron light sources around the world and 7 operating in the U.S., with more either planned or under construction. These light sources together support the research of tens of thousands of
scientists worldwide. Within the U.S., the four DOE synchrotron light sources support more than eleven thousand users annually, and the demand for access to the unique tools at these light sources continues to increase. This phenomenal growth is limited mainly by the resources required to support the user community, and is expected to continue. Research conducted at modern synchrotron light sources is very cost effective because these centralized facilities can exploit the economies of scale by operating sophisticated instruments for a large number of users and sharing staff with unique expertise.

The increasing level of complexity and cost of instrumentation required for synchrotron research has also led to a profound transformation in many research fields, driving them from the tradition of “small” science, where most research is conducted in individual research groups, to increasingly larger collaborations, where the community must work closely together to identify research priorities, raise funds, specify and design instruments and share the resources in an open and transparent fashion. Although adapting to this transformation presents a significant challenge and requires a close collaboration between the research communities and synchrotron facilities, it is remarkably valuable: the macromolecular crystallography community has successfully made the transition, leading to a tremendous growth of both the community and the scientific output.

These developments, both technical and sociological, as well as the broad scientific and societal impact of research conducted at synchrotron light sources have made these facilities an essential part of the research infrastructure for many nations.
3 Stanford Synchrotron Radiation Lightsource

SSRL began in 1972 with seed funding from the Stanford Center for Materials Research and in 1973 with a small grant from the Materials Division of the National Science Foundation (NSF). It was initially called the Stanford Synchrotron Radiation Project (SSRP). The first user run followed in 1974. SSRP was the first facility in the world to exploit the stability and brightness of a multi-GeV electron storage ring, SPEAR, and provide the entire spectral region, from VUV/soft x-ray to hard x-ray, for scientific research. In 1977 SSRP became the Stanford Synchrotron Radiation Laboratory (SSRL). Many experimental techniques and accelerator technologies routinely used today were developed and pioneered at SSRL.

SSRL became a fully dedicated synchrotron radiation source in 1992 and, in 2004, successfully completed a major upgrade of SPEAR, with joint funding from the Department of Energy (DOE) and the National Institutes of Health (NIH), transforming the storage ring into a third-generation synchrotron light source - SPEAR3. At the start of user operations in early 2004, SPEAR3 operated at 3 GeV with the design emittance of 18 nm-rad and a current of 200 mA with injection every 8 hours. Today, SPEAR3 is operated at 3 GeV, with 9.6 nm-rad emittance and top-off injection at a current of 500 mA with a reliability of over 97%. There is an active accelerator research and development program to continue improving the performance and reliability of the accelerator complex, including emittance improvements to less than 6 nm-rad and the development of short pulse operation in the few psec to ultimately sub-psec range. SSRL is expanding its undulator beam lines and continuously upgrading existing ones, including new optics and instrumentation.

SSRL, being the premier hard x-ray source serving the western U.S., currently supports the research of more than 1600 users annually and operates >30 scattering, spectroscopy and imaging experimental stations, with capacity for ~45 beam line stations and the ability to serve more than ~2200 users. It is a highly productive scientific user facility with high user satisfaction, generating more than 400 peer-reviewed publications annually. Research conducted at SSRL continues to have major impacts in condensed matter physics and materials sciences, structural biology, and environmental science. SSRL also serves an important educational function, with graduate student users typically completing >50 doctoral theses annually. Many leaders in synchrotron research around the world having received their initial synchrotron-radiation training at SSRL.

Roger Kornberg, Professor of Structural Biology at the Stanford University School of Medicine, was awarded the 2006 Nobel Prize in Chemistry for research into how the DNA genetic blueprint is decoded and translated into messages that are used to direct the synthesis of proteins – a process essential for all life. Kornberg's studies at SSRL first revealed the atomic-level structure of the molecular machine (RNA Polymerase II) which unwinds DNA, reads the base-pair sequence, and creates a message (m-RNA), which is then used by another cellular machine, called the ribosome, to synthesize proteins (the process being known as transcription). Since transcriptional regulation underlies all cellular metabolism, his work is also shedding light on how the process can go awry and cause birth defects, cancer, and other diseases, and how new drugs can be designed to control or cure such diseases.

In the early 1990s, SSRL identified Kornberg's research on RNA Polymerase II as high-risk high-award, and granted regular access to the high-brightness Macromolecular Crystallography beam lines, which he used to reveal the complex structure of RNA Polymerase II. SSRL's development of sample mounting robotics and high-throughput automated sample screening systems significantly accelerated the process, making it possible to efficiently screen hundreds of crystalline samples to select the few most optimal for diffraction studies. The graphic highlighting the related Science article illustrates the structure of the first transcription complex, determined to atomic-level resolution.
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 NIH and the National Science Foundation (NSF). SSRL also works with a diverse community of researchers to develop new capabilities, as well as provide research infrastructure and support to enhance scientific productivity, and attract and educate new user communities. The main SSRL user and staff research areas are in materials science, chemistry and catalysis, interfacial science, and structural biology - and within these are special focus areas that can be described within the paradigms of ‘materials by design’, ‘emergent behavior from complexity’, and ‘complex bio-processes’.

3.1 Looking into the Future: Building a New User Facility Paradigm at SSRL

In the coming decade, high-brightness synchrotron radiation will be increasingly accessible to the scientific research community as new facilities around the world are brought on line. This presents an enormous opportunity for the scientific community to address large-scale and complex problems, working increasingly across facilities and even national boundaries, while expanding into new areas of applications. During this time, facilities need to both focus on their own strategic directions through interactions with key stakeholders—in particular their user community—as well as coordinate and collaborate with other facilities.

Scientific opportunities

SSRL focuses on the scientific opportunities and research priorities identified by the Office of Science and other agencies, and works with researchers from academia, industry and government to develop new experimental and analytical techniques, design and construct state-of-the-art instruments, as well as provide research infrastructure and support to enhance scientific productivity, and attract and educate new user community.

Partnership with scientific community

For a given scientific focus area, SSRL will build partnerships with the leaders and the community to identify the most important problems in the field, guide the development of new experimental techniques, beam lines, instrumentation and research facilities optimized for pursuing those problems, and provide support to the community for efficient access, successful experiments, and scientific results.

Discovery to deployment

Discoveries from basic research often lead to technology developments that have significant societal impact; and requirements from industry and national security often inspire new basic research directions. National user facilities are the ideal places to promote collaborations between researchers from academia, industry and government laboratories. SSRL will facilitate and strengthen these interactions and the exchange between basic and applied research.

Dedication to users' needs

SSRL is working 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 experiment cycle. From proactively reaching out to new
scientific communities to building the needed tools and support for experiment design, data collection and analysis, 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.

**Light Source enhancement**

Finally, to support the current and future scientific program, SSRL will expand on its an accelerator improvement program to further enhance the performance of SPEAR3, both in source brightness and new operation modes, as well as ensure the reliability of the accelerator complex. SSRL will also contribute to future light sources through a coordinated effort on the development of new accelerator concepts as well as by identifying and developing the science drivers that define the performance requirements of future light sources.

### 3.2 Scientific Foci

The main SSRL science focus areas are Materials Science, Chemistry and Catalysis, and Structural Molecular Biology. SSRL’s strategic plan aims to pursue a range of scientific grand challenges, as related to these areas, and as derived from the roadmaps of the major funding agencies, including the DOE Office of Basic Energy Sciences (BES). SSRL’s roadmap is further refined with input from the scientific community, guided by the advice of its Scientific Advisory Committee and Machine Advisory Committee, and through interaction with the SSRL Users’ Organization. Globally, the foci can be described within the paradigms of Materials by Design, and Emergent Behavior from Complexity.

#### 3.2.1 Create Materials by Design

“Materials by Design” is the ultimate goal in materials science. Recent progress in theory, computation power, materials synthesis, and characterization tools has brought this goal within reach. Synchrotron light sources, with their exceptional properties, are playing an essential role in providing a wide range of powerful characterization tools that allow the materials research community to understand the relationship between structure and function as well as the relationship between processing conditions and structure, at an unprecedented level of detail. The challenges are to provide access to these tools in a timely fashion so that they can effectively guide the theory and synthesis of new materials and to develop sophisticated new tools that can address increasingly subtle scientific questions related to materials structure-function relationships and processing.

#### 3.2.2 Understanding Emergent Behavior from Complexity

In most complex systems, including strongly correlated electrons in high temperature superconductors, cell biology, and bio-remediation, unique system-level behaviors and properties often emerge from the interactions among the constituents or properties of the system. The challenge is to understand the individual interactions and how these lead to the emergent system level properties, which can be accomplished by developing:

- Tools with increasing detection sensitivity for chemical speciation and orbital and spin moments, in combination with extreme sample environments, to allow the study of individual and collective properties
- Tools with higher spatial and temporal resolution for in-situ studies, to allow the hierarchical study of the function of complex systems as a whole
4 Science at SSRL

4.1 Materials Science at SSRL

Advanced materials are at the heart of our technically advanced society. The increasing rapid development of functionally useful materials is due to the recent advances in theory, synthesis and characterization enabling the realization of “Materials by Design”. Synchrotron light sources are playing an important role here by providing effective characterization capabilities. SSRL focuses on several specific areas within materials sciences where we can have the most important impact.

