LCLS STRATEGIC PLAN 2023-2028

September 2023, Prof. Mike Dunne (LCLS Director)

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Enabling a new era of transformative X-ray science

Introduction and Background

A new scientific frontier opened in 2009 when the world's first X-ray free-electron laser (XFEL), the Linac Coherent Light Source (LCLS), began operations at the SLAC National Accelerator Laboratory, operated by Stanford University on behalf of the US Department of Energy, Office of Basic Energy Sciences (DOE-BES).

The scientific start of LCLS has arguably been one of the most vigorous and successful of any new research facility, impacting a broad cross-section of fields ranging from atomic and molecular science, ultrafast chemistry and catalysis, fluid dynamics, clean energy systems, structural biology, high energy-density science, photon science, and advanced materials

The major scientific accomplishments of LCLS within the first few years of operation are reflected in both the number of publications (over 1600 to date) and the number of users attracted by this novel source (over 3000 unique users and 13,000 user visits, in approximately a thousand experiments - mostly within the limitations of a single beamline). As such, the scientific productivity of the facility is incredibly high - and is distributed over a broad set of areas (see Figure 1). The scientific impact of LCLS during the first five years was summarized in 2015[1], and the scientific highlights of the first 10 years was celebrated in 2019.

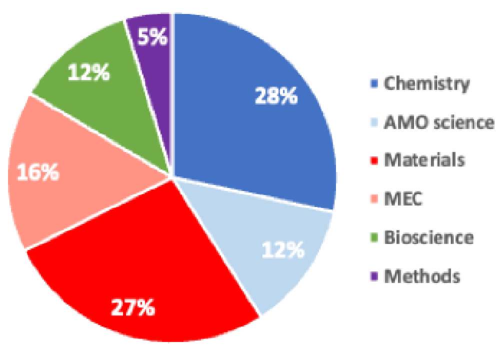

Figure 1 Typical breakdown of the scientific proposals received from the user community

The scientific impact of LCLS has been enhanced by a suite of remarkable developments in the facility's capabilities[2], with examples shown in Figure 2. LCLS can now provide ultrashort pulses (from ~200 attoseconds (as) to >100 femtoseconds (fs)), with unprecedented peak power and peak brightness[3], in SASE or seeded-mode operation, over an energy range from ~250 to ~25,000 eV at 120 Hz. LCLS can provide dual-pulses with relatively arbitrary separation in time (from fs to ~0.5us), with the option of dual color, and variable linear/circular polarization. Recent work has increased the peak power up to 1000 GW and has delivered 4 independent pulses in a train that can be separated in increments of 0.35ns to cover a time window of up to ~500ns.

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[1] Bostedt, et al., "Linac Coherent Light Source: The first five years", Rev. Mod. Phys, 88, 015007 (2016).
[2] See details of operating modes: https://lcls.slac.stanford.edu/machine-faq
[3] Typically 10^{33} ph/s/mm^2/mrad^2/0.1% BW and up to 10^{35} when seeded, with up to 1 Terawatt peak power.

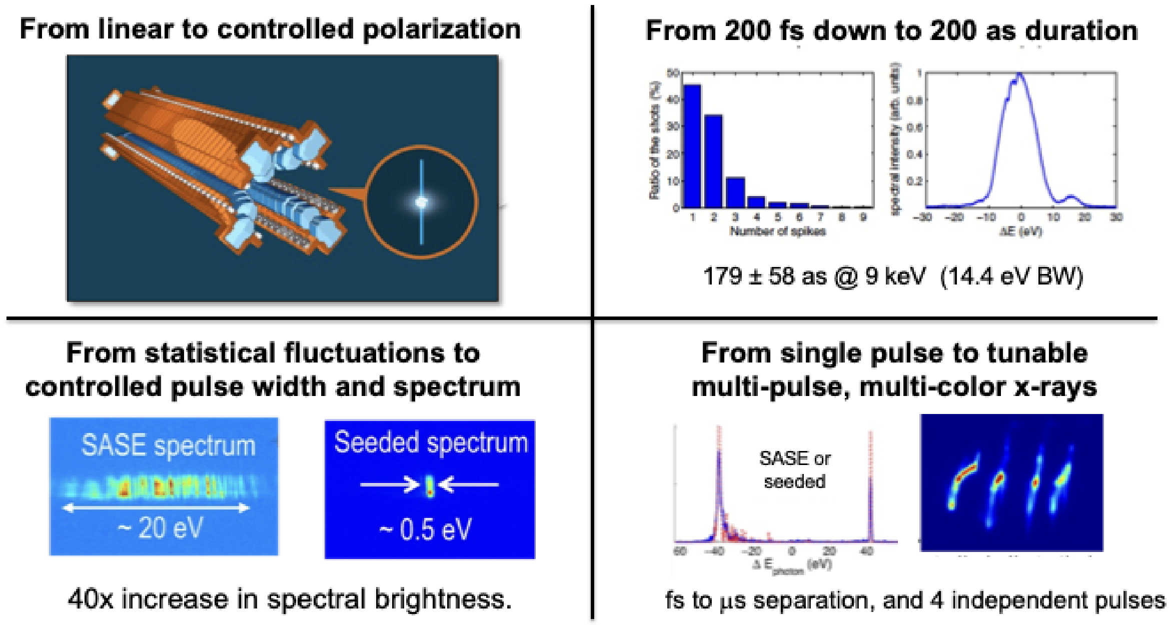


Figure 2 Example advances in XFEL beam performance over the past few years

The success of LCLS has been accompanied by the rapid development of other hard-X-ray FEL facilities (Figure 3), including SACLA (Japan), the European XFEL (Germany), PAL-XFEL (Republic of Korea), Swiss-FEL (Switzerland), and construction of SHINE (China), as well as soft X-ray facilities such as FLASH (Germany), Fermi@Elettra (Italy) and SXFEL (China).

