Advanced Light Source
Strategic Plan
2018–2022
Executive Summary

Despite our wealth of knowledge about the structure of molecules and solids, we still are not able to make the energy storage systems we need, form desired chemical bonds at will, or process information with energy efficiency near the thermodynamic limit. These basic science challenges directly impact energy issues of major societal impact. They will often be addressed using hierarchical assemblies of cooperatively functioning nanoscale materials. For example, a catalytic network will arrange catalytic centers in space to perform a multistep chemical synthesis with high efficiency and selectivity; an adaptive material will dynamically redirect the flow of energy or charge to maximize energy storage or control energy conversion efficiency; a neuromorphic information processing element might connect multifunctional oxide nanostructures to amplify and use their extreme sensitivity to external stimulus.

Such structures exemplify emergence, in which the function of a composite system differs markedly from the properties of its atomic and nanoscale components. Developing predictive power for emergent properties lies at the core of the BESAC Grand Challenges (2007) and Transformational Opportunities (2015) documents and is a common theme of many recent BES Basic Research Needs reports. How can we rationally assemble multiscale structures, often with imperfect interfaces, to achieve a desired function? How do we control non-equilibrium processes to maintain desired fidelity and high efficiency over long periods of time?

Accomplishing these goals requires analytical tools that combine spatial resolution at the nanoscale, where macroscopic properties begin to emerge, with structural, chemical, and magnetic sensitivity, which are directly related to the targeted functional properties.

Soft x-ray (SRx) tools are particularly powerful in this regard because they allow us to probe the important valence levels with resonant excitations from shallow core levels, and thereby to determine chemical bonding, kinetics, magnetism, and many other properties related to useful function. The vision laid forth in the Advanced Light Source (ALS) Strategic Plan is to continue to develop and support cutting-edge SRx tools, along with complementary techniques spanning from the infrared through the hard x-ray regime, to understand and control emergent properties.

For 25 years the ALS has led the scientific community in developing new techniques and protocols, many of which are now deployed at other x-ray facilities around the world. The new and upgraded tools described in this strategic plan suggest this ALS innovative spirit will continue apace for years to come. Demand from the user community for access to ALS instruments has grown enormously since the facility was commissioned, and stretches our capacity. Demand for Approved Program status, which is a measure of aspirations to form strong partnerships with the ALS and to develop new capabilities, continues to grow.

These ongoing advances in ALS science capabilities were enabled by a synergistic program of accelerator improvements and upgrades. These have dramatically improved beam stability, provided complementary and cost-effective hard x-ray capacity, and increased source brightness by over an order of magnitude since 2008. The ALS Accelerator Physics group spearheaded a proposal to install an ultrahigh brightness multibend achromat lattice at the ALS, an upgrade called ALS-U. The ALS-U project team is working toward a Conceptual Design Report and a
CD-1 review in summer, 2018. ALS-U is crucial to maintaining ALS world leadership in SXR science and is deeply connected to the focus of this strategic plan since high brightness is directly correlated with our ability to probe the spatial, temporal, and spectral structure of heterogeneous materials and hierarchical material and chemical assemblies. ALS-U is a top LBNL priority and has garnered significant laboratory resources.

The ALS will continue to incorporate the latest technologies into existing instruments and to repurpose beamlines to serve the most pressing science needs. These efforts will enhance ALS capabilities and are a key feature of preparing for science after ALS-U is commissioned. We have engaged our user community about ALS-U in annual User Meetings, workshops, online forums, and crosscutting reviews. Ideas for ALS-U science opportunities are being melded with the ALS priorities discussed in this strategic plan, a process that will continue until ALS-U is commissioned.

ALS scientists are also actively participating in an LBNL planning process to renovate the “old town” area. This will replace several post-World War II buildings near of the ALS, some of which provide low quality but needed ALS office and technical space, with modern laboratory and office space. This space will support science activities that strongly overlap ALS/ALS-U capabilities and will dramatically expand our ability to serve the ALS user community.

The ALS works closely with the community to stay abreast of emerging science areas and to expand the breadth and depth of our capabilities. The ALS is part of the LBNL Energy Sciences Area and participates in valuable strategic planning with the other primarily BES-funded divisions. We have longstanding partnerships with the LBNL Chemical Dynamics Program and the Center for X-Ray Optics, and a growing number of partnerships with the Molecular Foundry and other LBNL user facilities. ALS scientists also maintain active and productive collaborations with the Earth and Environmental Sciences, Energy Technologies, Biosciences, Physical Sciences, and Computing Sciences Areas. We maintain typically 25 approved programs, which include several Energy Frontier Research Centers (EFRCs), DOE Energy Hubs, EERE-funded centers, and other initiatives from around the country. The ALS accelerator group maintains a number of collaborations with other BES x-ray facilities to leverage research of mutual interest.

The ALS seeks regular advice on its operation through interrelated activities that feed this strategic plan. We engage our Users’ Executive Committee (UEC) several times each year to discuss how we might help users be more productive. The UEC also organizes our annual User Meeting, which includes workshops organized by our staff and users. The user demand noted above is managed with advice from our Proposal Study Panel (PSP). The ALS Scientific Advisory Committee (SAC), with experts from many different disciplines, meets twice per year to provide high-level advice on our program. The SAC also oversees crosscutting reviews of entire ALS sub-disciplines to seek focused advice on how to optimize our capabilities.

The excellent ALS staff has established and maintains a productive and highly collaborative environment to accomplish the ALS mission, which is to support users in doing outstanding science in a safe environment. Motivated by that spirit, our strategic plan outlines a path to a future that is even brighter than our outstanding past.
I. A Synopsis of 2018-22 ALS Strategic Priorities

A. Introduction

Functioning chemical, material, and biological systems rely on structures that are hierarchical in space and in time. The capacity and lifetime of a battery are determined by atomic-scale diffusion, the structures of nanometer-scale interfaces and porous membrane separators, the organization of an electrolyte and submicron-scale grains of cathode and anode materials, and the packaging of a macroscale device. Protein molecules assemble to form the nuclear pore complex to regulate transport through the nuclear membrane, thereby controlling cell, tissue, and organism function. But an arbitrary multiscale structure does not necessarily do anything useful; a complex correlation between different scales is a key ingredient that endows multiscale structures with useful function. Chemical reactions, for example, could not occur but for the complex interplay of high energy electronic and low energy nuclear vibrational motion.

Fig. 1: ALS images of spatial scales in quantum matter, clockwise from the upper left: (a) Near field far-infrared study of plasmon-polaritons in graphene, 20 nm resolution (O. Khatib, et. al. Nat Phot., submitted); (b) Tunable spin splitting in WSe$_2$ Studied with micro-ARPES on MAESTRO, which offers spatial resolution between 100 nm and a few microns (Katoch, et. al., doi:10.1038/s41567-017-0033-4); (c) Conducting domain walls in Nd$_2$Ir$_2$O$_7$ studies with hard x-ray microdiffraction, 1 µm resolution (E. Ma, et. al., DOI: 10.1126/science.acc8289); (d) Electrical switching of spin vortices measure with photoelectron microscopy, 30 nm resolution; Li, et. al., doi:10.1063/1.4990987).

The ALS offers a unique suite of multiscale, multimodal imaging and scattering tools to probe such hierarchical structures in space. Fig. 1 indicates how the complementarity of soft x-ray (SXR), hard x-ray, and infrared tools can be applied to study spin, quantum, and photonic materials in new and incisive ways. A similar story could be developed around our unique combination of soft, tender, and hard x-ray scattering tools to study chemical and soft material structures. Spectroscopic contrast has empowered ALS users to apply these imaging and scattering techniques to magnetic/spin nanostructures, to orbital structures in organic materials and complex oxides alike, to helical phases in spin and liquid crystal materials, to energy storage materials, and to many other current issues in chemical, material, biological, and environmental
science. ALS tools have been applied in a pump-probe modality to study multiscale chemical and material dynamics, and the increasing SXR coherent power and source stability derived from ongoing ALS accelerator improvements are being leveraged to probe a broad range of spontaneous motion as well.

The ALS owes its success to a deep connection to current research trends driven by strong partnership with an outstanding user community, with other LBNL divisions and user facilities, and with research groups at universities, companies, and institutes from around the world. These partnerships drive continued innovation in instrumentation and experimental protocols, a focused program of accelerator upgrades, a strong commitment to user support, and constant attention to all aspects of safety.

The ALS upgrade (ALS-U), currently approaching a CD-1 review in 2018, is a major step in this process since it will significantly expand the accessible spatial and temporal scales. ALS staff and users are heavily engaged in planning for ALS-U experimental systems and science opportunities, and this ensures that ALS and ALS-U stay in sync throughout the project execution. A significant fraction of this ALS Strategic Plan reflects our efforts to be ready for ALS-U through continued aggressive and innovative instrument development activities.

While ALS will continue to impact a broad set of research disciplines, in the following sections we classify our plans into the general areas that are highly visible in the BESAC Grand Challenges (2007) and Transformational Opportunities (2015) documents as well as a series of more focused BES Basic Research needs documents:

A) **Mapping electronic, ionic, and chemical pathways in diverse systems**: utilize the chemical contrast and spatial resolution of ALS tools to discover structure-function relationships in hierarchical chemical processes, e.g., catalysis, earth and environmental systems, and energy storage and conversion.

B) **Enabling development of new functional spin, quantum, and topological materials for novel electronic applications**: deploy the spatial sensitivity, spectral contrast, and temporal resolution of ALS tools to discover and understand emerging materials, e.g., to support emerging quantum, spintronic, and neuromorphic information processing modalities.

C) **Understanding complex biological, environmental, and soft condensed matter interactions across large temporal and spatial scales**: harness the power of existing and emerging ALS imaging, scattering, and spectroscopic tools to understand natural and artificial processes at their most relevant length and time scales.

This ALS Strategic Plan describes how the facility’s innovative culture will evolve over the next 5 years, through the ALS upgrade, and for decades to come by enhancing our ability to support the most important basic energy research having the broadest long-range impact. Sec. II elaborates how the ALS will marshal its resources to develop and incorporate the latest technologies to optimize and upgrade existing instruments, seeking efficiencies wherever possible, and repurposing existing beamlines to serve the most relevant science needs. Sec. III discusses ongoing and planned accelerator upgrades that enable ever more powerful tools. A particular focus is the planned ALS Upgrade (ALS-U) for which a vigorous effort to develop a
complete conceptual design is underway. In Sec. IV we describe activities to ensure safe operations, to maximize our user and community engagement in setting strategic priorities, and to develop strong programs in optics, detectors, and data management to optimize our operation.

In the remainder of this introductory section, we briefly summarize ALS strategic priorities for 2018-2022 in the areas of beamlines and end stations (Sec. I.B), accelerator and facility upgrades and improvements (Sec I.C), and other ancillary capabilities (Sec. I.D).