SSRL’s materials science programs will provide and further develop a comprehensive set of tools and methodologies in support of the national “Materials Genome” initiative, focusing on materials for sustainable energy as identified in SLAC’s energy strategy, specifically materials for energy storage and use (batteries and solar cells). Second, they will provide and develop tools and methodologies to understand the wide range of phenomena emerging from complex systems, in particular strongly correlated electron materials, such as high temperature superconductors, topological insulators, multiferroics as well as the magnetic materials and semiconductors needed for emerging technologies. Special emphasis will be given to the following areas:

- Enhancing in-situ, real-time capabilities for the study of structure-function relationships of materials, material responses under realistic operational conditions, and material synthesis and processing
- Developing tools and integrated approaches to probe materials over multiple length-scales and time-scales
- Coupling experimental techniques closely to theory and modeling

We will broaden the impact of SSRL through partnerships with a number of institutions in sustainable energy materials research, including the Energy Frontier Research Centers (ERFCs) - for example playing an integral part in the Center for Inverse Design, the National Renewable Energy Laboratory (NREL), and Stanford’s Institutes, Centers and Departments (e.g., Precourt Institute for Energy). Often SSRL hosts EFRC- and other institutionally-affiliated students and postdoctoral scholars, with SSRL staff acting as mentors for the young researchers. We will closely coordinate with other DOE Office of Science user facilities to enhance industrial research, and support initiatives supported by DOE technology offices, for example, the Bay Area Photovoltaic Consortium (BAPVC) and the Batteries for Advanced Transportation Technologies (BATT), supported by EERE.

Finally, in close collaboration with Stanford University and through introductory workshops for new synchrotron users, one-on-one mentoring for undergraduate and graduate students, and a dedicated materials-science teaching beam line, we will carry on SSRL’s long tradition of educating and training the next generation of scientists and engineers.

In the following, we will focus on the scientific challenges in the major materials science research directions at SSRL, and new instrumentation being developed and planned.

4.1.1 Materials for Sustainable Energy

The development of sustainable energy solutions to power humanity is one of the most important scientific and technical challenges of our time. Dramatic improvements in energy conversion, transmission, storage and usage are critical to maintain the economy, environment and our quality of life. A SLAC task force on Energy Research has recommended the establishment of a center of excellence in sustainable energy research at SLAC focusing on atomic-scale design of materials for chemical energy conversion (catalysts), advanced photon conversion (solar cells) and electrochemical energy storage (batteries). SSRL is playing a major role for detailed characterization and understanding of the structural and electronic properties of a wide variety of sustainable energy materials. This includes organic and inorganic photovoltaics, transparent conductors, battery electrodes and catalytic particles.
This work will continue to be an important and growing effort at SSRL involving x-ray scattering, spectroscopy and imaging studies of materials’ structure-function relationships; often these will be conducted in-situ, in-operando, or during processing/synthesis. Furthermore, these materials are often hierarchically complex at the mesoscale, and it is essential to characterize them over a range of length scales - from Å to μm. An example of this, for organic solar cells, is shown below. It is also anticipated that studies of interfaces will become increasingly important, since interfacial regions are crucially important in almost all materials used for sustainable energy. The atomic and molecular structural properties of interfaces affect the functioning of devices used for energy conversion, storage and use. Although buried interfaces (between two condensed phases) are difficult to characterize at an atomic level, x-ray scattering offers an unparalleled method of obtaining detailed interface specific structural information.

(Left) Schematic diagram of the active layer in a bulk-heterojunction solar cell, composed of an intimate meso-scale mixture of donor (blue, here a polymer) and acceptor rich (red, here a fullerene) phases. The schematic illustrates the complicated nature of this multiphase system in which a large range of length scales, from the Ångström to the micrometer, are present. (I) Nanoscale phase segregation between the donor and acceptor materials. (II) Molecular ordering, orientation and disorder in the polymer. (III) Relative orientation and charge transfer dynamics between organic-organic, and organic-inorganic interfaces. (IV) Composition, molecular orientation and quantification of the molecularly intermixed phases.

(Right) When a photon is absorbed by the polymer, excitons (shown by the blue oval in the figure on the right) are created. These can move to low-energy traps (indicated by dashed blue arrow) located on extended polymer chains (red oval). If a fullerene molecule is close to the exciton, the exciton dissociates (converts into separate positive and negative charges) as shown by the solid blue arrow, which can be used to drive a current. The crucially important nature of the polymer-fullerene interface is unknown.

This increasing importance of energy materials motivates improved SSRL capabilities in structure and morphology studies with scattering, imaging and spectroscopy:

- **SAXS/WAXS:** The wide range of important length scales in these materials drives the approach to simultaneously probe both atomic scale structure (wide angle x-ray scattering; WAXS) and longer length morphology (small angle x-ray scattering; SAXS), and SSRL’s plan for a new beam line for simultaneous SAXS/WAXS. This instrument will be used, for example, to investigate, in-situ, processing of organic photovoltaic structures where it is important to correlate and understand how, in real time, the processing conditions impact the resulting structures and how this affects the photovoltaic properties. Experiments investigating the simultaneous SAXS/WAXS of nanoparticle catalysts (e.g., for oxygen reduction) and battery electrodes will lend insight into the degradation mechanisms.

- **Interface Scattering:** The importance of interface structure in energy materials requires an undulator source with a state-of-the-art diffractometer for accurate measurements of interface specific diffraction (e.g., ‘truncation rods’). This allows determination of the interface atomic and molecular structure, which affects the functioning of devices used for energy conversion, storage and use. The use of this methodology for buried interfaces is a unique strength of hard x-ray diffraction.

4.1.2 **Strongly Correlated Electron Materials – Quantum Materials**

One of the five grand scientific challenges identified by DOE-BES is to understand emerging properties of matter from complex correlations of constituent components. Important examples of such properties are the collective and nanoscale phenomena in quantum matter, such as high temperature superconductivity, colossal magnetoresistance and multiferroics. The complexity of these emergent phenomena stems from the strong correlation between electrons that is present in these materials, leading to a strongly-coupled many-body ground state. Many of the
degrees of freedom available to a solid, namely the spatial arrangement of spins, charges, and orbitals, interact in a complicated way so that the material’s fundamental properties cannot be predicted by understanding the properties of the material’s individual constituents.

As better controlled model systems become available, a sophisticated understanding on the universality of these diverse materials will lead to great revelations influencing science beyond these specific properties. There is no doubt that surprising discoveries will be made that dramatically advance our understanding of these materials, such as the recent, unexpected discovery of iron-based high temperature superconductors. Just as these new materials have emerged, the light source tools for their study have also evolved substantially. In studying strongly correlated electron materials, a number of synchrotron-based experimental tools have gained prominence. Amongst the most important is:

- **Angle-resolved Photoemission Spectroscopy (ARPES):** With the extremely high angular and energy resolution now achievable, this technique reveals the electronic structure with unprecedented precision and sophistication – information which forms the foundation for a comprehensive understanding of complex materials. As demonstrated by its strong impact on the high-Tc superconductors and topological insulators, high-resolution ARPES is the most direct and powerful experimental probe to gain insight into the electronic structure of these materials and their novel physics. SSRL has a long tradition and strong local expertise in photoemission spectroscopy and among its users are world-leading experimental groups. To maintain this area of scientific excellence at SSRL, a series of upgrades are planned. A new undulator branch line is in construction at beam line 5. This upgrade will completely modernize and greatly expand the capabilities of the existing Normal Incidence Monochromator (NIM) branch-line with higher polarization control and extended photon energy range, as well as significant improvement in flux and beam spot size. Complemented by the ultra-high resolution capability of the NIM branch line, we expect this beam line will become a leading photoemission facility in the world. We plan to integrate spin-resolved capability to the new ARPES end station. This adds a new dimension to this powerful technique by providing unparalleled insight into the spin dynamics in novel magnetic materials and strongly correlated electron systems.

- **X-ray Scattering:** In addition to charge, spin and orbital degree of freedom, the atomic structure of the strongly correlated electron materials is of considerable importance, as it dictates the emergent electronic properties. This is especially important for hetero-interfaces in metal oxides, such as LaAlO3/SrTiO3, where the precise atomic arrangements determine if the interface is doped n- or p-type. We will build on SSRL’s strength in materials scattering to develop a vibrant program in oxide heterointerface structure that is closely coupled to Stanford and the SSRL spectroscopy program. This will be a significant complement to ARPES and will allow a more complete physical picture of the emergent phenomena at metal oxide interfaces. We also expect to extend the program to the interface structure for energy materials; these measurements require an undulator source.