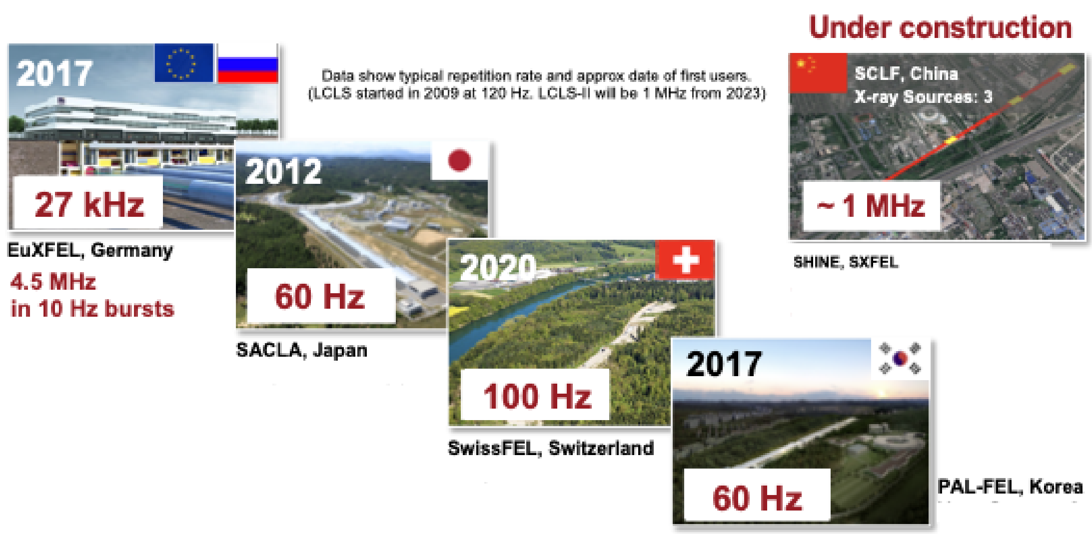


Figure 3 Summary of the world's hard X-ray FEL facilities, with nominal pulse repetition rates.

To keep the LCLS facility in a preeminent state, SLAC and the US Department of Energy Office of Science are pursuing a vigorous series of developments, captured as a multi-phase plan in Figure 4. The scientific priorities that motivate these developments have been derived from the set of Grand Challenges and Transformational Opportunities identified by the DOE-BES leadership and its advisory committees, with specific directions informed by Basic Research Needs reports, focused roundtables, and dedicated LCLS community workshops.

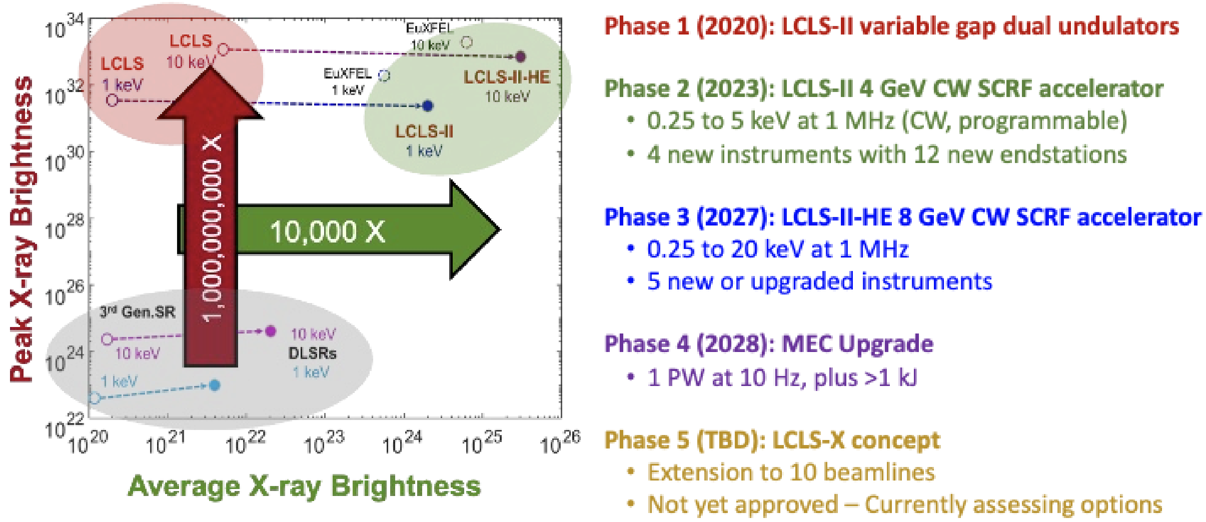


Figure 4 High level development plan for the LCLS facility over the near/medium term

The [LCLS-II Project] represents over a billion dollars investment that has delivered a superconducting accelerator in the first kilometer of the SLAC linac tunnel, able to deliver X-rays from 0.2 to 5 keV at up to 1 million pulses per second (compared to the prior operation at 120 pulses per second). This leap in repetition rate, and the corresponding average brightness, will transform the scientific breadth and impact of the facility. A suite of new instruments, known as L2S-I, is being deployed to take full advantage of this new source.

Beyond this, an extension to higher X-ray energy at high repetition rate has long been requested by the LCLS user community[4]. In response, DOE launched the LCLS-II-HE ("High Energy") project. Due to come online in 2028, this will double the energy of the superconducting linac to 8 GeV, which will extend X-ray energy from a current cutoff of ~5 keV to up to 20 keV.

LCLS-II and -HE will be transformative tools for energy science. They will qualitatively change how X-ray scattering, spectroscopy and imaging are used, showing how natural and artificial systems function, revealing dynamics on timescales down to the attosecond regime, and mapping spatial response down to sub-atomic levels. They will enable powerful new methods to capture rare chemical and material events, characterize fluctuating heterogeneous complexes, and reveal underlying quantum phenomena in matter using nonlinear, multi-dimensional, and coherent X-ray techniques only possible with a true X-ray laser.