**B. Instruments to Address High Impact Research Problems**

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

**2016:**
- An infrared beamline at ALS source point 2.4 devoted to IR tomography and near-field IR imaging (partly funded by SUFD to help NSLS IR users)
- A tender energy x-ray scattering beamline and end station at 5.3.1 focused on soft and environmental systems
- The MAESTRO complex at 7.0.2 for ARPES, PEEM-ARPES, and nanoARPES, all coupled to diverse material growth capabilities (partly SUFD SISGRS funded)

**2017:**
- A magnetic spectroscopy station with a 4T superconducting “octapole” magnet (ARRA)
- A soft x-ray branch line (purchased in the Wisconsin SRC ‘fire sale’) installed at 9.0.1 to extend the breadth of the ALS/LBNL CSD chemical dynamics program capabilities
- The COSMIC scattering branch at 7.0.1.1 and end station for soft x-ray ptychographic imaging with sub-10 nm resolution (SUFD midscale funding)
- A new superbend beamline at 12.2.1 to upgrade the chemical crystallography program previously on 11.3.1
- An upgrade of the 7.3.3 SAXS beamline to allow push-button control of detector distance for flexible, high throughput operation.

The top part of Table 1 summarizes additional ALS beamline and end station projects with a total cost over $0.5M presently being commissioned or under construction. The first five rows list beamline projects that are approaching completion and will start taking friendly users over the next 6 months. The sixth row describes QERLIN, an aggressive “double-dispersion” design concept that will increase throughput for resonant soft x-ray inelastic scattering (RIXS) by about a factor of 100 over existing designs, to start commissioning in spring 2019.

By mid-FY2019 we will have finished major construction on all of the beamline projects listed in Table 1, and we will be ready to start designing and scheduling additional beamline and end station projects. An initial and non-prioritized list of candidate beamline projects is provided in the top part of Table 2. We emphasize the importance of keeping the ALS strategic plan in sync with the plan for experimental systems in the ALS-U project budget. Both of these planning processes are informed by workshops, online user forums, and a round of crosscutting reviews of existing beamlines, and are overseen by committees reporting to ALS and ALS-U management. The 2019-23 version of the ALS strategic plan will provide an updated and prioritized list of ALS projects that is tightly integrated with the ALS-U plan.
Table 1. ALS Accelerator and Experimental Systems Projects in Progress*

<table>
<thead>
<tr>
<th>Source point</th>
<th>Project Title</th>
<th>Target comm.</th>
<th>Partners &amp; Funding</th>
<th>Scope and Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>9.3.1</td>
<td>Tender energy spectroscopy</td>
<td>Now</td>
<td>JCAP, JCESR, ALS EQU</td>
<td>Upgrade vacuum crystal monochromator &amp; optics; tender energy ambient pressure XPS at the solid/solid and solid/liquid interface</td>
</tr>
<tr>
<td>7.3.1</td>
<td>Soft x-ray spectroscopy</td>
<td>Now</td>
<td>JCAP, ALS EQU</td>
<td>Update monochromator; increase capacity for in situ/operando SXR spectroscopy; complements undulator-based capacity on 8.0.1 and AMBER</td>
</tr>
<tr>
<td>7.0.1.1</td>
<td>Coherent scattering - XPCS</td>
<td>April 2018</td>
<td>DOE midscale, ALS EQU</td>
<td>Half-length undulator and SXR beamline for XPCS studies of spontaneous fluctuations in spin, quantum, and topological materials</td>
</tr>
<tr>
<td>6.0.1</td>
<td>AMBER</td>
<td>Sept 2018</td>
<td>PNNL, JCAP, JCESR, ALS EQU</td>
<td>Repurpose undulator; multimodal SXR in situ/operando spectroscopy studies of catalysis, earth &amp; environment, and energy conversion</td>
</tr>
<tr>
<td>2.0</td>
<td>GEMINI:</td>
<td>Sept 2018</td>
<td>HHMI, LBNL, LBNL/MBIB</td>
<td>In-vacuum undulator monochromator; microfocus optics for macromolecular crystallography; advanced detectors; robotic sample handling</td>
</tr>
<tr>
<td>6.0.2</td>
<td>QERLIN</td>
<td>March 2019</td>
<td>Moore Foundation, ALS EQU</td>
<td>Repurpose undulator; soft x-ray RIXS beamline &amp; double dispersion design for high throughput &amp; resolution; spin &amp; quantum materials</td>
</tr>
</tbody>
</table>

**Experimental Systems**

**Accelerator Systems & Conventional Facilities**

<table>
<thead>
<tr>
<th>Source point</th>
<th>Project Title</th>
<th>Target comm.</th>
<th>Partners &amp; Funding</th>
<th>Scope and Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>SRRF Upgrade</td>
<td>Finish July 2018</td>
<td>ALS AIP</td>
<td>Update aging RF system; eliminate potential major single-point failures; serves ALS and ALS-U (nearly complete)</td>
</tr>
<tr>
<td></td>
<td>Controls Upgrade 2.0</td>
<td>Finish Jan 2019</td>
<td>ALS AIP</td>
<td>Update aging storage ring control system; serves ALS and many components will serve ALS-U (nearly complete)</td>
</tr>
<tr>
<td></td>
<td>Non-linear kicker</td>
<td>July 2018</td>
<td>LBNL-Director funds</td>
<td>Decreases perturbation to ALS users during injection. Can potentially operate in future ALS-U accumulator ring.</td>
</tr>
<tr>
<td></td>
<td>HVAC/energy efficiency</td>
<td>2018</td>
<td>SLI GPP</td>
<td>Stabilizes ALS environment for improved beam stability; important for ALS and ALS-U</td>
</tr>
</tbody>
</table>

* List of acronyms is provided in Appendix 1.

We note that the total cost of all projects in Table 2 (experimental and accelerator systems) approximately matches our planned 10% investment annually of ALS funds in new projects. While the details might change by the updated strategic plan, this table illustrates the rough scope of projects we expect to accomplish with the ALS budget before ALS-U is commissioned.

While the ALS continues to innovate new and to upgrade existing experimental systems, the facility carefully balances its suite of instruments with the staff it is able to support so as to maintain efficient and sustainable operations. The design, commissioning, and operation of most of the projects listed in Tables 1 and 2 is being or will be handled by existing ALS scientific staff.
who have been managing the beamlines and instruments being upgraded, or in some cases being shut down. Overall, these projects are intended to be net staffing neutral. The ALS maintains a summary of beamline metrics that provides a snapshot of beamline staffing, user demand, usage, operational complexity, and overall productivity. This is used to help maintain an appropriate and balanced level of support on different beamlines. Increasingly, ALS staff are trained across different beamlines to enhance operational efficiency.

### C. Accelerator Upgrades to Enable Improved ALS Tools

Cutting-edge beamline and end stations provide only part of what is required for continuous ALS renewal and obviously do not capture the totality of the ALS innovative spirit. Current strategic priorities for the existing ALS accelerator for 2018-2022 are summarized in the lower portions of Tables 1 and 2 and are further elaborated in Sec. III of this document. For the last 5-6 years, the ALS has been in the process of modernizing most major existing accelerator systems: power supplies, beam position monitors, control systems, rf system, and a host of smaller components. Conversion to top-off operation and addition of 48 sextupoles to the lattice has increased the source brightness by more than an order of magnitude in the past decade. As indicated in the bottom part of Table 1, replacement and upgrade of two other main accelerator subsystems (RF

### Experimental Systems

<table>
<thead>
<tr>
<th>Source point</th>
<th>Project title</th>
<th>Partners &amp; Funding</th>
<th>Est. Cost</th>
<th>Scope &amp; notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.0.2</td>
<td>Quantum Microscope</td>
<td>ALS EQU</td>
<td>$2.5M</td>
<td>STXM for variable temperature, field, &amp; current microscopy of spin quantum &amp; topological materials</td>
</tr>
<tr>
<td>6.0.1</td>
<td>AMBER branchlines</td>
<td>ALS EQU</td>
<td>$3.1M</td>
<td>Scope may evolve depending on user advice</td>
</tr>
<tr>
<td>9.3.2</td>
<td>APXPS beamline replacement</td>
<td>ALS EQU</td>
<td>$2.5 M</td>
<td>Upgrade ancient SXR bend magnet beamline; scope may evolve depend on user advice</td>
</tr>
<tr>
<td>4.0.2</td>
<td>Magnetic spectroscopy, scattering</td>
<td>ALS AIP</td>
<td>$3.6M</td>
<td>Replace undulator &amp; vacuum chamber</td>
</tr>
<tr>
<td>8.0.1</td>
<td>SXR XAS and RIXS spectroscopy</td>
<td>ALS EQU</td>
<td>$5.0M</td>
<td>ALS: replace old beamline; ALS-U: chicane sector and build a second beamline; scope to be determined</td>
</tr>
<tr>
<td>10.0.1</td>
<td>Beamline replacement</td>
<td>ALS EQU</td>
<td>$5.0M</td>
<td>ALS: replace old beamline; ALS-U: chicane sector and build a second beamline; scope to be determined</td>
</tr>
</tbody>
</table>

### Accelerator Systems

| Linac and injector upgrade | ALS AIP | $2.2M | Replaces ALS linac modulators and related subsystems; readies aging accelerator system for ALS-U |
| SR corrector vacuum upgrade | ALS AIP | $550K | Replaces thick aluminum chambers with thin stainless steel to increase BW of fast orbit feedback system |
and controls) is nearly complete. The bottom of table 2 indicates that a major upgrade of the injector is planned for the next few years. All of these accelerator upgrades are necessary to keep the ALS accelerator up to date, but are also important parts of preparing for ALS-U discussed briefly above and in Sec III. The list of emerging accelerator projects in the bottom of table 2 is incomplete and will be finalized in the next strategic plan update, in sync with ALS-U planning.