- **Resonant Soft X-ray Scattering (RSXS):** To paint a complete picture of strongly correlated electron materials, it is important to understand the rich variety of ordering phenomena in their novel ground states, such as charge/spin ordering in the stripe phase of high temperature superconductors, orbital ordering in manganites, and charge density waves in ReTe$_3$ (Re= rare earth), as well as the collective excitations, such as phonon, magnon, and d-d excitations. Here, resonant soft x-ray scattering (RSXS) can play an important role by directly probing these orders as exemplified by the detection of the charge ordering in La$_{2-x}$Ba$_x$CuO$_4$, a cuprate superconductor with static stripe order. SSRL will implement a program to develop RSXS on soft x-ray beam lines 13 and 10-1. This will complement the ARPES and (hard) x-ray scattering of quantum matter; this program will further benefit our soft materials efforts (photovoltaics) by enabling RSXS at the carbon (and other low atomic number elements) absorption edge.
Complementing the RSXS are soft x-ray scanning transmission x-ray microscopy (STXM) and holography and coherent scattering techniques. These techniques are appropriate for quantum matter as well as magnetic materials and nanostructures (e.g., spintronics), where it remains as a great challenge to understand the underlying microscopic mechanisms responsible for the magnetic properties. Photon-in photon-out STXM is inherently sensitive to bulk materials, buried layers and nanostructures and will enable unique investigations of nanoparticle functionalities in biomedical and magnetic applications. A soft x-ray instrument is coming into operation at beam line 13. X-ray holography and coherent scattering use the coherence of synchrotron radiation for lens-less imaging of magnetic domain structures. An x-ray holography end station is jointly operated at SSRL beam line 13 and the LCLS SXR beam line. Future STXM and coherent scattering research will emphasize femtosecond laser pump - x-ray probe experiments and x-ray photon correlation schemes via time resolved detection for accessing the few picosecond timescale. These make use of the unique SPEAR3 low-α mode operation and bridge the gap between conventional synchrotrons and FELs.

4.1.3 Cross-Cutting Theme: In-situ Scattering, Spectroscopy and Imaging of Reactions and Materials Synthesis

The ability of hard x-rays to penetrate materials enables real time (in-situ and in operando) studies of materials processing and reactions. While much has been done at SSRL and elsewhere in the past decades, with the emergence of novel nanomaterials and the increasing importance of sustainable energy materials, hard x-ray scattering, spectroscopy and imaging will play a vital role in better understanding these reaction processes. This will facilitate the rational design of novel functional materials. The structure and morphology of supported nanomaterials used as catalysts changes during the catalytic reaction and this can have an effect on the subsequent reactivity. Thus, to better understand these effects, it is important to probe these changes in situ and in real time. This can be accomplished with in-situ imaging (using an upgraded transmission x-ray microscope (TXM)), spectroscopy (new advanced spectroscopy beam line) and in-situ, simultaneous SAXS/WAXS on the new undulator beam line. Similarly, for electrochemical energy storage, in-situ studies of how the anode and cathode morphology and physical and chemical structure change during discharge and charge are important for understanding capacity fading, an outstanding issue for electrical vehicle batteries (see Figure below).

X-ray scattering, spectroscopy and imaging will also enable better understanding of advanced materials processing. Since the ultimate structure and morphology of a material depends on its synthetic conditions, studying this in real time provides a way to favorably tune the structure and morphology. For example, if organic solar cells are to have an impact on our energy landscape, they must be fabricated by low-cost printing. Through in-situ x-ray scattering of the printing process (see figure), SSRL will explore the role of printing in the formation of organic solar cells and to quantitatively relate the performance of organic solar cells to the material’s microstructure. An in-situ materials synthesis capability that combines Pulsed Laser Deposition (PLD) and Molecular Beam Epitaxy (MBE) is being developed for the new ARPES end station on beam...
A combination of the state-of-the-art ARPES system and a sophisticated thin film growth system will greatly enhance the applicability of ARPES. We also envisage both in-situ scattering and spectroscopy of atomic layer deposition (ALD) working with Stanford's Center on Nanostructuring for Efficient Energy Conversion (CNEEC) and of printed batteries.

4.1.4 Enabling Technology: High Repetition Rate Pump-Probe Science

Condensed matter consists of large numbers of atoms that can be arranged in a fine balance between bonding, electronic and magnetic forces. Important properties of these materials are driven by how the atoms are perturbed when subjected to an external stimulus and then regain their equilibrium. If the external stimulus is sufficiently large, then often the perturbed state, instead of regaining its original equilibrium structure, transforms to a new arrangement through a phase transition or a chemical reaction. Understanding how condensed matter responds to such an external stimulus is, therefore, essential for not only deciphering mechanisms and pathways of scientifically interesting and technologically important chemical reactions but for designing new materials with precisely tailored properties. Pump-probe experiments are thus at the heart of several of the present scientific and technological challenges (from strongly correlated materials to artificial photosynthesis).

X-rays are an attractive probe of the response of matter to an external stimulus, since they can directly probe the arrangement of atoms and their electrons. Lattice structures and phonons are probed through specular and diffuse scattering, electronic structure through photoemission and absorption spectroscopy, and magnetic structure through polarization dependent spectroscopy and scattering. The intensity of the pump is a key control. A low intensity pump perturbs the system only slightly and the experiment probes the shape of the energy minima at equilibrium by monitoring oscillations in the non-equilibrium states. Increasing the pump intensity probes states further away from equilibrium, and at even higher pump intensity the experiment probes energy barrier(s). Often what is desired is a probe beam with low peak intensity but high average intensity, since this results in a large enough x-ray signal. These high repetition rate pump-probe studies are best performed at SSRL's high-brightness beam lines and they complement LCLS work. SSRL will develop instrumentation and further evolve accelerator timing-mode lattices (such as the current low-α mode) for such capabilities.

4.1.5 Summary of Planned Future Capabilities

The scientific strategy is driving the need for and planned around the following beam line and instrument developments:

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<th>Science themes</th>
<th>Experimental technique / beam line / instrument</th>
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<td>Strongly correlated electrons</td>
<td>Spectroscopy; Undulator beam line; diffractometer</td>
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<tr>
<td>Information technology</td>
<td>Spectroscopy; Undulator beam line; diffractometer</td>
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<tr>
<td>Energy: Photon conversion and batteries</td>
<td>Spectroscopy (x-ray inelastic scattering); Undulator beam line; diffractometer</td>
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<td>in-situ growth and synthesis</td>
<td>Spectroscopy (x-ray inelastic scattering); Undulator beam line; diffractometer</td>
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<td>Picosecond time domain</td>
<td>Spectroscopy (x-ray inelastic scattering); Undulator beam line; diffractometer</td>
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4.2 Chemistry, Catalysis and Interface Sciences

Catalysis is the essential mechanism for directing and accelerating chemical reactions. The development of efficient and selective catalysts is key to enabling use of alternative sources of fuels and chemicals, directly or indirectly based on renewable resources, to meet the growing energy needs while reducing environmental impact. Recent advances in theory aim to design catalysts on the basis of understanding the basic catalytic mechanisms, the materials properties determining them and the chemical reaction pathways, and to enable catalyst synthesis. Fundamental to this understanding is also that of chemistry and chemical processes in general, as applied catalysis, but also to pure chemical systems, biogeochemistry, environmental chemistry, biochemistry, and materials chemistry. The chemistry, catalysis and interface chemistry program encompasses all of these science areas.

SSRL’s chemistry, catalysis and interface science program will expand its existing specialized spectroscopy, imaging and scattering capabilities to work with the user community to develop molecular-level characterization of catalysts under in-situ reaction conditions, as well as for high-throughput characterization of synthetic models. SSRL will also focus on enabling the understanding of the fundamental underlying electronic and structural properties, and course of chemical reactions, on relevant scales of space, time and energy, for chemistry and catalysis.

In the coming years, the emphasis will be on selected areas, such as those related to producing hydrogen from solar water splitting, alcohols from the cellulose of plants, and hydrocarbons from recycled carbon dioxide. Special emphasis will be given to the following developments:

- In-situ, real-time characterization tools, based on hard and soft x-ray absorption (XAS) and emission (XES, PES) spectroscopies, inelastic scattering-based methods, XAS imaging, x-ray scattering, and x-ray microscopy and tomography with XANES capabilities, over multiple time and length scales
- Integrating non-synchrotron based characterization and analytical tools, such as mass spectrometry, Raman, infrared and UV-vis spectroscopy with the synchrotron techniques and facilities
- Bringing together surface and interface science, nanoscience, molecular science including bio-catalysis and environmental science
- Coupling the experimental techniques closely to theory and modeling

We will expand on and create new partnerships with a number of institutions in energy and catalysis research, including national laboratories, DOE Energy Innovation Hubs, Energy Frontier Research Centers (EFRCs) and Bioenergy Research Centers, industry and Stanford University Institutes, Centers and Departments. We will continue to grow our strong scientific partnership with the SUNCAT Center for Interface Science and Catalysis at SLAC and Stanford. We will expand on collaborations with national and international university programs and with Stanford University. We will closely coordinate with other DOE Office of Science user facilities to enhance industrial research.