In parallel, a major upgrade to the MEC instrument is being developed with the DOE Office of Fusion Energy Sciences (FES). This will significantly increase the peak power (from 0.1 to 1 Petawatt) and peak energy (from 0.1 kJ to >1 kJ) of the optical drive lasers, to open up a new era of precision plasma science and research into extreme material dynamics.

The layout of these upgrades is shown in Figures 5 to 7. More broadly at LCLS, a widespread series of developments are underway to integrate theory, simulation and experiments; pursue R&D in key technologies; ensure alignment between the local SLAC/Stanford science programs and the evolving facility; and engage the user community to exploit these new capabilities.

[4] See, for example: https://portal.slac.stanford.edu/sites/conf_public/lclsiihe2018/Pages/default.aspx and https://events.bizzabo.com/SLAC-UsersMeeting-2020/agenda/session/332876

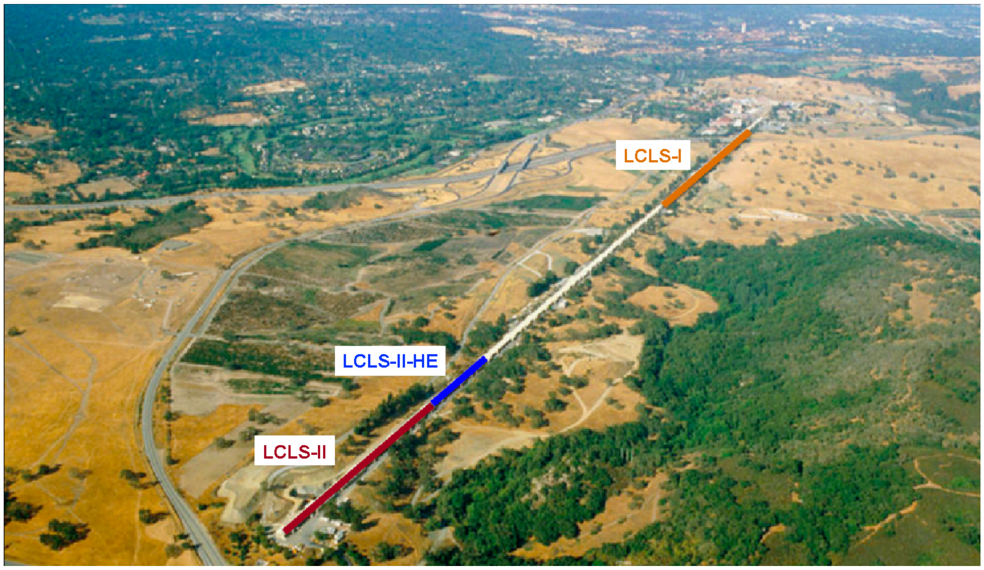


Figure 5 Layout of the accelerator upgrades for LCLS-II and LCLS-II-HE in relation to the existing linac (LCLS-I). The SLAC site and Stanford campus can be seen in the upper right.