Table 3. Ancillary Activities Supported by ALS, 2018-23

<table>
<thead>
<tr>
<th>Project</th>
<th>Commission</th>
<th>Funding Source</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>ALS EHS Program</td>
<td>Ongoing</td>
<td>ALS Ops</td>
<td>Continue to tune Work Planning and Control system</td>
</tr>
<tr>
<td>Strategic communications</td>
<td>ongoing outreach, workshops</td>
<td>ALS Ops</td>
<td>Maintain a robust and multi-faceted communications frameworks</td>
</tr>
<tr>
<td>Scientific Data Management</td>
<td>ongoing</td>
<td>ALS Ops, BES/ASCR</td>
<td>Work with LBNL computing divisions, CAMERA &amp; other facilities to maintain and expand our ability to transmit, store, manage, and analyze data streams</td>
</tr>
<tr>
<td>Advanced Detectors</td>
<td>ongoing</td>
<td>ALS Ops, SUFD R&amp;D</td>
<td>Continue development of detectors with high frame rate, high spatial resolution, or other specific characteristics</td>
</tr>
<tr>
<td>Optics &amp; Metrology</td>
<td>ongoing</td>
<td>ALS Ops, ALS-U</td>
<td>Ongoing optics upgrade for older ALS beamlines, support for nano-diffractive optic, and optical metrology, all with an eye toward ALS-U</td>
</tr>
<tr>
<td>User Portal</td>
<td>ESAF deployed; maintain</td>
<td>ALS Ops</td>
<td>Maintain modern portal to manage user access and to ensure their safe operation at the ALS</td>
</tr>
<tr>
<td></td>
<td>thereafter</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fellowship programs</td>
<td>ongoing</td>
<td>ALS Ops</td>
<td>Ongoing support of ALS Post baccalaureate, Doctoral, and Postdoctoral Fellowship Programs for user collaboration and staff development</td>
</tr>
</tbody>
</table>

D. Ancillary Capabilities to Support a Strong User Science Program

Table 3 summarizes several enabling ALS programs, projects, and technologies that support our strategic research priorities and engage the user community in strong partnerships. These include establishing efficient procedures to optimize facility usage, maintaining a strong safety culture, focusing on ALS staff professional development, engaging users in the strategic planning process, testing and regularly upgrading beamlines and optics, developing nanodiffractive optics that support advances in many ALS capabilities, developing and deploying state of the art x-ray detectors, and building the infrastructure needed to manage and to analyze the huge volume of data produced at the ALS. These are managed strategically and balanced against other instrument and accelerator needs, and are described in more detail in Sec. IV of this document.
II. New Tools to Probe Functional Materials and Structures

A. Mapping Chemical and Energy Pathways

Devices currently in use or being developed for selective and efficient heterogeneous catalysis, photocatalysis, energy conversion, and energy storage rely heavily on diverse multiscale phenomena, ranging from interfacial electron transfer and ion transport occurring on nanometer-picoscale to macroscale batteries that charge in hours and catalytic reactors with turnover rates of ~1/sec. Soft and hard x-rays can probe dense environments with atomic and chemical contrast spanning a large spatiotemporal range, thereby providing unique fundamental information about such functioning mesoscale devices. Such ‘nanokinetic’ measurements are essential to optimize complex multiscale chemical and electrochemical devices.

Existing ALS beamlines used for energy materials and catalysis research are among our most heavily over-subscribed beamlines. Tables 1 and 2 indicate that our strategic priorities increase both our capability and our capacity in this area, as elaborated below.

1. ALS soft and tender x-ray spectromicroscopy: COSMIC (2017)

Since 1995, the ALS has led the world in developing SXR scanning transmission x-ray microscopes (STXMs). STXMs on ALS beamlines 5.3.2.1/2 and 11.0.2 are in very high demand and are highly productive. Commissioning of the COherent Scattering and MICrscopy beamline (COSMIC) in began in 2017 and will maintain this world leadership. One branch of COSMIC will be optimized for ptychographic diffractive imaging with state-of-the-art scanning systems, high-data-rate CCD detectors matched to a high bandwidth data system, and diverse in situ sample environments. COSMIC will provide images with <5 nm nanometer resolution, ultimately combining 3D tomographic reconstruction with full chemical contrast. This will revolutionize our ability to probe ‘interphase’ regions in electrochemical systems, catalytic reactors, and environmental systems.

2. ALS soft and tender x-ray spectroscopy: 7.3.1, 9.0.1, 9.3.1, AMBER

In addition to the advanced imaging capabilities exemplified by COSMIC, ALS development of high throughput x-ray emission spectrographs and ambient pressure x-ray photoelectron spectroscopy (APXPS), complemented by new operando sample environments, has attracted many users wanting to address basic science issues in chemistry, catalysis, and energy conversion. For example, newly commissioned resonant inelastic x-ray scattering (RIXS) spectrographs on ALS beamline 8.0.1 combine very good throughput and energy resolution (Fig. 2). This is enabling previously impossible studies of electronic levels that are directly involved in chemical bonding, in diverse environments and often in functioning nanoscale devices.

Beamline 7.3.1 restart and upgrade (2018): To increase our soft x-ray spectroscopy capacity and thereby to address burgeoning user demand for these capabilities, we have updated and restarted ALS bend magnet beamline 7.3.1 and will install a simple soft x-ray spectroscopy end
Fig. 2: Left: CAD drawing showing the iRIXS endstation at Beamline 8.0.1 at the ALS. Center and right: RIXS maps of HOPG near the carbon K-edge. The 2.2 meter RIXS spectrograph, coupled to a 5 x 55 micron pixel CCD detector, achieves a resolving power of ~5000 and very high angular acceptance due to the efficient optical design employed (Rev. Sci. Inst., in press). The spectrograph is now available commercially.

station. This will access K-absorption edges up to aluminum, and will be used primarily for XAS studies of chemical systems in functioning environments.

**Beamline 9.3.1 upgrade (2018):** ALS has developed a new tender x-ray energy variant of APXPS on ALS beamline 9.3.1 to probe electrochemical reactions with operating electrodes/electrolyte systems (Fig. 3). This is becoming a very popular technique at ALS, but the beamline is in need of replacement. New vacuum crystal monochromator and optics have been delivered and commissioning began in late 2017.

**AMBER beamline (2018, 9):** Advanced Materials Beamline for Energy Research (AMBER) will be enabled by the repurposing sector 6 and will coordinate a suite of SXR tools on a single beamline. This will be optimized for advanced materials preparation and multimodal, high throughput, operando analysis of chemical and energy systems, thereby improving ALS capabilities and increasing capacity in this area. AMBER will provide in situ sample-preparation with RIXS and XAS spectroscopies and APXPS with at near-atmospheric pressure. AMBER is developed in partnership with PNNL and the JCAP and JCESR Energy Hubs. Commissioning of the first branch line will begin in 2018.

**SXR branch line at 9.0.1 (2017):** The ALS acquired a modern SXR monochromator from the Wisconsin Synchrotron Radiation Center when it ended operations. In collaboration with the LBNL Chemical Sciences Division, we installed and now co-manage this instrument on beamline 9.0.1 to expand the breadth and depth of ALS Chemical Dynamics programs. A particular focus will be on liquid interfaces using liquid jets, droplets, and other environments.

**3. Upgrade existing beamlines for chemical and material sciences**

**Upgrade of beamlines 8.0.1 and 9.3.2 (future development):** These beamlines have been very productive since the initial ALS commissioning, but both are outdated and are due for complete upgrades. The scope of these upgrades will depend on the outcome of the ALS/ALS-U planning process discussed above, and will be described in more detail in the 2019-23 strategic plan.
Fig. 3: Schematic of three-electrode electrochemistry setup in tender-energy APXPS system from Favaro, M. et al. doi: 10.1038/ncomms12695 (2016). (WE: polycrystalline Au, CE: polycrystalline Pt, RE: miniaturized Ag/AgCl/Cl-(sat.)); a: position of the electrodes before immersion (hydrated conditions); b: the electrodes are immersed into the electrolyte (0.1, 0.4, 1.0 and 80.0 mM KOH solution), where any electrochemical treatment can be performed within the APXPS chamber; c: after the ‘dip and pull’ procedure, the electrodes are finally brought to the operando APXPS position (chronoamperometry is performed at different potentials within the double layer region, while N 1s, O 1s and Au 4f core levels are measured) (APXPS: ambient pressure x-ray photoelectron spectroscopy; HEA: hemispherical electron analyzer).

**B. Spin, Quantum, and Topological Materials**

SXR spectroscopy, scattering, and microscopy tools have played a major role in discovering and understanding the exotic and fascinating materials physics of many new classes of spin, quantum, and topological materials over the past few decades: oxide and pnictide superconductors, manganites exhibiting colossal magnetoresistance, graphene and other 2D materials, topological insulators, multiferroics, and many others. Beyond the century-long endeavor, initiated with the discovery of quantum mechanics, to understand the electronic and magnetic structure of materials, these efforts also continue to provide the foundation for many existing and future electronic and information processing technologies.

The ALS supports instruments that probe the fundamental electronic and magnetic/spin structures and excitations that endow these materials with their unusual emergent properties, as well as complementary tools to discover, probe, and help optimize new emergent phase behaviors and functionalities. The combination of these two classes of technique is crucially important in helping us learn how to design new quantum materials and material structures with desired emergent functionality. For this reason, we are investing heavily to develop and apply powerful and complementary SXR nanoprobe spectroscopies in this science area.
The power of these SXR nanoprobe techniques will be dramatically enhanced by ALS-U, and our development efforts at ALS is closely connected to the ALS-U science plan. This is partly because intrinsic and/or designed nanoscale inhomogeneity often dramatically impacts the connection between fundamental interactions and the resulting functionality in these materials. Increasingly our users seek to combine these SXR techniques with other ancillary tools like scanned-probe microscopies and synchrotron infrared nanoscale spectroscopy (SINS). For example, staff from the Molecular Foundry/NCEM are actively involved in the MAESTRO complex described below, and are helping to plan the addition of scanned probe microscopy. Such multimodal instruments will enable a detailed understanding of the role of heterogeneity in determining the interesting and useful emergent properties these complex materials, particularly as they are deployed in patterned structures.

1. **Excitations and fundamental interactions**

New ALS capabilities designed to probe fundamental interactions in spin and quantum materials include:

**MAESTRO (2016-18):** ALS started commissioning the Microscopic And Electronic STRucture Observatory (MAESTRO) beamline in 2016. The beamline is now taking users, though the nanoAPRES system is scheduled for further commissioning and for work with friendly users. MAESTRO provides a unique combination of multimodal ARPES both with scanning micro- and presently 100 nm nanoprobe probes as well as full-field PEEM mode, with sophisticated samples prepared with multiple techniques such as pulsed laser deposition, molecular beam epitaxy, and mechanical exfoliation.

**qRIXS (2017) and QERLIN (2019):** A strength of ARPES is that it measures the coupling of electrons and holes to low energy excitations. However, it can be difficult to identify which excitation(s) lead to a particular emergent property. It is crucial to measure the dispersion relations of the low energy excitations directly, with high resolution, with SXR contrast, through crucial regions of the phase diagram, and over a large region of Fourier space. For this reason, one of the highest ALS priorities is to build and commission new SXR RIXS beamlines called qRIXS and QERLIN (Q- and Energy-ResoLved INelastic scattering). The qRIXS end station was commissioned in 2017 and deploys up to five 2.2 meter spectrographs similar to the one used to produce the results in Fig. 2, offering large angular acceptance, high throughput, and a resolving power of ~5000. The QERLIN beamline is enabled by the repurposing sector 6 following decommissioning of the ultrafast slicing sources, and is based on a novel optical design that involves multiplexing the incident beam across the face of the sample and the scattered beam across a high resolution pixelated detector. This will provide a resolving power >10,000 and will probe an entire map of photon energy in vs. photon energy out in parallel - a 100-fold increase in throughput.