Finally, we will continue our long-standing tradition of educating and training the next generation scientific workforce through introductory workshops for new users, summer schools for more advanced researchers, web-based experiment simulation tools, and mentoring of undergraduate and graduate students, and postdoctoral scholars.

In the following, we will focus on the scientific challenges in the chemistry and catalysis research directions at SSRL, new beam lines and instrumentation being developed and planned, and emerging plans for biogeochemistry.

4.2.1 Catalysts for Efficient Energy Production

Most chemical processes involved in energy conversion utilize catalytic chemical transformations. With the concept of “Materials by Design”, catalysis research is evolving to an integrated, continued cycle of theoretical modeling and prediction of optimized performance, synthesis of catalyst materials, and characterization in real time of catalyst structure and chemistry. Among the most important applications are catalysts for the synthesis of transportation fuels, and conversion of absorbed solar energy into chemical fuels through key transformations, such as production of H₂ and reduced hydrocarbons from CO₂, water, and sunlight. Also important is sustainable chemistry, where efficient synthesis of a few key molecules, such as methanol, ethylene and propylene - from non-fossil resources such as biomass - is the platform for some 50,000 industrial chemicals.

SSRL provides major beam line facility tools tailored to using x-ray absorption and emission spectroscopy and other techniques to characterize the electronic and geometric structures of catalysts, including supported metal
nanoparticles and clusters, metal complexes, oxides, silica-based co-catalysts and electrocatalysis materials for heterogeneous catalysis, as well as homogeneous catalysis involving organometallics, with increasing sophistication. New directions include \textit{in-situ} and \textit{in-operando} approaches including temperature, pressure, gases, and electrochemistry, with instrumentation implemented on existing insertion device beam lines and new bending magnet stations. The time domain will be addressed through rapid scanning techniques (minutes to milliseconds), energy-dispersive x-ray emission spectroscopy, and picosecond spectroscopy based on SPEAR3 low-\(\alpha\) modes.

- **Advanced Spectroscopy:** Since heterogeneous catalysts typically consist of one or more multi-element, nanometer sized active ingredients dispersed on high surface-area porous supports, development of techniques and sample environments to exploit high-energy resolution, hard x-ray emission spectroscopy will provide information about the interaction between the adsorbed molecule and the surface. Specific techniques include non-resonant x-ray Raman scattering, \(K\alpha\), \(K\beta\), and \(K\beta''\) x-ray emission, and resonant inelastic x-ray scattering (RIXS), and a new undulator-based “advanced spectroscopy” beam line will be implemented. Interpretation of the x-ray emission data to elucidating bonding between the molecules and surface atoms will be addressed through the development of new theoretical approaches.

- **High-throughput Spectroscopy:** New developments through, among others, the creation of SUNCAT at SLAC, DOE’s Energy Hubs (such as JCAP) and Energy Frontier Research Centers, and PNNL’s Institute of Integrated Catalysis, will dramatically accelerate the production of new catalytic materials that will require high-throughput x-ray spectroscopic characterization. SSRL will optimize and automate most parts of this process, from sample handling, measurement, online data visualization to data analysis, to meet the needs of rapid screening of large numbers of samples, and furthermore enable this to be performed via remote access to the experiment by the researchers.

- **In-situ X-ray Absorption Spectroscopy:** To enable in-situ characterization of catalysts under operand conditions through x-ray absorption spectroscopy (edge and EXAFS) a bending magnet port will be dedicated for buildout of two stations, with focused and unfocused optics capabilities, and including specific instrumentation for reaction controls.

An important building block of a new sustainable energy infrastructure is the transition of the transportation sector from inefficient internal combustion engines towards electric drives. Proton exchange membrane fuel cells (PEMFCs) are promising power sources since they can generate electricity from the electrochemical oxidation of a fuel, e.g. hydrogen or methanol. By preparing an ultrathin model catalyst, one Pt monolayer grown on a Rh(111) single-crystal surface, and using high energy resolution fluorescence detection techniques, unambiguous spectral fingerprints for surface Pt–O interactions were established, leading to insights of full cell performance. 

\textit{Phys. Chem. Chem. Phys.} \textbf{2011}, \textit{13}, 262. Figure at right shows: PEMFC fuel cell under \textit{in-situ} electrochemistry (left); image of beam impinging monolayer of Pt on Rh(111) surface (top right); \textit{HERFD} spectra at the Pt L\textsubscript{3} edge \textit{HERFD} spectra as a function of applied potential.

### 4.2.2 Surface Reactivity and Bonding

The description of the chemical bond between a surface and a molecule is the fundamental basis for understanding surface chemical reactivity and catalysis. The reaction rate is often related to the stability of specific intermediates on the surface. When a new catalytic material is researched, it is a matter of electronic structure design in order to create chemical bonds of a specific strength. The best material is often where the bond is neither too strong nor too weak. SSRL focuses on developing tools to probe the electronic structure of the adsorbed species on the surface to enable trends between different systems to be determined. In order to derive a simple picture, it is essential to provide surface-sensitive spectroscopic techniques that allow probing the electronic structure around one specific atomic site, in particular when investigating complex systems with many different sites.
Both soft x-ray emission and absorption spectroscopy provide an atom-specific probe of the electronic structure of low Z elements such as C, N and O. The atomic sensitivity arises from the creation of a core hole during the absorption process (see figure), and that this core hole can only be filled by valence electrons in the proximity of the excited atom. The final state of the x-ray emission process is a valence hole state similar to the final state in valence band photoemission, but here the valence electronic structure is projected onto a specific atom. Another essential aspect is that the polarization of the incident radiation and the direction of the emitted radiation allow directional sensitivity, providing a direct measure of the molecular orbital symmetry. For adsorbates with atoms of the same element but in different chemical surroundings, selective excitations can thus be used to obtain x-ray spectra from each specific atom in the system. We will continue to develop beam lines and instrumentation for the study of surfaces and interfaces for chemistry and catalysis:

- **Soft X-ray Surface Spectroscopy:** The SSRL soft x-ray beam line 13-2 incorporates a surface science experimental end-station with a newly developed high-throughput soft x-ray emission spectrometer, which will enable advanced studies of many new catalytic materials as they undergo their reactions. A second end station for ambient pressure photoemission spectroscopy (APPEX) will allow measurements of surface species under near reaction condition (~50 torr at 500 eV).

- **Hard X-ray Surface Spectroscopy:** A third end station, for high-energy (5-20 keV) x-ray surface/interface photoemission spectroscopy under ambient pressure will be developed for catalysis research in, among others, artificial photosynthesis, and will be co-located on the new “advanced spectroscopy” undulator beam line.

### 4.2.3 Enzyme and Bio-Inspired Catalysts for Sustainable Energy

One of the key challenges in developing alternative energy sources is the availability of inexpensive and sustainable catalytic systems that are not based on rare, and economically non-viable, noble metal-based chemical systems. Fortunately, ‘blue-prints’ of such catalysts can be derived from understanding the function of metalloenzymes, in particular those that perform reactions such as producing hydrogen, converting nitrogen to ammonia, and producing hydrocarbon fuels from CO and H₂, for which Nature has evolved processes with highest sophistication and efficiency. To develop biohybrid or bioinspired production technologies, one needs to decipher these ‘blue-prints’ at the molecular level, both in terms of the location of atoms (geometric structure) and their electrons (electronic structure) in both resting and reactive intermediate states. The definition of physico-chemical parameters responsible for the impressive catalytic activity of such metalloenzymes is essential for understanding the overall mechanisms.

SSRL is playing a major national role in detailed characterization of the structural and electronic properties of metalloenzymes related to bioenergy and associated model systems. A novel research approach is multi-edge XAS measurements, where studies are performed at metal K and L edges, and at ligand (S, P, O, N, C) K-edges for a specific system, which due to complementarily allows for the experimental definition of the total electronic and geometric structure. This ability to conduct XAS experiments at a range of very soft to hard x-ray energies is a unique strength of SSRL. Similarly, instrumentation and methodology has been developed for polarized single crystal XAS, which provides unique capabilities for electronic and geometric structural determination of the active site.