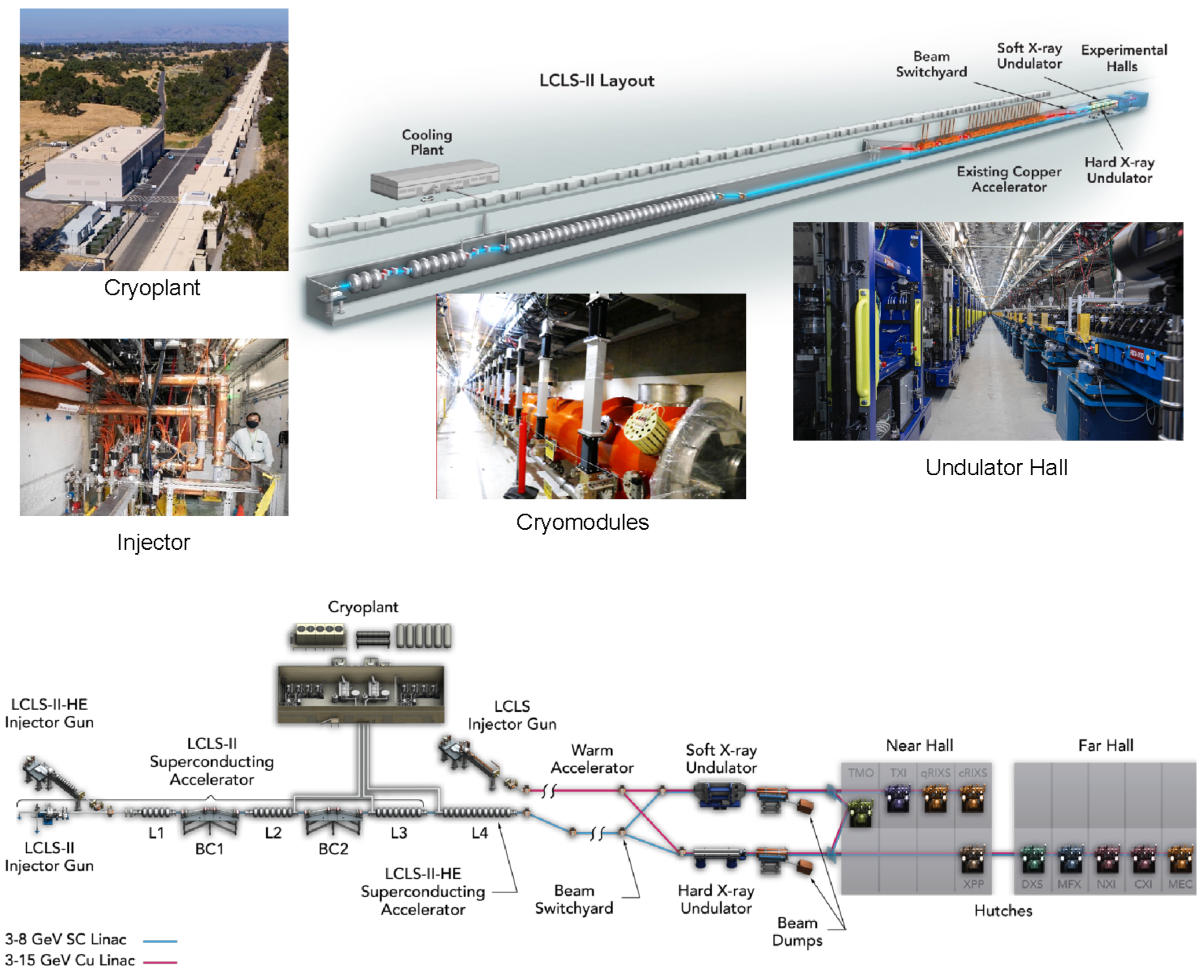
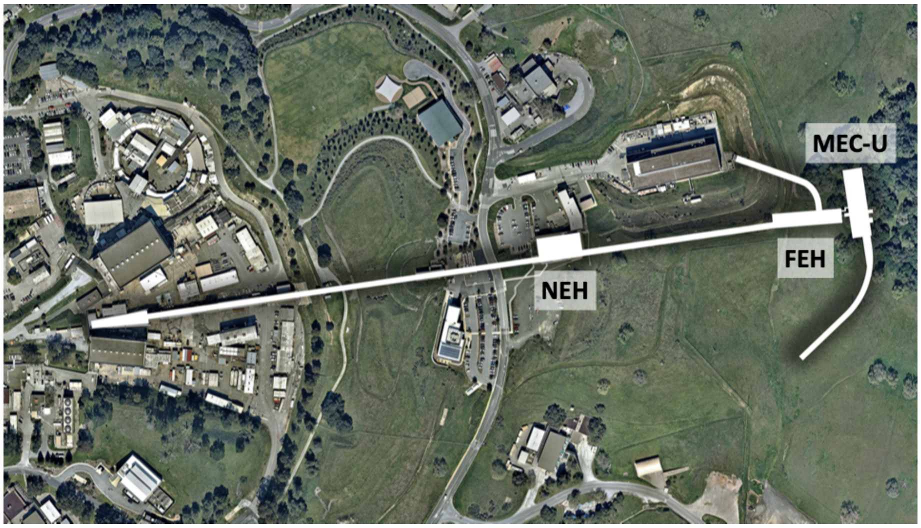
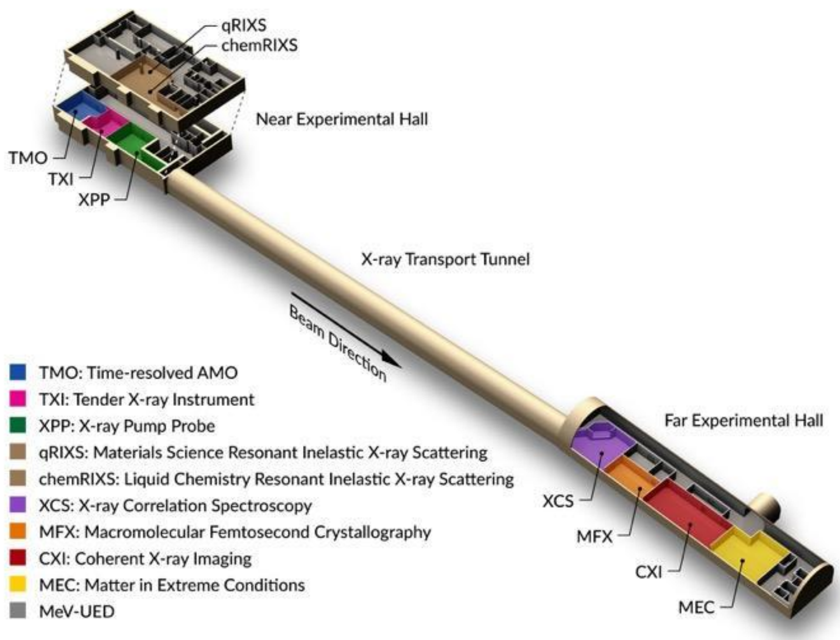
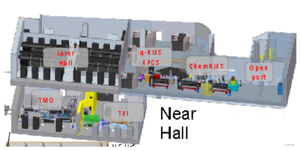


Figure 6 Schematic layouts of the accelerator upgrades LCLS-II and LCLS-II-HE



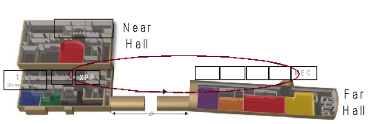


Soft X-ray (LCLS-II)



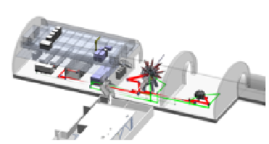
- Atomic physics
- Photo-catalysis
- Surface chemistry
- Quantum materials
- Single Particle Imaging
- Nonlinear X-ray science

Hard X-ray (LCLS-II-HE)



- Complex materials
- Semiconductors
- Biological function & dynamics
- Chemical catalysis
- Gas phase chemistry
- Quantum materials

MEC Upgrade



- Plasma physics
- High field science
- Extreme materials
- Lab astrophysics

Figure 7 LCLS instrument areas in the Near Experimental Hall (NEH), Far Experimental Hall (FEH), and the future MEC-Upgrade

Strategic Plan - Executive summary

The purpose of this document is to provide an overview of how the science opportunities defined by the LCLS user community are being translated into facility development activities and delivery of the user operations program for 2023-2028. Community feedback is sought.

The strategy is configured to take full advantage of the integrated nature of SLAC/Stanford and that of the wider DOE complex, fostering a vibrant research ecosystem to exploit these capabilities. A central aspect is nurturing our role as a full-service user science facility to provide transformative input from our staff at each stage of the research lifecycle, and to design and deliver the next generation of capabilities to keep LCLS at the forefront. This is augmented by coordination with SSRL and integration of MeV-UED and a suite of lab-scale facilities to develop people, techniques, new tools, and a diverse scientific portfolio. The strategy puts in place an integrated and adaptable approach to experimental delivery that drives the co-design of our accelerator/FEL, instruments, detector/data systems, sample environments, pump/probe lasers, X-ray beamline performance and associated systems.