**New spinARPES modalities (future development):** The ALS now has three undulator beamlines focused on ARPES, with a range of complementary capabilities. A recent crosscutting
review in this area to evaluate this suite of capabilities and advised on evolution over the next several years leading to ALS-U. Of particular interest is spinARPES, a capability not well-represented at other US facilities and which is highly relevant to emerging spin, quantum, and topological materials. Our plans in this area will be described in more detail in the 2019-23 strategic plan, which will be informed by the ALS/ALS-U planning process described above.

**nanoRIXS (future development):** We are starting to develop concepts for a nanoRIXS instrument as well, which will offer complementary information on neutral excitations and insulating materials that are not accessible to nanoARPES. Again, these plans will be clearer in the next ALS strategic plan.

### 2. Emergent phase behaviors

Powerful soft x-ray spectroscopy and scattering tools at ALS directly probe the fascinating emergent phase behaviors of functional spin and quantum materials in unique sample environments. These techniques are based on large near-edge soft x-ray magnetic circular (XMCD) and linear dichroism (XMLD), which provide high magnetic and electronic contrast with element-specificity and the ability to study interfaces and periodic structures such as charge and orbital ordering with a resolution down to a few nanometers. An important capability recently added is x-ray ferromagnetic resonance (XFMR), which provides very high sensitivity and has recently been used to detect pure AC spin currents. Other projects recently or soon to be commissioned include:

**High field end station (2017):** Over the past few years, the ALS has designed and commissioned a high field superconducting vector magnet that can produce a magnetic field up to 4T in arbitrary direction. This instrument will allow ALS users to uniquely probe orbital and spin anisotropies of complex magnetic materials. It has recently been commissioned and has produced first results in candidate high moment, high coercivity magnetic materials without rare earth elements.

**Resonant scattering:** ALS supports two productive resonant soft x-ray scattering instruments that probe the spatial distribution of chemical and material textures. One of these, located at 4.0.2, is devoted to probing spatial correlations in spin and quantum materials, and has recently been used, for example, to detect chiral domain walls in ferromagnetic films and to characterize polarization vortices in antiferromagnetic heterostructures. An analog of XFMR will soon be added to this scattering instrument to further enhance sensitivity, and a longer term goal is to turn this into a scattering microscopy (selected area diffraction). A branch of the COSMIC beamline and associated end station to be commissioned in spring 2018 will extend these scattering sensitivities into the time domain by enabling SXR photon correlation spectroscopy (XPCS) and various speckle metrology experiments. A long-range goal of the ALS strategic plan and the ALS-U science case is to connect the sensitivities of RIXS in the frequency domain using QERLIN and XPCS in the time domain using COSMIC to provide unique quasielastic scattering tools.
Quantum microscope (~2020): ALS SXR microscopes provide nanometer spatial resolution, which is a characteristic length scale of magnetic domains and domain walls, of spontaneously nano-phase-separated regions in many complex oxides, of spin textures like skyrmions, and of many other intrinsic heterogeneities in spin and quantum materials. While existing ALS microscopes already provide some capacity in this area, it is difficult to couple precision control systems with variable temperature and magnetic field. This seriously limits our capability for in situ microscopy of spin and quantum materials and in operando optimization of functional nanoscale structures. An important strategic ALS priority, which was strongly supported by a recent crosscutting review, is to develop a beamline optimized for SXR spectromicroscopy of magnetic, spin, and quantum materials and their nanostructured composites. This would be used, for example, to observe, understand and control the intrinsic electronic heterogeneity characteristic of many such materials, to measure these materials in patterned nanostructures that can be used to produce new emergent phases with new functionality like internal sources of spin currents, and to study the properties of domain walls and interfaces in these materials.

3. Upgrade existing beamlines for spin, quantum, and topological materials

Upgrade of beamlines 4.0.2 and 10.0.1 (future development): As suggested above, our user community has strongly advised that we build a microscope devoted to spin and quantum materials. A logical place to locate this is beamline 4.0.2, which already specializes in magnetic spectroscopy and scattering, but the beamline design is outdated and was not intended for microscopy. The elliptically polarizing undulator source on 4.0.2 was the first deployed at the ALS, and while it has been carefully optimized over the years for current applications, it has been limiting the efficiency of the beamline. We plan to upgrade that beamline and undulator before ALS-U commissioning over the next few years - another important step in preparing for ALS-U as well. Similarly, beamline 10.0.1 is based on aging technology and needs to be upgraded and redeveloped. Upgrading this beamline is also being considered inside the ALS-U project. The scope of these upgrades will depend on the outcome of the ALS/ALS-U planning process discussed above, and will be described in more detail in the 2019-23 strategic plan.

C. Understanding Complex Interactions in Soft and Biological Systems

The ALS and its partners supports scattering and imaging tools to probe soft, biological, and earth & environmental structures ranging from biopolymer molecules using macromolecular crystallography and solution SAXS to entire organisms using x-ray tomography (Fig. 5). A similar range of environmental structures can also be probed with chemical contrast. As in the other research areas discussed here, biological and environmental systems exhibit interesting and important phenomena that involve interactions across scales. The activity of an enzymatic center is determined by the secondary and tertiary structures of a protein molecule. The complex chemistry of a soil particle is determined by the availability of various species at the interfaces.
Fig. 5  The scales of structural biology illuminated by recent ALS results: a) protein structure of a gated ion channel (Brelidze, et. al., Nature 481, 530 (2012)); b) protein assembly to form the nuclear pore complex (Solmaz, et. al., PNAS 110, 5858 (2013)); c) single cell CAT scans with SXR nanotomography (Parkinson, et. al., J. Struct. Biol.,162: 380 (2008)); d) infrared tomography of living tissues with few-micron resolution(Martin, et. al., Nature Methods 10, 861 (2013)); e) x-ray tomography of living grape vines(McElrone, et. al., J. Vis. Exp. 74, e50162 (2013)).

The capabilities of infrared, soft x-ray, and hard x-ray imaging techniques to address biological problems pertain mostly to the images in Fig. 9, but the transitions between scales, indicated by the arrows, are of crucial importance to understanding how these complex systems function. What determines the function of a given protein molecule in a complex? How is a protein complex distributed in a cell to support and regulate cell function? How does intracellular signaling make a tissue work? We have many powerful tools to measure biological and environmental structures over a large spatial scale, but we have mostly an empirical understanding of how these scales interact. Addressing these questions will illuminate the connection between structural and systems biology, or environmental structures and environmental systems. Emerging tools serving environmental and biological science in Tables 1 and 2 will help fill this crucial gap in understanding.

**GEMINI beamline:** The macromolecular crystallography beamlines at the ALS have enabled outstanding scientific productivity, providing high-performance hard x-ray diffraction capabilities that have kept pace with the changing needs of the structural biology community (e.g., Fig. 9(a)). To continue to provide the highest possible performance, the Howard Hughes Medical Institute has recently funded a new high brightness protein crystallography facility called GEMINI in ALS sector 2. This will significantly expand our ability to probe small crystals with large unit cells, i.e., an emphasis on protein complexes like the nuclear pore complex in Fig. 9(b). This will include a high brightness in-vacuum undulator, eventually serving two branch lines simultaneously located in a single hutch. One of the branches will be served with diamond beam-splitters and operate at fixed wavelength; the other will be variable wavelength for multi-wavelength anomalous dispersion measurements. Design, procurement, and site preparation are underway and completion is expected in 2018.

**Infrared spectro-tomography:** The DOE’s Scientific User Facility Division provided funds to increase ALS infrared capacity to help the NSLS community through the dark time between the
shut down of NSLS and the commissioning of IR beamlines on NSLS-II. We have worked closely with NSLS staff to develop this plan and an ALS Approved Program proposal is now in place to serve their users needs and to establish a presence on the ALS floor. Using these funds we developed and commissioned source point 2.4, which will serve a full-field microscope with a focal plane array detector and has also increased our capacity on synchrotron infrared nano-imaging. Moreover, ALS staff collaborated with Carol Hirshmugl at the University of Wisconsin to develop infrared spectro-tomography at the SRC (Fig. 9(d)). This new IR station will be able to do full-field microscopy and tomography, thereby providing a new and valuable way to produce 3D images of living biological and environmental systems with ~5 micron resolution and the chemical contrast of infrared spectroscopy.

**Improved spatial resolution hard x-ray tomography:** The ALS hard x-ray tomography beamline provides submicron resolution tomographs that often provide a useful complement to other higher resolution imaging techniques. We are seeking funds to upgrade this beamline to allow insertion of focusing optics, thereby providing ~100 nm resolution in 3D in a zoomed in region.

**Multimodal x-ray scattering upgrades:** ALS offers an increasingly powerful suite of x-ray scattering capabilities over an unusually broad photon energy range, including the soft, tender, hard x-ray regimes. Recent additions to this portfolio include

- In 2017, access to wet environments was enabled in resonant SXR scattering (RSoXS) on polymer and soft matter at ALS beamline 11.0.2, in which sensitivity to molecular functionalities can be highlighted by tuning to near-edge features near.
- A tender resonant elastic x-ray scattering (T-REXS) beamline was commissioned in late 2017, enabling resonant scattering at the silicon through calcium K-edges
- An in-vacuum flight path with computer-controlled sample-detector distance was commissioned to simplify operation on this very high throughput SAXS/WAXS beamline.

**High throughput crystallography upgrade (2017):** We have formed a partnership with the LBNL Chemical Sciences Division to fund migration of our chemical and material crystallography beamline (11.3.1) to a superbend source (12.2.1). This was commissioned in Jan, 2018 and will provide ~1000x more flux at high energy than the currently-used regular bend magnet. This will increase capacity and precision, and will enable measuring micron-scale crystals. We will install robotic sample handling to enhance throughput and allow rapid materials screening and combinatoric experiments.
III. Accelerator Renewal and Upgrades to Maintain World Leadership in Soft X-ray Science and Technology

The ALS produces and delivers to users synchrotron radiation over a wide spectral range for science, i.e., from far infrared (IR) to hard x-rays with the core spectral region in the ultraviolet (UV) and SXR region. In this core region, relevant to chemistry, catalysis, surface science, nanoscience, life sciences, and complex materials, the ALS remains competitive with the newest synchrotron radiation sources worldwide. The quality of the science program is directly connected to the performance of the accelerator and therefore continued upgrades of the accelerator have always been a high priority activity for the ALS (see Tables 1 and 2 in Sec. I).

A. Recently or soon to be completed upgrades

Controls/Instrumentation upgrade: The controls and instrumentation upgrade is a four year project that is scheduled to be completed in FY18. Its goal is to modernize all control system hardware and software, as well as much of the beam diagnostics hardware. This will allow maintaining and improving the reliability of accelerator operations, reduce the effort necessary to support the control system in the future and provide improvements in performance, particularly in orbit stability. With the 20 times improved bandwidth of the new BPMs and existing corrector magnets, we expect a large improvement in the fast orbit feedback system. A large majority of the upgraded systems will be also used in the ALS-U.