- **Advanced Spectroscopy:** The new undulator advanced spectroscopy beam line will add a new dimension to these studies, as it will enable the combination of static and time-resolved x-ray absorption and emission experiments on systems such as nitrogenases, hydrogenases and photosystem centers. This will be coupled to genetic manipulations and/or chemical and photo-stimulated creation of reaction intermediates. Such intermediates might display minor but very indicative changes in the electronic structure, which will be detectable through new high-energy resolution x-ray emission spectroscopy. Added features will include in-situ monitoring, such as using UV-visible spectroscopy, or IR/Raman as appropriate.
• **Tender X-ray Spectroscopy:** A new low-energy (2-5 keV) bending magnet beam line will be instrumental in providing enhanced XAS imaging capabilities (at the micron level) as well as large area measurements for complementary ligand and metal L-edge x-ray absorption and emission studies.

• **Theoretical Modeling:** The experiments will be strongly coupled to theoretical modeling (SUNCAT) and development of new analysis tools.

Methane has potential as an alternative fuel but is also a potent greenhouse gas. The major source of methane produced in nature is the end product of the archaean decomposition of organic matter in strict anaerobic environments, such as lake sediments and the intestinal tract of animals. The protein methyl-coenzyme M reductase (MCR) catalyzes the final and rate-limiting step in the methane formation and is responsible for the generation of ~1 billion tons of methane every year. The catalytic site contains a nickel atom bound in a tetrapyrrolic ring. During the reaction, nickel changes oxidation state, and a short-lived intermediate where methyl is bound has been implicated. Through a combination of dilute solution and single crystal XAS (with electronic information provided by the K-edge structure, and geometric structural information from EXAFS), crystallography, spectroscopy and density functional theory calculations, a Ni$^{3+}$-methyl active site was established (Biochemistry 2009, 48, 3146; J. Am. Chem. Soc. 2011, 133, 5626).

4.2.4 Molecular Biogeochemistry, Environmental Chemistry and Interfacial Chemistry

Understanding and mitigating biological and environmental impacts of energy production are important to society. Fundamental research is needed to better understand and control carbon cycling and sequestration (in soils, oceans, the atmosphere, and geological repositories), safe disposition of nuclear waste, fate and mitigation of groundwater contaminants, and sustainability and resiliency of complex biogeochemical and environmental systems that support life on Earth. Key processes are driven by reactions occurring at the *molecular* scale at interfaces between water, minerals, and biological surfaces (e.g., biofilms), and in complex natural *mesoscale* systems in which dimensions range from 100 nanometers to millimeters. The exceptional capabilities of synchrotron techniques to provide information about bonding environments and electronic structure under *in-situ* conditions, over a continuum of length and temporal scales are crucial to enabling new discoveries and building our understanding in these research areas. Full understanding of these systems requires consideration of both “bio” and “geo” components and how they interact.

SSRL will identify strategies by which we can make the greatest scientific impacts in these societally important areas that we pioneered in the 1980’s. Emerging emphasis areas include the cycling of carbon, “biogeochemical carbon-critical” elements (including N, S, P, Fe), and contaminants in Earth’s subsurface and oceans; geological CO$_2$ sequestration, including reactive transport in mesoporous media; sustainable production and use of energy critical elements (including those in the platinum and rare earth element groups); developing mechanistic understanding of important biogeochemical reactions, including biomineralization; and the environmental reactivity and transformations of natural and anthropogenic nanoparticles. SSRL’s world-class strengths in x-ray absorption spectroscopy and imaging programs provide the foundation and leverage our competitiveness and impact of these programs.

Special emphasis will be given to the following developments:

• Specialized tools and integrated *in-situ* approaches to imaging the speciation and distribution of critical elements in complex natural biogeochemical systems at molecular to millimeter length-scales, at multiple time-scales, and under reactive conditions

• Enhancements to x-ray absorption and fluorescence spectroscopy and other experimental capabilities for detecting trace-element levels of different chemical species in complex environmental systems (see Figure below)

• Future STXM capabilities in the energy range of 0.2 to 2.5 keV for exploring chemistry accessible at the C, N, P and S K absorption edges

The development of high-throughput spectroscopy described previously is important for biogeochemical and environmental applications, as are the new beam lines. In particular, the new tender (2-5 keV) x-ray spectroscopy
bending magnet beam line will be essential in providing XAS imaging (at the micron level) and in determining the molecular-level speciation of the key elements P through Ca in aqueous solutions.

(Left) Acid mine drainage site at an abandoned Pb-Zn mine in Carnoules, Gard, France highly contaminated by arsenic (300 ppm As(III) in the water); (Right) [a] Thiomonus sp. bacteria (yellow arrows) were found to promote the precipitation of amorphous Fe(III)-As(V) hydrous oxides; [b] As(V) inner-sphere complexes on the Fe-sulfate mineral schwertmannite (after G. Morin et al., Environ. Sci. Technol. 2003, 37, 1705-1712; G.E. Brown, Jr. and G. Calas, Geochem. Perspect. 2012, 4-5, 483-742). The speciation of As was determined by XAS at SSRL and ESRF

4.2.5 Summary of Planned Future Capabilities

The scientific strategy is driving the need for and planned around the following beam line and instrument developments:

<table>
<thead>
<tr>
<th>Science themes</th>
<th>Experimental technique / beam line / instrument</th>
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<tr>
<td></td>
<td>Hard x-ray spectroscopy</td>
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<td>Catalysts for energy production</td>
<td>In-situ &amp; high throughput XAS (bending magnet)</td>
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<td>Advanced spectroscopy undulator (XES, XRS, RIXS)</td>
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<td>Tender x-ray XAS</td>
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<td>Surface reactivity and bonding</td>
<td>Hard x-ray ambient pressure surface spectroscopy</td>
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<tr>
<td>Enzyme and bio-inspired catalysis</td>
<td>Advanced spectroscopy undulator (XES, XRS, RIXS)</td>
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<td>Tender x-ray XAS</td>
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<td>Molecular biogeo-, environmental and interfacial</td>
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<td>STXM</td>
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<td>Picoscend time domain</td>
<td>Advanced spectroscopy undulator (XES, XRS, RIXS)</td>
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<td>Hard and tender x-ray XAS imaging</td>
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<td></td>
<td>upgraded TXM</td>
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4.3 Structural Molecular Biology

The goal of understanding biological structure and function, and applying this knowledge to solving grand challenge problems related to medicine, energy, and the environment is crucial to human health. 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 obtaining and utilizing biomolecular structural information on the nano-to-atomic scale to understand function (and malfunction) of biological processes. The SMB program has pioneered development of new and enhanced approaches for the investigation of biomolecular structure and function, making them widely available to the biomedical research community, contributing to both basic scientific knowledge and translational research. The SMB program uses a combination of macromolecular x-ray crystallography (MC), biological small angle x-ray scattering/diffraction (SAXS), x-ray imaging, and x-ray absorption (XAS) and emission spectroscopy (XES) to study the most challenging biological macromolecular systems.

4.3.1 Macromolecular Crystallography

Macromolecular crystallography (MC) will increasingly focus on the understanding of the complex biological machinery that drive the biology in cells. A first focus will be on structural studies of increasingly large and challenging macromolecular assemblies, crucial to advancing the understanding of complex biochemical processes. A second focus will be on membrane proteins, which are of major pharmacological importance, but exceptionally challenging to crystallize. While membrane proteins make up ~25% of an organism’s genome, less than ~1% of their structures have been determined. With advances in crystallization and synchrotron diffraction methods, a significant number of these structures will be within reach. A third area will be on controlling radiation damage to enable structure determination of specific chemical states of metalloproteins to understand enzymatic processes related to disease and bioenergetics. A fourth will be to continue developments of fully automated, high-throughput structure determination tools, working closely with the Structure Determination Core of the Joint Center for Structural Genomics, a NIH NIGMS funded center within the Protein Structure Initiative, and in collaboration with pharmaceutical industry. A specific effort will devoted towards structure-based drug design, which are critical not only for finding new drugs for the most serious illnesses, but also in the fight against the growing problem of drug resistance. The developments will build on the strong foundation of high automation with high reliability, full remote-access operation of all MC beam lines, specialized software for data collection and automation of data reduction and analysis, and high-capacity computing facilities. Specific emphasis will be given to the following developments:

- Novel crystallography data collection strategies for weakly diffracting samples, capitalizing on enhanced characteristics of novel detectors, micro-beam capabilities, and developments of sample delivery
- Sample handling techniques for room temperature and high throughput studies of chemically and mechanically sensitive samples
- Integrated non-synchrotron radiation spectroscopies for in-situ monitoring of electronic states in metalloproteins to follow biochemical processes and monitor beam induced changes
- Fully automated high-throughput, multi-crystal data collection pipelines to 1) accelerate fragment-based drug discovery, 2) mitigate radiation damage in weakly diffracting and/or microcrystal systems, and 3) preserve the oxidation state in metalloprotein active sites

A second generation microbeam undulator beam line is part of the future strategy. It will complement existing facilities, and will enhance the growing synergy with the Linac Coherent Light Source (LCLS) in the development of sub-micron and time-resolved crystallography described below.
4.3.2 Macromolecular Crystallography with LCLS