The next 5 years are centered on the design, delivery, commissioning and exploitation of a suite of major investments in the facility: LCLS-II, LCLS-II-HE, MEC-Upgrade, and associated scientific capabilities. For the longer term, it is noted that XFELs are still in their infancy and will likely define X-ray science in the 21st century, given their extreme peak and average power, and ability to study structure and dynamics with transform-limited pulses. SLAC is now developing its vision to fully realize this potential, aiming at a suite of optimized beamlines to meet the needs of the broad user community. This will allow the specialization necessary for full exploitation of each scientific area, yielding a step-change in the impact, breadth of use, and mode of operation of LCLS.

Success can be characterized as LCLS being the “facility of choice” for researchers across the community to address the most impactful scientific questions, producing seminal results. Key metrics will focus on integrated scientific impact, facility performance, long-term facility health and sustainability, responsiveness to sponsor priorities, and staff and user satisfaction.

At the highest level, the LCLS strategy can be expressed in 4 high level goals, with driving factors summarized for each area here, and specific objectives detailed in the main document:

GOAL 1 Establish a defining set of scientific priorities, with decadal-scale ambition

- Learn from the first decade of XFEL science to identify the most compelling directions for high impact science.
- Ensure flexibility to respond to a dynamic user program based on the emerging understanding of this rapidly-evolving field.
- Drive a transformation in X-ray science in the chosen areas, working with a broad user community
- Initiate community-wide science campaigns to tackle national priorities in clean energy, sustainability, human health, and microelectronics and the quantum revolution.

GOAL 2 Drive step-changes in source and facility performance

- Derive and deliver the facility performance requirements and the step-changes in capability needed with LCLS-II, HE and MEC-U to achieve the declared scientific goals.
- Push the boundaries of the field via exploration of new XFEL modes and instrument configurations to inspire new directions.
- Optimize facility performance via detailed Start-2-End modeling, precision diagnostics and feedback-based control systems.
- Undertake co-design of detectors, intelligent data reduction, and real-time massive-scale data analysis to take full advantage of the leap to the MHz XFEL era.
- Develop differentiating sample synthesis, delivery and environmental control methods.
- Lead the world in the definition and delivery of a third generation XFEL facility.

GOAL 3 Ensure mission success through operational excellence

- Provide world-class user support and infrastructure for sustainable operations.
- Maintain the highest standards for safety, research security, and financial probity.

GOAL 4 Empower societal and economic impact

- Foster a vibrant research ecosystem, taking advantage of the unified structure at SLAC/Stanford and within the DOE complex.
- Support a full-service science facility model, with transformative staff input at each stage of the research lifecycle to enhance the scientific quality, increase the likelihood of success, reduce the time to publication, and lower the barrier to entry for new users.
- Engage the widest possible set of potential user communities to ensure continued innovation to deliver sustained and transformative scientific and societal impact.
- Ensure strategic use of co-located facilities (LCLS, SSRL, Cryo-EM) and science labs, and coordination with light source facilities across the US and internationally.
- Cultivate a welcoming, inclusive, diverse, equitable and sustainable work environment.

Guiding Principles

The methods of delivery of the LCLS strategy are shaped by a set of 12 Guiding Principles. These inform the decision making process at each level in the organization:

1. Ensure safety, health, and mental wellbeing of staff and users are paramount, integrated into all aspects of our work.
2. Operate LCLS in the most scientifically productive and cost-effective manner, consistent with provision of an internationally-leading capability to a broad user community.
3. Nurture respect in the workplace as a bedrock value that provides a psychologically safe space for all to thrive - fostering a diverse, equitable and inclusive environment.

4. Provide attractive career development options for staff, driving a sustainable approach that protects the interests of individuals, teams, and the facility as a whole.
5. Optimize user access to maximize the value derived from the major DOE investments (e.g., via new multiplexing schemes; dedicated end-stations; revised operational models, Start-2-End models, offline test-stands, and the full-service user facility model)
6. Broaden the reach of LCLS to new user communities and science areas to ensure long-term scientific health and innovation.
7. Treat LCLS as an integrated facility when allocating funding, irrespective of where people sit in the SLAC organization, taking a system-level, facility-wide view of priorities.
8. Use ongoing LCLS experiments, and targeted in-house research, to refine the scientific priorities and assessments of delivery risk. Craft a set of credible pathways to the “ultimate experiments”, using a balance of technical studies, high impact intermediary science, theoretical modeling, and offline developments.
9. Ensure readiness for, and prioritize the exploitation of, the unique characteristics of LCLS-II (and subsequently LCLS-II-HE and MEC-U) compared to other XFEL and storage ring facilities (e.g., the use of continuous pulse structures; the ability to probe in the ultrafast domain; the use of X-ray beams of unprecedented average power and spectral brightness; and the availability of optimized instruments, detectors, lasers, optics, data systems).
10. Develop robust systems with high availability to users, configured to run with minimal intervention in ‘standard modes’ - in order to enable greater control of experiments by the users, facilitate remote access (to broaden community involvement), and to provide scalable, sustainable, and scientifically creative roles for LCLS staff.
11. Operate in an open, collaborative, and mutually-supportive manner with and between staff, users, vendor partners, collaborating institutions, and the DOE sponsors.
12. Provide sufficient investment in exploratory R&D to investigate next-generation concepts to keep LCLS at the forefront over the long term.