Storage Ring RF upgrade: The existing high power RF system was nearing the end of its useful lifetime and spares were becoming increasingly unavailable. Therefore an upgrade project is nearing completion with the goals of long-term maintainability, higher reliability, lower electricity consumption, and sufficient power reserves for all planned additions of new undulators, better immunity to ac line transients, and improved fast phase stability. The main risk factor of the system, the old Klystron, was replaced in FY12 and the project is planned to complete in summer of 2018. This upgraded RF system will also be used in the ALS-U.

B. Near-Term Upgrades

After the previously listed major upgrades are completed, many failure risks due to aging equipment will be retired. The largest remaining component is the injector RF system.

Injector RF upgrade: The RF systems in the ALS Injector are all, with the exception of the Booster RF Amplifier, original to the ALS from the early 1990's. Due to their age, many of these systems and in particular their components, are reaching the end of their serviceable life and in some cases, replacement parts are only available from single sources or are custom builds. We have not experienced significant long-term outages of the system, but shorter outages are common and the ALS RF engineering group spends a significant amount of time maintaining the injector RF systems. It is important to reduce the risk of prolonged beam outages caused by the inability to repair and maintain these systems and components. This includes the two 24 MW
modulators based on obsolete pulse forming network technology and trigger thyratron, the amplifiers for the sub-harmonic bunchers, the master oscillator and RF distribution system, and the low level RF controllers. Upgrading these systems would not only reduce this risk, but also give us an opportunity to increase performance and reliability and to provide the necessary lifetime to operate ALS-U in the future.

**HVAC/Infrastructure upgrades:** In addition, there are ongoing infrastructure upgrade projects, namely efforts to reduce the frequency of beam losses due to AC line voltage fluctuations, efforts to improve the temperature stability of the air in the end station area, and to stabilize the water temperature further. Several ongoing upgrades are also aimed at improving the overall energy efficiency of the ALS, both at the level of technical systems (RF, power supplies, injector operation modes), as well as building systems (HVAC).

### C. Other Accelerator R&D Activities

**Insertion device R&D:** Most of the insertion devices considered for renewal at the ALS and for the ALS upgrade are soft x-ray elliptically polarizing (EPU) insertion devices. Other devices could be short period undulators for tender energy photons (2-6 keV). EPUs are very popular because of the great versatility in the polarization they can provide. Along with other synchrotron facilities and evaluating synergies with the Linac Coherent Light Source, we are exploring possible avenues for improvement such as:

- Non-mechanically-moving EPUs and/or improved field shapes.
- In-vacuum EPUs.
- Cryogenically cooled permanent magnet undulators or
- Nb$_3$Sn based superconducting undulators for achieving ultimate brightness in the SXR range and for significantly higher brightness than now is achievable with wiggler sources.

There are 12 straight sections in the ALS. Currently 9 of these are populated with insertion devices. The remaining 3 – sectors 1, 2, and 3 – are presently being occupied with the injection systems (straight 1), RF and multibunch feedback kickers (straight 3), and camshaft kicker and other systems (straight 2). We are currently freeing up space in straight 2 to install one or two insertion devices while retaining the essential functionality for the storage ring. Among the ideas being considered and implemented are more compact multibunch feedback systems, replacing the 4 injection bumps with a single multibunch nonlinear kicker, and relocating equipment. In addition to freeing up space, the multibunch kicker should greatly reduce injection transients making top-off more transparent.

**Storage ring operating modes:** Pseudo-single-bunch (PSB) operation—a new operational mode at the ALS—can expand the capabilities of synchrotron light sources to carry out dynamics and time-of-flight experiments. In PSB operation, a single electron bunch is displaced transversely from the other electron bunches using a short-pulse, high-repetition-rate kicker magnet. Experiments that require light emitted only from a single bunch can use only radiation emitted
from this single bunch in its unique orbit and eliminate the light emitted from the other bunches using a collimator. Other beam lines will only see a small reduction in flux due to single displaced bunch. As a result, PSB eliminates the need to schedule multibunch and single- or two-bunch experiments during different running periods. Furthermore, the time spacing of PSB pulses can be adjusted from milliseconds to microseconds with a novel “kick-and-cancel” scheme, which can significantly alleviate complications of using high-power choppers and substantially reduce the rate of sample damage. On January 28, 2014 we introduced pseudo-single bunch into user time and the first experiments were done with the kicker set at 4 kHz.

Beyond the baseline of the completed brightness upgrade project, work is also investigating other possible modes of operation, including low alpha modes, which allow shorter electron bunch length for shorter x-ray pulses. These modes are enabled by the fact that the new sextupoles added in the upgrade allow control of the second order momentum compaction factor and consequently a potential reduction of the bunch length. This could enable substantial improvements for THz experiments in special operation modes. To support these experiments, we also consider modifying a vacuum chamber to enable larger acceptance angles for long wavelength IR radiation.

Presently the ALS vertical beamsize in the insertion device straights is just under 10 microns and the short term orbit stability about 0.6 micron rms (or ~6%). We are planning to reduce the coupling further and will add a number of additional EPUs. At that point the relative orbit stability would become significantly worse. The recently upgraded BPM system can potentially allow much greater orbit stability, however, to take full advantage of this requires a number (~20) of “fast” correctors – most likely air core magnets surrounding bellow shields and associated power supplies. Complementing the improvements to fast orbit stability with the ongoing instrumentation upgrade, we are also considering further improvements to the long term pointing stability of ALS photon beams by adding photon beam position monitors in beamlines.

D. Planning a diffraction-limited upgrade of the ALS

Evolutionary increases in storage ring source brightness over the past several decades like those described above, have supported an ever-increasing array of x-ray capabilities that have had a major impact on many disciplines – physics, chemistry, biology, material science, and others. A large capacity of storage ring sources has been developed around the world and is applied to diverse cutting-edge research problems. In recent years an additional, revolutionary increase in storage ring brightness has been proposed and is now being planned, developed, or deployed at facilities around the world. This increase will be accomplished by using storage ring lattice designs with electron beam emittance comparable to the diffraction limit of the (soft) x-rays that are produced. That is, the soft x-ray beams will be nearly diffraction limited, with smooth, transversely coherent wavefronts. Coherence means that all photons are ‘useful’ in demanding experiments that require focusing the beam into a small spot or encoding a material’s heterogeneity into a far-field speckle-diffraction pattern. For this reason a diffraction limited
storage ring (DLSR) is ideal for examining the nano- and meso-scale structure of materials, since they enable the highest possible spatial resolution coupled to broad temporal sensitivity and x-ray contrast mechanisms. Groundbreaking new applications to study heterogeneous materials and functional devices will be possible on a DLSR.

Motivated by the above thinking, ALS scientists and users have proposed to DOE BES a major upgrade of the facility to replace the existing storage ring with a multibend achromat lattice that would provide diffraction-limited soft x-ray beams up to about 2 keV. Such an upgrade would endow the ALS with the highest soft x-ray brightness and coherent flux of any storage-ring-based x-ray facility panned or under construction. It would manifestly increase our users’ ability to probe heterogeneous systems in ever-finer detail. It is a cost-effective upgrade that would allow a 25-year-old facility to maintain world leadership of soft x-ray science and technology for at least another 25 years. This project has recently achieved DOE CD-0 status, i.e., ALS-U is now officially a project, separate from, though strongly overlapping with ALS staff and strategic planning activities. ALS-U is scheduled for a CD-1 review in July, 2018. In this context, we are actively engaged in several long-range planning activities:

**User outreach**: We actively engaged users about the ALS-U project at the ALS User Meetings in October 2015, 2016, and 2017, and we followed up with workshops in October 2014 and January 2017 that focused on early science opportunities with ALS-U. An early science opportunities document with broad user input was completed in early 2017, and there is much enthusiasm for the upgrade among the community. In late 2017 and early 2018, under sponsorship of the ALS/ALS-U SAC and with active participation of the user community, we ran a series of crosscutting reviews that evaluated existing beamlines and instruments and suggested improvements, upgrades, and new construction, either by ALS or inside the ALS-U project. Based on all these inputs, we are conducting a process, again with user and ALS/ALS-U advisory committee involvement, to decide on ALS-U experimental systems. This process will also help inform the 2019-23 ALS strategic plan to be written in the summer/fall of 2018. Our goal is an overall ALS/ALS-U plan for new/upgraded experimental systems that is responsive to user needs and that will make ALS ready for early operations after ALS-U is complete.

**ALS-U accelerator physics**: We continue to explore various lattice and injection concepts for ALS-U. We are focusing in particular on the balance between transverse nonlinear dynamics, longitudinal dynamics and collective effects in an integrated way. The studies currently include numerical and analytical physics studies together with technology evaluation in the areas of magnets (DC+pulsed), vacuum systems, and RF systems (main and harmonic). In order to continue to serve the complementary hard x-ray community that coexists on the ALS we are also studying concepts for advanced radiation producing devices to incorporate intermediate x-ray sources into the lattice. An integral part is the optimization of possible injection schemes to enable high brightness lattices by on-axis injection. The study of possible lattice choices and accelerator technologies will be informed by parallel efforts to further develop the science case for soft x-ray diffraction limited light sources.
Merging ALS and ALS-U beamlines and instruments: A key feature of the planning process for ALS-U is to ensure the new lattice can be commissioned with a full complement of recently upgraded or new beamlines that are ready – and able - to take advantage of the impressive increase in source brightness. Key features of this emerging plan for beamline upgrades include:

- The on-axis injection scheme for ALS-U will enable an entirely new class of narrow gap and shorter period undulators that are a key component needed to achieve the highest possible brightness.

- Even though they have been continually upgraded, ALS undulator beamlines that are currently more than 10-15 years old will be approaching the end their useful lives when ALS-U is commissioned – particularly 4.0.2, 8.0, and possibly 9.0, 12.0. These will therefore need to be replaced or comprehensively upgraded for either ALS or ALS-U operation. We are seeking ways to support funding these beamline upgrades.

- ALS undulator beamlines constructed in the last 5-10 years are based on modern optical designs and have been maintained and upgraded regularly. They are mostly ALS-U ready, except a new generation of coherence-preserving optics will be needed to handle diffraction-limited SXR photon beams from ALS-U. Establishing the design parameters of such optics, especially how to handle the high power density, is presently an active area of R&D by the ALS-U team.

- Conceptualizing, designing and building new state of the art end stations is a constant process at the ALS; note for example that many entries in Tables 1 and 2 describe end station projects. These capabilities are being planned with ALS-U very much in mind.