The Linac Coherent Light Source (LCLS) is showing great promise for determining macromolecular structures from sub-micron sized crystals and possibly mitigating radiation damage altogether (diffraction-before-destruction). The LCLS also opens a new window in the time domain that is more than $10^3$ faster than currently accessible using synchrotrons for the study of biomolecular processes, opening access to a new regime of structural biodynamics and biochemical reactions. The SMB MC program is strongly engaged in the development of macromolecular crystallography at LCLS, both in scientific projects aimed at fundamental studies using an x-ray free electron laser as source, and in R&D. This is part of a larger initiative at SLAC with specific focus to develop parts of an open access, general user accessible ‘pipeline’ for nano- and micro-crystallography using LCLS, and to develop multiple methodologies for sample delivery, data acquisition, data reduction and structure solution. There is strong synergy and coordinated developments between SSRL SMB and LCLS, and these take into account complementary resources and facilities, such as instrumentation used at SSRL’s BL12-2 and LCLS stations CXI, XPP and XCS. This is rapidly evolving, and to an increasing degree involves scientists from other institutions than Stanford, such as Lawrence Berkeley National Laboratory, University of California at Berkeley and Los Angeles, and Caltech, with funding emerging from NIH NIGMS, DOE BER, and non-Federals sources as Howard Hughes Medical Institute. The SSRL SMB scientists will work closely with LCLS to help drive this area of strategic importance to SLAC, LCLS and SSRL, and for benefit of the scientific structural biology community.

4.3.3 Structural Genomics

The Structural Genomics Division at SSRL hosts the Structure Determination Core (SDC) of the Joint Center for Structural Genomics (JCSG). The JCSG operates a high-throughput structure determination pipeline as part of the NIH NIGMS-funded Protein Structure Initiative (PSI). The JCSG has partnered synergistically with the SSRL SMB program since its inception in 2000 to automate all steps in the x-ray crystallographic structure determination process - from crystal screening and data collection on the macromolecular crystallography (MC) beam lines, highly automated structure determination, and detailed, high quality structure refinement by a team of dedicated scientists.

The JCSG has contributed substantially to the development of HT structural biology worldwide as an innovative and highly productive structural genomics center, which has explored the structure, function and evolution of a diverse set of novel protein families. JCSG has developed a robust and scalable high-throughput platform to carry out all experimental steps, from identifying a target gene to depositing a 3-D structure in the Protein Data Bank (PDB). In the process, many new technologies and methods have been developed that are now in general use throughout the structural biology community, many in close partnership with the SMB MC group leading to rapid deployment.

As PSI evolved into PSI-Biology in 2010, the focus today is on high-throughput structural biology pipelines for large-scale biology partnerships that tackle several classes of challenging targets, including eukaryotic (mammalian) proteins and protein-protein / protein-nucleic acid complexes. Computational approaches are developed to combine low (from SAXS) and high resolution structural data to account for the dynamics of the component molecules that may occur during complex formation, and these methods are provided to the user community as they reach mature states.

The Structural Genomics Division is extending the publically available JCSG dataset repository to include and provide all datasets for solved and unsolved JCSG targets and also to provide access to screened diffraction images, to foster collaborations with methods developers, especially for challenging structures, and provide enhanced communication colleagues at remote locations. It will also actively engage members of the world-wide biological community to develop new biologically themes and projects and to carry out functional studies.

4.3.4 Biological Small Angle X-ray Scattering

Biological small-angle x-ray scattering and diffraction (BioSAXS) is one of the primary tools to study the structure of non-crystalline biological macromolecular systems in solution or as partially ordered arrays of biomolecules. Such studies can be performed under near physiological conditions, require small amounts of material and are well-suited for time resolved measurements, e.g. measuring the kinetics of conformational changes, or the identification of folding intermediates under biologically relevant conditions. As a structural technique of moderate resolution (~7-10 Å or lower), but with the capability of studying very large protein assemblies, SAXS complements higher-resolution techniques such as MC and NMR, since solution SAXS can model very large molecular complexes, whose overall
structure is unknown. Where structures of individual components are available they can be included in modeling to obtain a higher resolution perspective.

Scientific applications at SSRL focus on a number of systems with specific relevance for understanding disease and drug development, and will continue to drive developments at the BioSAXS beam line facility. Prime examples are the maturation process of virus particles or protein folding (time-resolved SAXS), amyloid precursor proteins (in-situ purification with sample delivery), protein families related to the human microbiome (automation and full pipeline), systems for drug delivery (fiber diffraction instrumentation), and mechanistic insights into biological process through understanding of conformational flexibility differences in solution and crystal forms (multi-method approaches). (The figure to the right illustrates time-resolved SAXS measurements and resulting particle structures for the maturation process for NwV virus.) Future developments also include the integration and simultaneous use of non-x-ray characterization tools.

The BioSAXS beam line 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 through a flexible camera approach. Specialized sample handling devices include an automatic fluid sample changer for high-throughput/small-volume measurements of large number of samples, in-situ FPLC with the sample measured as it is eluted from the column. The facility includes advanced instrument control and data processing software. Non x-ray characterization tools include dynamic light scattering instrumentation, providing at times critical sample characterization information. In addition to static solution scattering, BL4-2 maintains a premier experimental setup for time-resolved studies providing access to reaction time scales in the milliseconds and above.

Future developments will focus on

- Advanced automation with minimized sample volume and reduced measurement time, coupled with computational approaches to automate data quality assessment and data analysis, to create a fully automated pipeline, including remote access for users
- Enhancement of time-resolved SAXS capabilities to the sub-millisecond time regime and exploring new reaction triggering schemes
- Development of microfluidic approaches to high throughput solution scattering and time-resolved solution scattering experiments
- Development of SAXS-integrated biochemical separation methods coupled to in-situ non-synchrotron based characterization techniques to enhance sample integrity of sensitive samples

The development of an undulator-based SAXS/WAXS beam line for materials science will enable some specialized BioSAXS experiments that require such beam characteristics on a time-shared basis for the SMB program.

### 4.3.5 Biological X-ray Absorption and Emission Spectroscopy

Metal ions have key roles in biological structure and function - from being active sites of many enzymes to shuttling electrons in key metabolic pathways, having roles in signaling pathways and being key elements of cancer chemotherapies and disease-related biological malfunctions. X-ray absorption and emission spectroscopies provide exquisite local structural knowledge (electronic and geometric) about the metal active sites in biomolecules that address structure-function relationships. XAS spectromicroscopy provides spatially resolved information about metal distribution and speciation in materials of biological and medical relevance, including tissues. These spectroscopy techniques provide information that is highly complementary to that obtained by MC or SAXS in that they directly probe chemical properties of a chosen metal site in the macromolecule of any physical state.

The SSRL SMB BioXAS program has developed one of the largest dedicated and concentrated activities in the world with optimized beam lines and specialized instrumentation and analysis capabilities for enabling biological and biomedical research. The future emphases will be on the study of reaction intermediates, using polarized single crystal XAS with optical or chemical stimuli and with in-situ monitoring using non-SR spectroscopy approaches for
selected systems; and using time-resolved enzyme solution studies based on microfluidic device mixing and energy-dispersive XES at SSRL and LCLS. Detector developments for ultra-sensitive fluorescence measurements, and with fast read-out and processing capabilities, will be pursued in collaboration with industry and national laboratory development programs. Data analysis developments will include collaborations for inclusion of theoretical calculations for the interpretation of electronic and geometric structure, which will be critical to the interpretation of time-domain processes. Instrumentation and software developments for imaging of biological specimen, in length scales from mm to microns, and over energy ranges from soft to hard x-rays, will be further developed, and extended to XAS tomography and XAS confocal imaging. New facilities of particular importance include:

- **Advanced Spectroscopy**: The new undulator advanced spectroscopy beam line will be instrumental for the time resolved studies, as it will enable the combination of static and time-resolved x-ray absorption and emission experiments on systems, such as electron transfer proteins, oxidases and reductases, and complement developments for static solution and single crystal enzyme studies.
- **Tender X-ray Spectroscopy**: The new low-energy (2-5 keV) beam line will be instrumental in providing enhanced XAS imaging capabilities (at the micron level) for tissues, as well as large area measurements for complementary ligand and metal L-edge x-ray absorption and emission studies of biomedical systems.

As an integrated program within the Structural Molecular Biology center activity, we will educate and train the next generation structural biology scientists through tailored workshops, summer schools, web-based tools, mentoring of students and postdoctoral fellows, and by bringing the synchrotron to the home laboratory through advanced remote-access developments in tandem with rapid access beam time mechanisms. This will be coupled to developments of on-line learning tools, including simulation of experiments, in collaboration with Stanford University’s on-line teaching tool developers.