Goal 1: Establish a defining set of scientific priorities with decadal scale ambition

The scientific drivers for the LCLS facility are defined by an ongoing, iterative process to identify grand challenge objectives that are then used to set requirements for our facility development. These drivers are already published for LCLS-II, LCLS-II-HE and MEC-U following community input, along with the facility plans to allow ongoing comment and improvements via regular workshops and formal reviews. Regular peer review of LCLS “science and instrumentation” is held to assess impact to date and future directions (most recently in the areas of material science (Sept 2019), bioscience (Feb 2020), condensed phase chemistry (Feb 2021), AMOS and gas phase chemistry (Feb 2022) and HED science (Dec 2023), complemented by DOE Triennial Reviews (most recently Oct 2021) and a decadal retrospective (2019).

A broad cross-section of the scientific and technical community are engaged in this multi-year, iterative approach to define and peer review our priority research directions and associated facility development priorities. This cycle is captured in Figure 8, with individual areas explained in more detail in section 3.2.2.

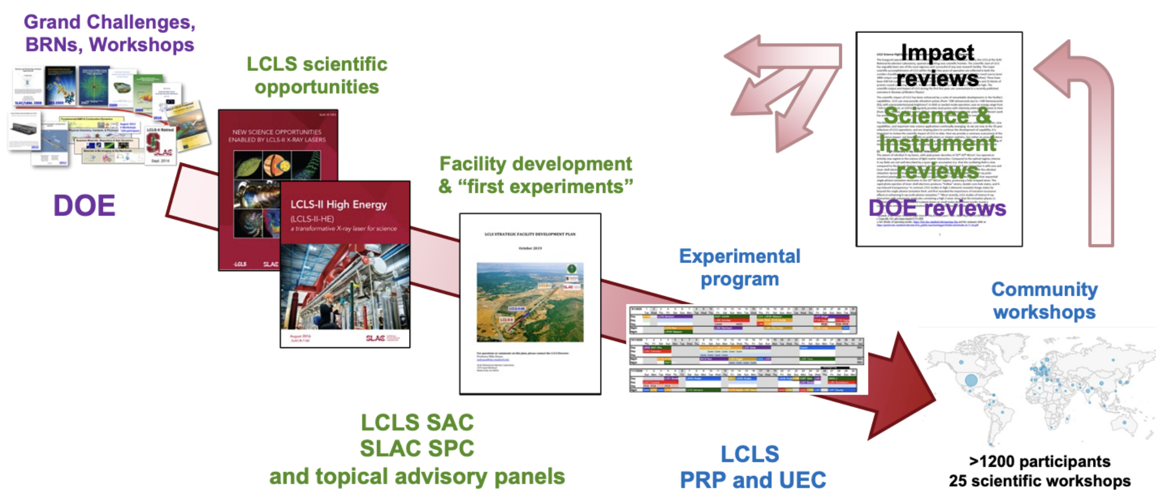


Figure 8 The overall LCLS process to derive its scientific priorities

The emphasis of LCLS over its first decade of operation has primarily been on fundamental research, in which the important benchmarks of science impact and significance are “grand challenges” where results from LCLS have led to qualitative advances or new thinking in the respective fields of science. For the DOE-BES science mission, important references are the basic research needs (BRN) report series[5], and the two “grand challenges” reports[6,7] that articulate science challenges that cut across all BES BRN reports. For science areas beyond

[5] *DOE Office of Science, Basic Energy Sciences, Basic Research Needs Reports:* *http://science.energy.gov/bes/news-and-resources/reports/basic-research-needs/*

[6] *"Directing Matter and Energy: Five Grand Challenges for Science and the Imagination,"* *https://doi.org/10.2172/935427* *(2007)*

[7] *"Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science - BESAC Report" http://science.energy.gov/~/media/bes/besac/pdf/Reports/CFME_rpt_print.pdf (2015)*

BES (e.g. biology, fusion energy, matter in extreme environments etc.), grand challenges are derived from equivalent prominent reports from expert panels in the respective fields.

In addition, as the world's first XFEL (with capabilities ~10^9 beyond previous X-ray sources), much of the early research at LCLS focused on: (1) discovery science, opening and exploring new scientific frontiers, (2) advanced X-ray method development to fully exploit the transformative capabilities of XFELs, and (3) pushing the frontier in X-ray capabilities, e.g. from ~100 fs to ~0.2 fs pulse durations, terawatt peak power pulses, two-color pulses and pulse trains etc. These significant science and technology advances are considered as underpinning, enabling steps for the thematic areas discussed below. These advances very much drive the frontiers of science in a new field, and should be considered as a central element of the facility's overall scientific impact and strategic direction.

The future strategic directions of LCLS are informed by these early results, of which a representative selection is summarized in Appendix 1, providing examples of where XFELs have made major advances to date, to inspire new ideas and directions

1.1 Drive a transformation in X-ray science

The LCLS facility has opened up a new era in X-ray science via the coupling of unprecedented beam performance, innovative instrument design, and leading-edge laser, detector and data systems. Going forward in the immediate term, LCLS-II will qualitatively change the way that X-ray imaging, scattering and spectroscopy can be used to study how natural and artificial systems function. It will enable new ways to capture rare chemical events, characterize fluctuating heterogeneous complexes, and reveal quantum phenomena in matter, using nonlinear, multidimensional and coherent X-ray techniques that are possible only with X-ray lasers. Later this decade, LCLS-II-HE will enable precision measurements of structural dynamics on atomic spatial scales and fundamental timescales. Such measurements are needed to underpin many of the transformative opportunities identified by BESAC, by providing detailed insight into the behavior of complex matter in real-world heterogeneous samples on fundamental scales of energy, time, and length. Alongside this, a complete reimagining of the Matter in Extreme Conditions instrument, known as the MEC-Upgrade, will for the first time combine high repetition-rate petawatt lasers with kilojoule lasers and an XFEL - opening up unprecedented opportunities for the study of fusion energy and laboratory astrophysics.

In the following, we briefly summarize six broad areas of science in which the unique capabilities of the upgrades to LCLS can address critical knowledge gaps at the new scientific frontiers of matter and energy. A more extensive description of these science opportunities can be found via the LCLS-II, LCLS-II-HE and MEC-Upgrade websites.