Planning the lattice changeover: Removing the existing ALS lattice and replacing it with the ALS-U multibend achromat lattice is estimated to require 9-12 months and is itself a major engineering project. Planning for this changeover is already a major focus of the ALS-U project.
IV. Ancillary Capabilities and Activities

A. Safe Operation on the ALS Experimental Floor

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

Integrating Floor and Accelerator Operations: ALS cross-trains floor operators, who directly work with users and ALS scientists and who play a key role assuring safety on the floor, and accelerator operators, who would otherwise have limited interaction with users and floor safety. This leads to better integration of these two activities and provides more staff trained to understand safety procedures and to notice potential hazards on the floor. Similarly, there are more staff who understand safe accelerator operations. This leads to a better and more efficient operation overall. This has further evolved, with new training modules designed to further the knowledge and capabilities of all operators.

Management Walk-Arounds: ALS management schedules regular weekly walk-arounds and more in depth monthly visits to beamlines in individual sectors to understand and evaluate floor operations, with a focus on safety. In addition, supervisors within the direct Line Management chain participate in the annual safety reviews conducted at each beamline.

Introduction of new Work Authorization Process: ALS and matrixed Engineering staff have adopted the new LBNL-wide Work (WPC) and Control Activity Manager program to authorize their work. This system ensures that a complete evaluation of work scope, hazards, and mitigating controls has been performed prior to work authorization.

User ISM Support: As discussed in more detail in Sec. IV.F, a primary goal of developing a new User Portal is to develop a simple and intuitive web-based input tool for users to create safety analysis forms for each of their experiments. Accordingly, the ALS is commissioning new software to facilitate an on-line ISM process for each and every study performed by users and staff. This will enhance communication between users and the ALS safety team to insure that hazards are identified early on in the planning process so that the appropriate controls are understood and in place for efficient and safe use of scheduled beamtime.

Beamline/Accelerator Renewals and Upgrades: The scope and nature of both beamline and accelerator projects is constantly evolving, and multiple ALS- and LBNL EHS-review processes are now in place to thoroughly evaluate all safety, engineering and operational concerns. Many projects involve upgrades of current systems, and an ‘abbreviated’ review protocol has increased the efficiency of the review process without compromising safety at ALS. Also, operating experience with safety management systems such as top-off critical apertures, beamline shielding end-points, beamline radiation safety training, and have been incorporated to make the reviews more effective and efficient. Lastly, current DOE trends in accelerator safety including
unreviewed safety issues, configuration control, readiness reviews, etc. are integrated into ALS processes.

**Technical Capabilities:** The ALS Safety Program has collaborated with other elements of the ALS in a number of areas: developing the capabilities of the user biology lab and its technical support function, continuing development of chemical lab support such as glove boxes, additional lab capabilities in the ALS mezzanine, and *in situ* capabilities for flame, low/high temperature, high pressure, laser, and other potentially hazardous environments, and improved support in the handling of low level radioactive materials.
**B. Strategic Engagement to Maintain Excellence and Set Scientific Priorities**

The quality and impact of the ALS’s research depends on an engaged and innovative user community as well as input from other internal and external sources. In collaboration with our scientific staff, our users bring forward key ideas that fuel our facility. As such, our strategic plan is guided by their diverse input, which we seek on a regular basis. Advisory committee meetings, reviews, workshops, and other formal and informal meetings provide additional avenues to shape our priorities. Our primary paths of engagement are as follows:

- **Our Users’ Executive Committee (UEC)** serves as an interface between ALS staff and users. We engage them formally and informally several times per year to identify ways to help users be more productive at the facility. The UEC is elected from the user population and generally represents the spectrum of research activities at the ALS.

- **Our annual User Meeting** is organized by the UEC and includes 12–15 topical workshops planned collaboratively by our staff and users (see http://tinyurl.com/als-um-workshops). The meeting is well attended and provides invaluable advice on emerging opportunities and research priorities. The ALS financially supports the User Meeting in recognition of its impact on the ALS’s strategic direction.

- In addition to the regularly held User Meeting, we also convene **special ad hoc workshops**. For example, a workshop to develop the science case for the ALS Upgrade was held in January 2017 and enabled many key users and other outside experts to guide our vision.

- The ALS **Scientific Advisory Committee (SAC)**, composed of national and international experts from many disciplines, meets twice per year to provide high-level advice to LBNL and ALS management. All of our strategic plans and priorities are discussed in detail with the SAC.

- With oversight from the SAC, the ALS recently organized a round of **crosscutting reviews** of all beamlines, organized by entire sub-discipline,s to seek focused advice on how to optimize our capabilities to address important research problems. This was part of the process to select ALS-U experimental systems and also will inform the 2019-2023 ALS Strategic plan. The long term intent is to review all ALS beamlines every 3-4 years.

- As part of LBNL’s **Energy Sciences Area (ESA)**—the heart of DOE’s Basic Energy Sciences activities at the laboratory—our management team participates in area meetings with partner divisions, providing and receiving valuable collaborative strategic advice. The insights and guidance of our fellow ESA divisions will be critical to developing the capabilities and science plans for the ALS Upgrade.

- **Approved Programs (APs)** provide longer-term, guaranteed access to beam time for an individual or group proposing a high-quality research program, as evaluated against the General User (GU) population. AP proposals are evaluated by the Program Study Panel (PSP), which also evaluates regular GU proposals. APs contribute to the ALS’s strategic direction by helping develop significant new capabilities. The final recommendation on an
AP proposal is made by the SAC, which also gauges the research and development plans in terms of the overall ALS program.

• The ALS’s strong ties to many faculty and research groups from UC Berkeley and other UC campuses also contribute to our strategic thinking.

• In a fashion similar to the Approved Programs, the ALS Doctoral and Postdoctoral Programs, described in Sec. IV.G, provide yet another channel to engage strong users, to develop the next generation of synchrotron science experts, and to leverage ALS resources toward future strategic priorities.

• The ALS Communications Group is responsible for highlighting the facility’s capabilities and amplifying highly impactful research carried out by our users and staff to a diverse set of audiences. By promoting our capabilities and scientific outputs to current and potential users, DOE, other synchrotron facilities, and the general public, we attract a talented and innovative user pool and garner the support of the public and government agencies for our work. Distribution channels include the recently revamped ALS website and our monthly newsletter, ALSNews, which has more than 7,000 subscribers. The group also collaborates with LBNL’s Public Affairs office to increase the visibility and reach of our research outputs.
C. Addressing Data Handling and Analysis Challenges

1. Meeting User Needs

Before describing ALS computing capabilities, it is useful to describe two types of user needs. First, in the area of experiments where large data rates and volumes and/or the need for fast, complex, and advanced analysis mean that it would be impossible for users to succeed at their experiments without relying on the network, computing, and software infrastructure of the ALS and ALS computing partners. Second, as the ALS expands its impact into new areas of science, this by definition brings in researchers who are not already experts in ALS techniques and at least initially rely on the computing hardware, software, and expertise of the ALS and its computing partners.

The areas in which the ALS has focused its efforts have been to provide:

- Fast data transfer, from the acquisition systems to temporary then archival storage, and to users’ home institutions
- Robust data management, including the ability to use advanced search on archived data
- Real-time feedback based on fast data processing
- Easy-to-use optimized analysis that allows users to analyze all of their data and extract maximal information

To do this, the ALS has developed a number of capabilities, but has also pioneered the “superfacility” concept, in which users are simultaneously given access to multiple DOE facilities, including NERSC and ESnet. These capabilities are described in more detail below.

2. Network and Computing Infrastructure

ALS staff have worked closely with experts in LBL and DOE networking, computing, and IT groups to design a reference architecture for the networking and computing hardware located at the beamlines (see Figure 6). The network architecture relies both on the ALS network, LBLnet, and ESnet, and takes advantage of the ScienceDMZ model. In addition to equipment located at beamlines, some of the computing and networking hardware is located in a server room in the User Services Building (building 15). In particular, there are a number of GPU servers there, which are used for fast data processing. The ALS Visualization and Analysis Lab also has computing and visualization workstations which are connected to the system. For the past few years, the ALS has had an allocation at NERSC, including 400 TB of project disk space, access to the many-Petabyte HPSS tape storage system, and millions of compute hours (40 million in 2016).

3. Systems for Data Management

The ALS has been a synchrotron trailblazer when it comes to developing advanced data management capabilities that take advantage of collaborations with computing facilities. The set of tools and systems developed at the ALS with partners in the LBNL computing divisions are
referred to as SPOT Suite. Versions of this have been deployed at beamlines 7.3.3, 8.3.2, 12.3.2, and COSMIC. The tools include software that runs at the beamline to detect new data and launch packaging and transfer, database servers that register the data with its associated metadata to allow subsequent search and organization, and workers, message passing systems, and workflow tools that allow automated processing to be launched on data sets using resources at supercomputing centers as data arrives. Users can access all of this powerful infrastructure from an easy-to-use web portal, where they can view or download results during or after beamtime.

To date, SPOT Suite contains hundreds of thousands of data sets and multiple petabytes of data. But while SPOT Suite has proven that this kind of work is both essential and enormously impactful, the ALS is at a crossroads in terms of determining next steps. SPOT was initially funded as part of an LBNL LDRD, and was deployed in prototype mode at 3 beamlines. It has not subsequently received any significant funding that would allow it to expand throughout the ALS or to expand into true production mode at the beamlines at which it has been deployed. The ALS has proven is has the capability to be a leader in this area, but would require a dedicated, funded group to continue its leadership. We are actively communication with the LBNL computing divisions about how to develop and maintain these ALS-ESNET-NERSC interfaces.

4. Algorithms and Software for Data Processing and Analysis

There is an enormous amount software--along with the underlying theory and algorithm development--created by ALS staff and provided for users. A very abbreviated list includes:

![Simplified schematic of network and computing hardware at an ALS beamline, and how these are connected to NERSC.](image-url)
• XPCS analysis software (Sujoy Roy)
• Software for automation of small molecule crystallography analysis (Simon Teat, Dinesh Kumar)
• Software for robotic data collection and subsequent automated analysis for SAXS/WAXS (Alexander Hexemer)
• NEXAFS analysis and information extraction for contribution to the Materials Project (Alpha N’Diaye, Sean Fackler)
• XMAS/FOXMAS for microdiffraction analysis (Nobumichi Tamura)
• Machine Learning for both image processing and scattering analysis (Alexander Hexemer)

In addition, ALS participates in the Center for Advanced Mathematics for Energy Research Applications (CAMERA). That program is not part of the ALS Operations Budget. It is jointly funded by the office of Advanced Scientific Computing Research (ASCR) and BES Scientific User Facility Division (SUFD). James Sethian, UC Berkeley & LBNL Computational Research Division, is the PI. The CAMERA's Mission states “We have assembled a coordinated team of applied mathematicians, computer scientists, beam line scientists, materials scientists, and computational chemists….to accelerate the transfer of new mathematical ideas to experimental science.” Information about CAMERA can be found at [www.camera.lbl.gov](http://www.camera.lbl.gov).