**4.3.6 Summary of Planned Future Capabilities**

The scientific strategy is driving the need for and planned around the following beam line and instrument developments:

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<thead>
<tr>
<th>Structural biology area</th>
<th>Experimental technique / beam line / instrument</th>
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<td></td>
<td>Diffraction</td>
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<tr>
<td>Macromolecular crystallography</td>
<td>Micro-beam undulator for micro- to nano-crystallography</td>
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<td>Biological SAXS</td>
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<td>Biological XAS and XES</td>
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<tr>
<td>Picosecond to femtosecond time domain</td>
<td>Micro- to nano-crystallography instrumentation at LCLS</td>
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5 Operational Excellence

5.1 Accelerator Improvement Plan

The SSRL accelerator, SPEAR3, provides a 3-GeV electron beam to deliver high brightness and high average power photons to multiple experimental stations over the soft to hard x-ray energy spectrum. SPEAR3 is operated with top-off injection at a current of 500 mA and with a reliability of typically above 97%. The SSRL strategy for SPEAR3 is to continually improve beam quality and innovate to keep SSRL competitive with synchrotron light sources around the world. An accelerator improvement plan has been developed with the following key elements:

- Accelerator performance improvements
- Accelerator reliability improvements
- Accelerator research and development
- Advancing the next generation light sources

5.1.1 Accelerator Performance Improvements

Acceleration performance improvements include improvements in beam quality, optimization for time-resolved experiments, and injector enhancements to increase the range of injection options.

Improvements to Beam Quality

- **Lower emittance**: Optimization of the SPEAR3 brightness by reducing the horizontal emittance from approximately 9.6 nm-rad to 5 nm-rad. The emittance can be reduced to approximately 6 nm-rad by increasing the tune and dispersion, and by modifying the injection septum to maintain the dynamic aperture for injection. The emittance can be further reduced to 5 nm-rad with the addition of superconducting damping wiggles.
  
- **Multi-bunch feedback** - this will improve beam stability in three ways:
  - Reduction of transverse damping time to reduce transient motion due to top-off injection.
  - Enhancement of the single bunch purity as required for timing mode user experiments by clearing charge adjacent to timing buckets.
  - Mitigation of the multi-bunch instabilities associated with future in-vacuum undulator (IVUN) and ion instabilities at 500 mA.

The following figure shows emittance plotted against dispersion, as a function of all possible SPEAR3 lattices. The blue area indicates the allowed values based on current SPEAR3 operating parameters. The black dots show the realized values and projected values based upon the accelerator upgrade described above.
The following figure shows the emittance from light sources around the world including the proposed SPEAR3 emittance reduction to 5 nm-rad.

**Optimization for Time-resolved Experiments**

- **Low-α mode** - Installation of a sub-ps laser to perform a cross correlation pulse length measurement to improve user support for time resolved experiments.
- **Diagnostics upgrade** - We plan to upgrade the SPEAR3 and transport line beam position monitors (BPMs) to measure position and arrival time with improved resolution for short-pulse, low-α experiments where the single-bunch charge is low. The ability to monitor and study turn-by-turn non-linear dynamics under these conditions will also assist in providing the user community with stable beam conditions and long beam lifetime.

**Injector Enhancements**

SPEAR3 is currently operating with top-off injection, which maintains the stored current at better than 1% accuracy. Since the injector was not designed to operate in this mode, the following upgrades are planned to improve injector performance, including raising the constancy of the storage ring current to a level that is commensurate with other storage rings.

- **Bunch-by-bunch current monitor** - Optimization of the stored beam bucket pattern by targeting the best bucket for injection, to optimize the fill pattern
- **Booster power supply upgrade** - Replacement with a direct drive power supply, allowing reduction of the time between injections in order to reach current constancy of order 0.1%
- **Pulse train injection** - With an injector rf system matched to the SPEAR3 frequency and photo-cathode gun operation (see section below) we will be able to inject pulse trains instead of single bunches into SPEAR3. This will significantly increase injection rates and reduce the number of injection transients, which affect users with sensitive measurements
5.1.2 Accelerator Reliability Improvements

The projects in this category will improve the mean time between failure (MTBF) and the mean time to repair (MTTR). This is especially important for the injector, which is now over 20 years old and with some rf components over 30 years old.

- **RF Upgrade**
  - Linac RF upgrade - Addition of a pulsed 2.856 GHz klystron with IGBT based modulators and upgraded low level rf controls to improve reliability and reproducibility.
  - Booster RF upgrade - This project will replace the 30 year old rf system with a modern rf system matched to the SPEAR3 frequency. The change in rf frequency will enable pulse train injections (described above) and significantly improve the injector reliability.

- **SPEAR3 Safety System Component Upgrade** – Upgrades to permit additional beam lines, allow individual beam lines to close in response to beam line-specific faults, make the system compatible with current standards, replace aging beam shut off ion-chambers, and upgrade control system to monitor power supply status.

- **Timing System Upgrade** - Replacement of the obsolete injection timing system with a fiber-based timing system in use at LCLS, improving reliability and making distribution of timing signals inexpensive.

- **Controls Upgrade** –Replacement of CAMAC hardware, upgrade of power supply controllers to a SLAC standard Ethernet controller, and updating of booster control software to be compatible with SPEAR3 controls.

- **Injector Corrector Magnet Power Supply Upgrade** – Replacement of the obsolete injector corrector power supplies (CEBAFs) with a standard SLAC power supply.

- **Vacuum Chamber and Power Supply Spares** – Stocking of spares for the vacuum chambers and power supplies for the accelerator; this is critical in order to provide meet uptime goals, since these spares can require weeks or months to fabricate.

- **Photo-emission Gun Operation** - Replace obsolete electrostatic chopper with Q switched laser to gate electron beam. This along with the injector rf upgrade will also permit pulse train injection described above.

5.1.3 Accelerator Research and Development

The following ongoing research and development is in progress to keep SPEAR3 at the cutting edge of synchrotron radiation research as well as more generic research that will also benefit the greater accelerator community.

**SPEAR3 R&D**

- **THz beam line optimization** - Dipole chamber for extracting THz coherent synchrotron radiation from SPEAR3.

- **Multi-pole injection kicker study** - This study will determine if the SPEAR3 Lambertson injection method can be replaced with a multi-pole injection kicker design that does not disturb the stored beam and thus makes injection nearly transparent to users.

- **Photo-emission lifetime optimization** – A study to determine methods to maximize the lifetime of thermionic cathodes operated in photo-emission mode to enable conversion of SPEAR3 cathode to full time photo-emission.

- **High charge, short bunch R&D** – A study to determine the limitations and feasibility of operating with two additional accelerator cavities at different frequencies to enable simultaneous long and short bunch operation has begun. Where the two rf frequencies constructively interfere, strong longitudinal focusing leads to a short bunch but with high bunch charge instability threshold. Likewise where the frequencies destructively interfere the weak focusing yields a long bunch. The method requires very high rf voltages since the pulse length is inversely proportional to the square root of the rf gradient and thus high gradient superconducting rf cavities are necessary. We are investigating how to mitigate the higher order modes generated in multi-cell superconducting cavities for use in the SPEAR3 storage ring as well as other effects.
Generic Accelerator R&D

- **Non-linear dynamics** - This will improve the agreement between the non-linear model and non-linear dynamics measurements. As we push to lower emittance and the dynamic aperture becomes smaller, models with improved accuracy are critical. This work is also important for the design of future diffraction limited storage rings such as PEP-X.

- **Photo-cathode R&D** - SPEAR3 staff contribute to LCLS-related cathode research, including measurements of cathode performance and theory development for new designer cathodes. Research is also in progress to improve ion resistance for III-V photocathodes in high current guns.

- **Rf undulator testing** - Determine the feasibility of transporting an electron beam through a radio frequency (rf) undulator with the polarization rotated and switched on/off at kHz frequencies.

- **Ultrafast electron diffraction and microscopy** – The first high energy (MeV) ultrafast electron diffraction (UED) experiment was conducted at SSRL and staff continue to investigate ways to optimize high energy accelerators for use as UED and ultrafast electron microscopy applications.

### 5.1.4 Advancing the Next Generation Light Sources

New techniques have recently been developed to build diffraction limited storage rings that could bring a new range of capabilities to SLAC. The diffraction limited PEP-X accelerator could be realized by converting the existing PEP-II storage ring (2.2 km circumference) on the SLAC site into an x-ray source that will produce x-rays with an average brightness that exceeds any other storage ring light source, existing or planned, by greater than a factor of 10, and SPEAR3 by greater than a factor of 1000. PEP-X would capitalize on existing hardware and infrastructure (high-power rf accelerating system and utilities such as electrical and cooling networks) from the recently decommissioned PEP-II, much as the LCLS and LCLS-II capitalized on the existing SLAC linac hardware and infrastructure.