Coupled Dynamics of Energy and Charge in Atoms and Molecules

Charge migration, redistribution and localization, even in simple molecules, are not well understood at the quantum level - but these are the fundamental processes that drive chemical reactions and store or release energy, with applications ranging from combustion to natural and man-made molecular systems that convert sunlight into fuels. Understanding and controlling these processes remains a fundamental science challenge, in large part because the movement of charge is closely coupled to subtle structural changes of the molecule, with indirect evidence pointing to the importance of quantum coherences. However, we have not been able to directly observe these processes to date, and they are beyond the description of conventional models.

High-repetition-rate soft X-rays from LCLS-II enable dynamic molecular reaction microscope techniques that will directly map charge distributions and reaction dynamics in the molecular frame. LCLS-II-HE will image dynamics at the atomic scale via hard X-ray scattering and coherent diffractive imaging (CDI) to reveal the coupled behavior of electrons and atoms with unprecedented clarity. New nonlinear X-ray spectroscopies offer the potential to map quantum coherences in complex chemical environments in an element-specific way for the first time.

Grand-challenge science areas addressed:
- Control Matter at the Level of Electrons
- Emergent Properties from Complex Electronic and Atomic Correlations
- Master Energy and Information on the Nanoscale

Catalysis, Photocatalysis, Environmental & Coordination Chemistry

A deeper understanding of the fundamental processes in catalysis, photocatalysis, and interfacial chemistry is essential for directed design of new systems for chemical transformations, energy storage, and solar energy conversion that are efficient, chemically selective, robust, and based on Earth-abundant elements.

LCLS-II and HE will reveal the critical (and often rare) transient events in these multistep processes, from light harvesting to charge separation, migration, and accumulation at catalytically active sites. Time-resolved, high-sensitivity, element-specific scattering and spectroscopy enabled by LCLS-II will provide the first direct view of atomic-scale chemical dynamics at interfaces, making it possible to pinpoint where charge carriers are lost (within a molecular complex or device) — a crucial bottleneck for efficient solar energy conversion. The penetrating capability of hard X-rays will probe operating catalytic systems across multiple time and length scales. The unique LCLS capability for simultaneous delivery of hard and soft X-ray pulses opens the possibility to follow chemical dynamics (via spectroscopy) concurrent with structural dynamics (substrate scattering) during heterogeneous catalysis. Time-resolved hard X-ray spectroscopy with high fidelity, enabled by LCLS-II-HE, will reveal the fine details of functioning biological catalysts (enzymes) and inform the design of artificial catalysts and networks with targeted functionality.

Grand-challenge science areas addressed:
- Beyond Ideal Materials and Systems
- Mastering Hierarchical Architectures in Matter Beyond Equilibrium
- Imaging Matter across Scales
- Data, Algorithms and Computing

Emergent Phenomena in Quantum Materials

There is an urgent technological need to understand and control the exotic quantum-based properties of new materials – ranging from superconductivity to ferro-electricity to magnetism. These properties emerge from the correlated interactions of the constituent matter components of charge, spin, and phonons, and are not well described by conventional band models that underpin present semiconductor technologies.

Fully coherent X-rays from LCLS-II will enable new high-resolution spectroscopy approaches that will map the collective excitations that define these new materials in unprecedented detail. Ultrashort X-ray pulses and optical fields will facilitate new coherent light-matter approaches for manipulating charge, spin, and phonon modes to both advance our fundamental understanding and point the way to new approaches for materials control. A comprehensive description of the ground-state collective modes that appear at modest energies, 1-100 meV, where modern X-ray sources and spectrometers lack the required combination of photon flux and energy resolution, is critical to understanding quantum materials. High- resolution hard X-ray scattering and spectroscopy with LCLS-II-HE at close to the Fourier limit will provide important new insights into the collective modes in 5d transition metal oxides – where entirely new phenomena are now being discovered, owing to the combination of strong spin-orbit coupling and strong charge correlation. The ability to apply transient fields and forces (optical, THz, magnetic, pressure) with the time-structure of LCLS-II and HE will be a powerful approach for teasing apart intertwined ordering, and will be a step toward materials control that exploits coherent light-matter interaction. Deeper insight into the coupled electronic and atomic structure in quantum materials will be achieved via simultaneous atomic-resolution scattering and bulk-sensitive photoemission enabled by LCLS-II-HE hard X-rays and high repetition rate.

Grand-challenge science areas addressed:

- Emergent Properties from Complex Electronic and Atomic Correlations
- Harnessing Coherence in Light and Matter

Nanoscale Materials Dynamics, Heterogeneity & Fluctuations

The properties of functional materials are often defined by interfaces, heterogeneity, imperfections, and fluctuations of charge and/or atomic structure. Models of ideal materials often break down when trying to describe the properties that arise from these complex, non-equilibrium conditions. Yet, there exists untapped potential to enhance materials performance and create new functionality if we can achieve a much deeper insight into these statistical atomic-scale dynamics. Important examples include: structural dynamics associated with ion transport in materials for energy storage devices and fuel cells; nanostructured materials for manipulating non-equilibrium thermal transport; two-dimensional materials and heterostructures with exotic properties that are strongly influenced by electron-phonon coupling, light-matter interactions, and subtle external stimuli; and perovskite photovoltaics where dynamic structural fluctuations influence power conversion efficiency.

Ultrashort X-ray pulses from LCLS-II will provide element-specific snapshots of materials dynamics to characterize transient non-equilibrium and meta-stable phases. Programmable trains of soft X-ray pulses at high repetition rates will characterize spontaneous fluctuations and heterogeneities at the nanoscale across many decades of time. LCLS-II-HE will open an entirely new regime for time-domain coherent X-ray scattering of both statistical (e.g. XPCS) and triggered (pump-probe) dynamics with high average coherent power and penetrating capability for sensitive real-time, in situ probes of atomic-scale structure. This novel class of measurements will lead to new understanding of materials, and, ultimately, device performance, and will couple directly to both theory efforts and next-generation materials design initiatives.