ALS also has an annual facility level allocation from ASCR/BES at the National Energy Research Scientific Computing Center (NERSC) of 35,000,000 massively parallel processing (MPP) hours ([http://www.nersc.gov/users/accounts/user-accounts/how-usage-is-charged/](http://www.nersc.gov/users/accounts/user-accounts/how-usage-is-charged/)) and 15,000,000 storage resource units (SRUs) in the NERSC High Performance Storage System ([http://www.nersc.gov/users/storage-and-file-systems/hpss/hpss-charging/](http://www.nersc.gov/users/storage-and-file-systems/hpss/hpss-charging/)). These allocations are managed by beamline scientists for the benefit of data intensive ALS users. Over the last three years, these allocations have processed more than 200,000 datasets, managed 2.0 PB of data, and launched more than 3 million jobs. The facility allocation is re-competed annually.
D. ALS Detector Development Program

The ALS Detector Development Group focuses on the development of novel soft x-ray detectors that enhance the productivity of the ALS, enhance the facility’s scientific reach, and help plan and optimize capabilities for ALS-U. Soft x-ray detection has challenges not present in hard x-ray detection: Signal-to-Noise (1/10th the energy of hard x-rays), in-vacuum operation and detection efficiency (shallow penetration of soft x-rays into a detector).

Several of the techniques and beamlines described above (Ptychography and STXM, COSMIC, qRIXS, QERLIN, …) are enabled by detectors we have developed.

The FastCCD, developed in collaboration with the Detector Group at APS, is now deployed at ALS, APS, LCLS, NSLS-II and XFEL. It is used for scanning microscopies at ALS, and several new deployments at ALS beamlines are planned.

The VeryFastCCD, the next generation of the FastCCD, is being developed in collaboration with SLAC as an LCLS-II soft x-ray detector, and will be an obvious upgrade for scanning microscopies at ALS as brightness increases.

The SpectroCCD, a very fine pitch (5 x 45 μm²) detector for (1D) RIXS, has proven key to obtaining the resolution needed for qRIXS (see Fig. 2). The detector is being commercialized through the STTR program, and deployments for qRIXS are planned.

QERLIN presents the challenge of high spatial resolution for 2D RIXS, at comparatively high rate. Here, the group has leveraged its experience in pioneering CMOS detectors for electron microscopy to develop a 5x5 μm² soft x-ray, high rate CMOS detector.

Future soft x-ray detector advances will be needed to cope with the higher rates provided by improvements in optics and sources, notably ALS-U. For example, we are actively collaborating with the UC Space Sciences Laboratory to investigate and develop hybrid detectors that combine channel plate sensors that feed pixelated CMOS TimePix detectors for several of these applications – fast XPCS, time resolved spectroscopy, and high resolution RIXS.

As faster detectors means higher data rates, our activities are intimately connected with efforts on "big data." We are developing a 100,000 frame/s electron detector for STEM in close collaboration with NERSC, and we will apply data reduction and transport techniques learned here to detectors for ALS.

Workshops (every 1-2 years) at ALS Users Meetings and elsewhere are forums to collect community need and interest, and, together with Experimental Systems and Scientific Support groups, drive our priorities. ALS operating funds are used to deploy the detectors we develop, and to adapt them to specific experiments and beamlines.
E. ALS X-ray Optics and Metrology Programs

This section describes the tools and techniques that are being developed to enable the construction of a new generation of beamlines and end stations, as outlined in Section I.B, Table 2. This period will see the replacement of old beamlines such as 8.0 and 4.0.2 and addition of major new capabilities, such as the AMBER beamline for energy research and the QERLIN beamline for soft x-ray inelastic scattering. These two are due to be completed in FY18 and are designed to take full advantage of the present ALS source. They will be upgraded as part of the ALS-U program.

The replacements for 8.0 and 4.0.2 will be designed to be compatible with the new ALS-U source from the outset. This means that they must be able to transport, focus and condition beams of soft x-rays up to 1000 times brighter than we have today. One of the challenges in doing so will be to cope with beam sizes in the horizontal direction that are 30 times smaller than the beams we have today. This requires horizontally focusing mirrors to be of much higher quality, and to have a surface figure under load that deviates from the theoretically perfect figure by less than 1 nm. The absorbed power load is typically a few hundred watts. Such tolerances require large improvements in fabrication quality and in mirror cooling technology. Fortunately over the last decade, major advances in fabrication have been made, and even fairly complex figures can now be made to the requisite tolerance.

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

In addition to manufacturing and thermal tolerances, vibration becomes a major factor in the performance of a beamline at this tolerance level. One area of work is centered in reduction of cooling fluid induced vibration. Turbulence and cavitation in cooling lines can excite the natural vibrational modes of a structure, leading to excessive motion of the optics. To counter this, we are doing R&D on the modelling of turbulence in cooled systems, the use of optimum geometry and diffuser structures to reduce vibration, and on implementation of stiffer support mechanisms. Part of this ongoing work is to survey the vibration we currently have on the ALS floor, and in some of our ID beamlines.

Another area of concern is slow drift of optics due primarily to ground motion and relaxation of support mechanisms. One way to counter this is to monitor the beam position and angle along the beamline. This is difficult to do at ALS where we have many variable polarization devices. The normal type of centroid measuring devices do not work for such undulators, due to the
rotation of the radiation pattern as the polarization is changed. To sense the beam location, we must image the beam. To do this, we are embarking on R&D to examine a number of potential solutions. One methodology which looks promising is to reflect off-axis light from a wavelength defining multilayer mirror onto an image sensor. Although the pattern will be complex, we believe that by image analysis combined with an understanding of the physics of the radiation generation, we will be able to find the centroid of the radiation pattern to high accuracy. The result of this work should be a new toolbox of techniques in mirror cooling, mounting, alignment, stabilization and beam monitoring which should significantly improve the quality of beam that is delivered to users.

An integral component of the optics program at ALS is the X-ray Optics Laboratory (XROL). This assures the quality of the optical components installed in beamlines or used in endstations. This entails measurement of mirrors to ensure vendor compliance to specifications, calibrating and adjusting parameters for adjustable mirrors, as well as thorough alignment, tuning, and characterization of the opto-mechanical systems. For example, we must ensure that the mounting system of mirrors does not cause undue deformation in operation, and that the system under adjustment or water flow has the desired characteristics. The XROL checks that the opto-mechanical systems as installed in the beamlines will work according to specifications.

XROL has been in operation in a new laboratory space in the ALS User Support Building since 2014, with comprehensive control of environmental conditions. This is a cleanroom facility a factor of ~5 better than class 1000, with temperature stability better than ±30 mK over a day. The lab equipment includes a phase-shift interferometry microscope, a two-interferometer system (with capability for measurements of small radius of curvature, crucial for sagittally shaped x-ray mirrors), two slope-measuring long-trace profilers (upgraded LTP-II and DLTP), an atomic force microscope, optical microscopes, a differential laser Doppler vibrometer, and various systems for development of new x-ray optics and metrology techniques. With these instruments, the XROL delivers the state-of-the-art optical metrology required to build and maintain high performance operations of the ALS beamlines. For example, the upgraded LTP-II and DLTP are capable of one-dimensional surface slope profiling with a proven accuracy of tangential slope measurements with flat optics of ~60 nrad [root-mean-square (rms)] and with significantly curved optics (radius of curvature of ≥15 m) of ~200 nrad limited by the profiler’s systematic errors. The increasing brightness of ALS is driving our program to even higher measurement accuracy. For example, for next generation optics we need absolute accuracy of 50 nrad and a height accuracy of < 0.5 nm in many cases. In close collaboration with optics teams from other DOE BES facilities as well as with our colleagues around the world, we are developing new methods that should take us to these goals within a few years.

Specific optical metrology challenges to be addressed are the development of the required ultra-high accuracy x-ray mirror and diffraction grating characterization instruments. The major XROL efforts will be directed to research and development of a new Optical Surface Slope Measuring System (OSSMS) capable of two-dimensional (2D) surface-slope metrology at
accuracy below 50 nrad (absolute). The key elements of the new instrument that are a high-precision granite gantry system with air-bearing translation systems and a precision air-bearing stage for tilting and flipping the SUT have been specified, purchased, installed, and commissioned at the XROL in 2015-2016. The system is capable of precise 2D scanning over the surface under test (SUT). The next goal is to develop state-of-the-art optical sensors for the OSSMS. The work is in progress at the XROL. Another promising technique is stitching interferometry, similar to the MSI/ RADSI (micro-stitching interferometry/relative-angle determinable stitching interferometry) system recently developed at the Ultra-Precision Machining Laboratory at Osaka University.

Finally a third component of our work is to develop unique optical elements, where required by the ALS experimental program. For example, we require diffraction gratings with very high efficiency and resolution for resonant inelastic x-ray scattering (RIXS). Maximizing the efficiency requires the use of multilayer coatings, which in turn require the grating facets to be atomically smooth. We have developed this technology and it will be deployed for the first time in the high resolution Qerlin RIXS spectrometer. An offshoot of this work has been the development of very high efficiency blazed reflection gratings with very low scattered light for a number of beamlines. Similar optics will be developed for compact nano-RIXS spectrographs in the next few years. In addition we will be developing reflection zone plates as simple high efficiency monochromators, and ultra-high resolution zone plates using zone patterning techniques to go beyond 10 nm focused resolution, in collaboration with colleagues in the center for x-ray optics (CXRO).
F. Continuing Development of a Modern User Portal

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

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

In order to meet ALS needs for at least the next decade, ALS has an ongoing project to further develop ALSHub to service all ALS needs related to users and to ensure the system runs on a technologically updated platform that will mitigate risks associated with older software. The ALS approach to the continuing development of the user portal is to plan upgrades, which will provide useful tools at each step.

The final major part of the project to develop tools to Manage Experiment Safety started in July 2016 and is currently being commissioned and deployed. The new Experiment Safety Approval System (ESAF) replaces the existing Experiment Safety Sheets. Using data from the ALS Scheduler, users are automatically reminded to complete an ESAF. All user data entry, experiment review, approval and authorization is completed online. Safety staff and beamline staff can customize questionnaires to obtain the required sample, equipment and experiment details. Hazard controls are assigned semi-automatically and adjusted during the review process and inspection setup is facilitated. Electronic signatures are used for user compliance agreement, safety management approval and work lead authorization.

At this point ALS will undertake a rolling program of assessing and, if necessary, upgrading each component to ensure the user services system remains fit for purpose. Updating the user services interface for ALS users is seen as critical to ensuring safe and efficient user operations.
G. ALS Professional and Workforce Development

The success of the DOE synchrotron radiation facilities depends strongly on developing a knowledgeable and highly trained community of users and beamline scientists who apply existing and innovate new tools, often collaboratively, to pursue a diverse array of research frontiers. The ALS takes its role in professional and workforce development very seriously.