### 5.2 Beam Line Development and Technical Capabilities

Based on the scientific drivers and with the aim to match those to the optimum sources, SSRL has developed a long-term beam line build-out plan that will significantly increase both beam line capability and capacity. The light source currently features 27 operating beam lines (equipped with 33 stations): 9 independently operating bending magnet beam lines on 4 bending magnet sources and 18 independently operating insertion device beam lines on 9 insertion device sources. When fully built-out, SSRL will have 36 operating beam lines: 15 independently operating bending magnet beam lines on 7 bending magnet sources and 21 independently operating insertion device beam lines on 13 insertion device sources (see Table below). Coupled with innovative hutch equipment and state-of-the-art detectors, this promises competitive instrument performance for productive science over the coming decade.

This plan revitalizes existing beam lines and sets in motion an ambitious program of developing new undulator beam lines. SPEAR3 can accommodate five additional insertion device beam ports within the existing building footprints, offering impressive brightness and flux in the intermediate x-ray regime (see Figures on the following page). A further three bending magnet beam ports are also available for expansion into existing buildings. With more significant building modifications, further bending and insertion device beam ports could be instrumented. Beam line upgrades will optimize each source and associated beam line optics for the intended application while leveling station demand. Overall, the plan seeks to accommodate additional users in the near-term by rapidly adding capacity at "workhorse" beam lines, leading to increased productivity. Through a carefully orchestrated sequence of upgrades and application relocations, this plan will affect this transformation with a minimum of disruption to users.

**SSRL beam line sources and science disciplines served circa 2013 and those envisioned after further optimization of the existing beam lines and the addition of new beam lines. In the 2013 count, three beam lines serve multiple scientific disciplines so the beam line count by discipline does not equal the total number of beam lines.**

<table>
<thead>
<tr>
<th>Circa 2013 (three BLs shared between disciplines)</th>
<th>Fully future built out</th>
</tr>
</thead>
<tbody>
<tr>
<td>27 BLs (15 wiggler, 1 IVU, 2 EPU, 9 bend)</td>
<td>36 BLs (11 wigglers, 8 IVU, 2 EPU, 15 bend)</td>
</tr>
<tr>
<td>10 Chemistry &amp; Catalysis (7 ID &amp; 3 bend)</td>
<td>12 Chemistry &amp; Catalysis (7 ID &amp; 5 bend)</td>
</tr>
<tr>
<td>7 Structural Molecular Biology (6 ID &amp; 1 bend)</td>
<td>7 Structural Molecular Biology (6 ID &amp; 1 bend)</td>
</tr>
<tr>
<td>13 Material Science (7 ID &amp; 6 bend)</td>
<td>17 Material Science (8 ID &amp; 9 bend)</td>
</tr>
</tbody>
</table>
5.2.1 New Undulator Beam Line Developments

The lower emittance of the SPEAR3 accelerator upgrade, coupled with incremental further lattice improvements that have pushed the demonstrated SPEAR3 emittance almost three-fold lower than the SPEAR3 project design goal, make in-vacuum undulators (IVU) extremely well-suited insertion device sources for the production of high brightness, intermediate energy x-ray beams. The first IVU beam line on SPEAR3, BL12-2, was developed for macromolecular crystallography of small samples. This beam line has demonstrated the efficacy of teaming a high brightness, IVU source on SPEAR3 with stable, emittance-conserving optics and state-of-the-art experimental equipment and detectors. In the next few years SSRL plans an aggressive program to develop additional IVU-sourced beam lines.

BL12-1, a sister macromolecular crystallography beam line to BL12-2, is planned for the un-used insertion device straight of the BL12 10 mrad chicane. Taking advantage of the experience gained operating the BL12-2 small gap IVU, the new BL12-1 IVU (chicane IVU18, cf. Figure above) will be designed for smaller magnet gap allowing the incorporation of 162 poles in the same length insertion device as the older 134-pole BL12-2 IVU. This higher brightness source will be teamed with state-of-the-art Kirkpatrick-Baez (KB) mirrors and the proven SSRL LN$_2$-cooled monochromator design. The optical system will be designed to maximize source demagnification yielding a focus optimally sized for crystallography of ≤ 10µm samples with beam stabilization servo systems to ensure stable illumination of small samples. The hutch equipment will include the evolving SSRL SMB macromolecular crystallography instrumentation for micro-crystal applications.

In addition, as all of the existing SPEAR3 straight sections are IVU-capable, SSRL has many other opportunities for more high brightness IVU beam lines similar to the one described above. These include two currently in process / planned for implementation in standard straight sections (std. strght. IVU21, cf. Figure above) for an advanced spectroscopy beam line and a small/wide angle scattering materials beam line.

5.2.2 Revitalization of Existing Insertion Device and Bending Magnet Beam Lines

As noted above, the goal of SSRL’s long term beam line upgrade plan is to optimize the each source and associated beam line optics for the intended application while leveling station demand. This plan also includes the addition of bending magnet beam lines for targeted applications. The Figure below graphically illustrates the currently planned distribution of techniques across the different beam lines at the end of this upgrade process as well as showing those sources which are currently available for expansion.
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 research life cycle from beginning to end to ensure that users 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 to the right and described below.

Reaching Out to New and Diverse Scientific Communities

SSRL has remained at the forefront over the facility’s ~40-year history by continually enhancing the synchrotron source, developing new methods, beam lines and instrumentation, and bringing in new ideas from users, staff and faculty. The facility has successfully fostered several new scientific communities in areas including structural molecular biology, hard x-ray scattering, photoemission spectroscopy, imaging, and catalysis, while encouraging networking with established and emerging scientific research centers. Of the approximately 1,600 scientists who annually participate in experiments at SSRL, over 35% are first-time users. With our strategic plan that includes lowering the emittance, running at one of the highest-current levels on any mid-energy source world-wide, expanding in capability and capacity, we have a goal to continue the growth and the support of existing and new communities.

SSRL staff scientists reach out to new users and communities through their participation in scientific conferences related to key scientific topics, organizations and educational programs. In the coming years, SSRL will continue to educate future generations of scientists and will increase the number of SSRL facility tours for local and visiting scientists who have an interest in conducting synchrotron research.

To reach industrial researchers, SSRL networks and collaborates with both local start-ups and large multi-national companies to pursue opportunities in energy research, biotechnology, and information technology.

Finally, SSRL staff members are increasing their coordination with other light source facilities to create shared outreach materials, including Lightsources.org, a website that provides light source information to the academic, scientific, and industrial communities.
Providing Introductory Workshops to Potential New Facility Users

After reaching out to new user communities, SSRL staff members follow up with introductory workshops in selected areas of science and techniques. These workshops, including “Demystifying the Synchrotron Experience,” first held at SLAC in autumn 2011, offer interested scientists the background they need to make informed decisions on how synchrotron research may further their science.

Providing Tools for Experiment Design

SSRL provides multiple online resources to help users best design their experiments, and plans to increase these resources in the coming years. The Structural Molecular Biology Division at SSRL has received glowing feedback from users for its remote access systems that integrate an interactive interface with both real and simulated beam lines. SSRL is using lessons learned from the implementation of macromolecular remote user program to extend rapid throughput and other web-based visualization and simulation platforms across facility beam lines.

Reviewing Proposals and Allocating Beam Time

To ensure the facilities are leveraged for the most fruitful and important research, requests for beam time are peer reviewed on the basis of scientific merit and impact. To enable timely and current research, SSRL also provides a rapid-access proposal process for urgent requests. SSRL also 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.

Running Hands-on Tutorials

To ensure effective usage of beam time, meaningful 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 as well as short courses and workshops that focus on synchrotron techniques.

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 the following resources to help scientists make the most of their beam time:

- 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, and anaerobic chambers
- Assistance with sample preparation
- Remote access where applicable, allowing users to collect and process data remotely using a remote desktop application and beam line automation
- User facilities including an on-site guest house, exercise facility and, in the next five years, a central check-in and orientation point for all SLAC users
- Multi-lingual support staff and safety training courses

In the next five years, SSRL will seek to increase staff and one-on-one training to help researchers optimize beam time and subsequent analysis.

Providing Tools and Support for Data Analysis

To optimize the productivity of users, the SSRL scientific staff has developed several data analysis software programs that are made available for users during the experiments, and for download to home institutions in general. Training on how to use the software is provided during experiments and as topics during workshops and summer schools.
Assisting with Communicating Results

Nearly 500 papers are published annually as a result of research at SSRL, totaling over 10,000 publications since the facility began in 1974. SSRL staff members make a concerted effort to communicate these results with the general public, the media, the local community, and other scientists through public lectures, press releases, science articles, and brochures. SSRL also produces a monthly electronic newsletter that disseminates scientific results and new facility capabilities with the scientific community.

Training the Future Science Generation

Throughout the research lifecycle, SSRL actively participates in building a pipeline of future scientists and engineers. In addition to the workshops and tutorials described above, more than half of the experiments at SSRL are conducted by undergraduate students, graduate students, or postdoctoral scholars. Students generally come to SSRL as part of a larger university-based research team led by an experienced researcher. The 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 scientific discoveries.