Professional development for ALS scientific staff: The ALS innovative spirit so evident in this document is dependent in part on the excellence of our scientific staff. While there is not one approach to success at the ALS, our most successful and strongly engaged beamline scientists establish very strong records of collaborative research, so that they are equal partners with users in our some of the strongest research activities at the ALS. Postdocs with external fellowships now regularly seek to come to the ALS to work collaboratively with these strong staff; at present there are 3–4 such external postdoctoral fellows at ALS.

The ALS Division Staff Committee (DSC) is charged with advising on personnel issues and tracks the career progress of ALS scientific staff. For example, the DSC has placed renewed emphasis on nominations for promotion to LBNL Senior Staff Scientist, the rough equivalent of a full professor at a university. We achieved three such promotions in the last two years, and there are now have five senior scientists on the ALS scientific staff.

The ALS seeks internal and external recognition for its scientific staff, particularly the beamline scientists who are at the heart of our success. The ALS has established an awards committee composed of the Division Deputy for Science and the leaders of the Scientific Support Group and the Experimental Systems Group, with others as needed, to focus on organizing nominations for these awards in timely fashion. We have regular successes on internal ALS, LBNL, and DOE awards and external recognition as well. A sampling from the last three years includes

- Two ALS scientific staff (Rotenberg and Kevan) were awarded the American Physical Society (APS) Davisson and Germer Prize in 2017, and Peter Denes, who is in the LBNL Engineering Division and leads the ALS detector development program, won the 2017 APS Keithley Award. Several other scientific staff have been elected fellows of the APS in the past three years.
- Our scientific staff have also won a few conference awards in the past three years.
- A large group of ALS and LBNL engineering staff won a DOE Achievement Award in 2016 for the recent sextupole brightness upgrade.
- ALS scientific staff fared very well in the LBNL Staff Recognition process the past two years, bringing home several awards for both scientific and technical developments.
- ALS scientific staff are regular recipients of annual ALS awards for excellence in research, instrumentation, and service – the Shirley, Halbach, and Renner Awards (see https://als.lbl.gov/past-meetings/). These are awarded during the annual users meeting and selections are made by the ALS Users Executive Committee.
• Two LBNL staff stationed and working full time at ALS were finalists in the 2016 R&D 100 award.

• ALS management focuses on developing strong candidates for DOE Early Career Research Awards. Our first success occurred a few years ago with with Alex Hexemer. A key feature of success in this was simply nominating an exceptionally strong candidate who is also an exceptionally strong, collaborative, and productive beamline scientist. We have several more young candidates who fit that mold and who were nominated this year.

We are very proud of the above list. External recognition for beamline staff is not common since the portfolio of a beamline scientist does not map very well onto the criteria for external awards, which tend to be heavily oriented toward individual research contributions.

Workforce development activities at the ALS: It is also very important is to establish a strong pipeline of talented candidates to become facility staff - at the ALS and at other facilities - in the future. Aside from the user training activities that happen daily on the experimental floor, the facility sponsors three related programs that directly impact the professional development of young scientists, from college undergraduates to advanced postdoctoral associates:

• **ALS post-baccalaureate and internship program:** The ALS spends ~$100K/year to support undergraduate interns and recent college graduates for part- or full-time employment at the facility for a period up to one year. These students are assigned to work closely with an ALS staff scientist and to help with a project that will update or expand the capabilities of an ALS beamline or end station. Alumni of this program are competitive in applying to the best graduate programs in the US, and regularly select an ALS user as their doctoral thesis advisor. Other alumni have been hired for technical support positions at the ALS, elsewhere at Berkeley Lab, or in the high technology industry.

• **ALS Doctoral Fellowship Program:** The ALS spends ~$200K/year to support typically a dozen doctoral fellows in steady state. This program is highly competitive and attracts superb young talent to the ALS. The ALS offers each Fellow stipend support of about 50% of a typical graduate student pay. The Fellow’s thesis supervisor generally provides the balance of financial support as well as university benefits. In addition to training, other goals of the program are to engage the thesis advisor deeply in ALS research activities and to provide a career development opportunity and supervisory responsibility to ALS staff scientists. The program was established in 2003 and has developed an impressive list of alumni – some now ALS staff and users.

• **ALS Collaborative Postdoctoral Fellowship Program:** The ALS allocates ~$600K/year to this program, and operates in a similar collaborative approach as the doctoral program described above. The strength of the ALS in applying x-rays to frontier research problems attracts a very strong pool of applicants. The financial arrangements are more diverse than for the doctoral program, but the funds are similarly leveraged and a primary intent is again to engage faculty as well as PI’s in other Berkeley Lab divisions in strong collaborations.
There is a sizable flux of students from one of these programs into the next: a few interns and become Doctoral Fellows, and several Doctoral Fellows become ALS postdocs, either in the fellowship program or supported by an LDRD proposal. Given this training it is to be expected that many of the Postdoctoral Fellows continue their careers as beamline scientists or active users of synchrotron radiation facilities. These workforce development programs have a significant long-range impact on the synchrotron radiation community at large and on the ALS user program specifically, even though fellows are not allowed to engage directly in user service.

The programs have been approved and supported by the DOE and are part of the ALS Field Work Proposal. These are training programs that qualify for a significantly reduced Berkeley Lab burdens, which, combined with the leveraging described above, makes them very cost effective.

Committees formed from the ALS staff and user community oversee the fellowship programs and help maintain a high degree of leveraging and ensure strong alignment of the programs with the facility’s strategic plan. Applications for Doctoral Fellowships are solicited annually, and files are evaluated by an ad hoc committee composed of the ALS Division Deputy for Science (DDS), the head of the ALS Science Support Group, a beamline scientist and usually two faculty who conduct strong research programs at the ALS. A separate committee composed of the DDS and ALS beamline group leaders. More detailed information about the fellowship programs is provided on the ALS web site at

https://als.lbl.gov/about/career-opportunities/als-doctoral-fellowship-in-residence/
https://als.lbl.gov/about/career-opportunities/als-collaborative-postdoctoral-fellowship-program/

ALS beamline scientists have learned how to leverage resources available to them, including their own small beam time allocation, beam time of their close collaborators, funds from these fellowship programs, and other resources brought by their collaborators and provided by the ALS. The fellowship programs are a crucial ingredient of this process, both in supporting existing beamline scientists and training new ones.
Appendix 1: List of acronyms

ALS: Advanced Light Source
ALS-U: Advanced Light Source Upgrade
ALSHub: Portal used by users to engage the ALS proposal system
AMBER: advanced materials beamline for energy research
AP: ALS Approved Program
APS: Advanced Photon Source or American Physical Society
APXPS: ambient pressure x-ray photoelectron spectroscopy
ARPES: angle resolved photoelectron spectroscopy
ASCR: Advanced Scientific Computing Research, a division in the DOE office of Science
BATT: LBNL Batteries for Advanced Transportation Technologies program
BCSB: Berkeley Center for Structural Biology
BER: DOE Biological and Environmental Research
BER/BSISB: BER funded Berkeley Synchrotron Infrared Structural Biology Program
BES: Department of Energy Basic Energy Sciences
CAMERA: Center for Advanced Mathematics for Energy Research Applications (CAMERA)
COSMIC: COherent Scattering and MICroscopy beamline (ALS 7.0.1 complex)
CSD: LBNL Chemical Sciences Division
CRD: LBNL Computational Research Division
CXRO: LBNL Center for X-ray Optics
DDS/ALS-DDS: ALS Division Deputy for Science
DLSR: Diffraction-Limited Storage Ring
DMSE: BES Division of Materials Science and engineering
DSC: ALS Division Staff Committee, the personnel committee for scientific staff
EES: LBNL Earth and Environmental Science Division
EHS: ALS or LBNL Environmental Health and Safety Division
EPU: elliptically polarizing undulator
ESA: LBNL Energy Sciences Area
ESAF: Experiment Safety Assessment Form
ESNet: Energy Sciences Network
EUV: Extended UltraViolet lithography
GEMINI: new protein crystallography beamline
GU: ALS General User
GUP: General User Proposal
HHMI: Howard Hughes Medical Institute
HVAC: Heating, Ventilation, Air Conditioning
ISM: Integrated Safety Management
JCAP: Joint Center for Artificial Photosynthesis, a DOE Energy Hub
JCESR: Joint Center for Energy Storage Research, a DOE Energy Hub
LCLS: LINAC Coherent Light Source, a free electron laser at SLAC
LDRD: LBNL Laboratory Directed Research and Development
LUXOR: Lightsource Upgrade for X-Ray Optics Renewal
MAESTRO: Microscopic And Electronic STructure Observatory (ALS 7.0.2 complex)
MBA: Multibend Achromat accelerator lattice
MF: LBNL Molecular Foundry
MOF: Metal Organic Framework nanoporous material
MSD: LBNL Material Sciences Division
nanoIR: near field IR microscopy delivering ~20 nm resolution
NCEM: National Center for Electron Microscopy in the LBNL Molecular Foundry
NERSC: LBNL National Energy Research Supercomputing Center
NEXAFS: Near Edge X-ray Absorption Fine Structure
NSLS-II National Synchrotron Light Source (-II)
OML: ALS Optical Metrology Laboratory
PBD: LBNL Physical Biosciences Division
PEEM: photoelectron emission microscopy
PSB: Pseudo-Single Bunch operation at the ALS
PSP: ALS Program Study Panel
QERLIN: Q- and energy resolved inelastic scattering beamline
qRIXS: ALS end station to enable parallel-detection RIXS with q-resolution
RAPIDD: Rapid Access, Industrial, and Director Discretionary beam time proposal
RIXS: resonant inelastic x-ray scattering
RSoXS: Resonant Soft X-ray Scattering
SAC: ALS Scientific Advisory Committee
SAXS: Small Angle X-ray Scattering
SCBG: BES Chemical Sciences, Geosciences & Biosciences
SEMATECH: Semiconductor Manufacturing Technology Consortium
SINS: Synchrotron Infrared Nanoscale Spectroscopy
SUFD: BES Scientific User facility Division
spinARPES: spin-resolved ARPES
STXM: scanning soft x-ray transmission microscope
SXR: Soft X-ray
SXE: Soft X-ray Emission spectroscopy
SYBYLS: Berkeley Lab Structurally Integrated Biology for the Life Sciences Program
TEM: Transmission Electron Microscopy
TI: topological insulators
UEC: A:S Users Executive Committee
USUP: User Services User Portal
WPC: LBNL Work Planning and Control safety management system
XAS: x-ray absorption spectroscopy
XFEL: X-ray Free Electron Laser in commissioning in Hamburg
XM1: X-ray Microscope #1 (ALS beamline 6.1.2)
XPCS: x-ray correlation spectroscopy