Grand-challenge science areas addressed:

- Beyond Ideal Materials and Systems
- Mastering Hierarchical Architectures in Matter Beyond Equilibrium
- Imaging Matter across Scales

Biological Function and Dynamics

Biological function is profoundly influenced by dynamic changes in protein conformations and by interactions with molecules and other complexes — processes that span many decades in time. Such dynamics are central to the function of biological enzymes, cellular ion channels composed of membrane proteins, and macromolecular machines responsible for transcription, translation and splicing, to name just a few examples. X-ray crystallography at modern synchrotrons has transformed the field of structural biology by routinely resolving simple macromolecules at the atomic scale. LCLS has already demonstrated a major advance in this area by resolving the structures of macromolecules that were previously inaccessible by using the new approaches of serial nano-crystallography and 'diffract before destroy' with high peak power X-ray pulses.

The high repetition rate of LCLS-II portends another major advance by revealing biological function through its unique capability to follow the dynamics of macromolecules and interacting complexes in real time and in native environments. Advanced solution scattering and coherent imaging techniques will characterize the conformational dynamics of heterogeneous ensembles of macromolecules – both spontaneous fluctuations of isolated complexes and those initiated by the presence of specific molecules, environmental changes, or by other stimuli.

At high repetition rates, serial femtosecond crystallography (SFX) will advance to address some of the most pressing challenges in structural biology for which only very limited sample volumes are available (e.g. human proteins); or only very small crystal sizes can be achieved (<1 μm); or where current structural information is significantly compromised by damage from conventional X-ray methods (e.g. redox effects in metalloproteins). In all of these cases, high throughput and near- physiological conditions of room temperature crystallography will be qualitative advances. X-ray energies spanning the Se K-edge (12.6 keV) will further enable de novo phasing via molecular replacement and anomalous scattering. Time-resolved SFX and solution SAXS will advance from present few-time snapshots of model systems at high photolysis levels to full time sequences of molecular dynamics that are most relevant for biology. Hard X-rays and high repetition rates will further enable advanced crystallography methods that exploit diffuse scattering from imperfect crystals, as well as advanced solution scattering and single particle imaging methods to map sample heterogeneity and conformational dynamics in native environments.

Grand-challenge science areas addressed:

- Imaging Matter across Scales
- Characterize & Control Systems away from Equilibrium
- Data, Algorithms and Computing

Materials in Extreme Environments

Studies of extreme materials are important for fusion, fission and aerospace materials applications and provide important insights into planetary physics and geoscience. The unique combination of capabilities from LCLS enable high-resolution spectroscopic and structural characterization of matter in extreme states that is far beyond what is achievable by other means. High peak brightness combined with high repetition rates and high X-ray energies are required to: (i) penetrate dynamically heated dense targets and diamond anvil cells (DAC), (ii) achieve high signal-to-noise data above the self-emission bremsstrahlung background, (iii) probe large momentum transfers on atomic scales to reveal structure and material phases, and (iv) measure inelastic X-ray scattering with sufficient energy resolution and sensitivity to determine the physical properties of materials.

Grand-challenge science areas addressed:
- Characterize & Control Systems away from Equilibrium
- Beyond Ideal Materials and Systems
- Pursuit of Fusion Energy

1.2 Target key national priorities

Key national priorities to achieve climate and economic competitiveness goals are outlined in a 2022 report: *U.S. Innovation to Meet 2050 Climate Goals: Assessing Initial R&D Opportunities*, and in a 2023 report: *The U.S. National Blueprint for Transportation Decarbonization*. These priorities are further reflected in the DOE's Energy Earthshots initiative which integrates program development and execution across the basic energy sciences and energy technology offices of DOE to achieve ambitious goals for abundant, affordable, and reliable clean energy solutions – achievable within the next decade.

It is further recognized that persistent innovation and ongoing advances in fundamental research provide an essential foundation for addressing some of the most pressing challenges facing the U.S. over the next several decades. Similarly, U.S. national health priorities and bio-preparedness plans rely prominently on foundational science for biohazard identification, disease prevention treatments, interventions, and cures.

The solutions to many important challenges – such as developing sustainable sources of energy, revolutionary microelectronics, mitigating environmental and climate problems, creating new green technologies, and developing precision medical therapies – depend on a transformation in our predictive understanding and ability to control complex matter, materials and devices, at the atomic scale, and on the fundamental timescales that determine functionality.

This informs the LCLS strategy, as outlined below. In each area, LCLS seeks to galvanize multi-investigator, multi-disciplinary teams to address the key challenges, providing long term access to beamtime, coordinated use of offline sample synthesis and preparatory studies, and directed development of new instrumentation and data analytic solutions.

Clean Energy

The global commitment to transform the energy economy requires many parallel advances to be achieved and continually improved. A key element is the development of new materials and devices with goals that include: (1) efficient use of solar and thermal energy to drive chemical processes for creating renewable fuels; (2) the generation of clean hydrogen using renewable energy and feedstocks; (3) efficient and scalable processes for carbon capture and storage associated with legacy fossil fuels; (4) invention of efficient, durable, recyclable materials for photovoltaics and energy storage systems; (5) development of advanced nuclear processes (fission and fusion) and associated confinement of hazardous materials and high surety treatment of waste.

The LCLS strategy to contribute to meeting these challenges is to drive qualitative advances in our understanding and ability to control excited state photo-chemistry, catalysis, complex chemical transformations, and non-equilibrium chemical processes. One illustrative example is the natural process of photosynthesis – solar-driven water-splitting and CO_2 uptake to create oxygen, and hydrocarbons – the original source of all fossil fuels on Earth. A much deeper understanding of these processes will lead to the development of design principles for artificial or chemical-synthetic approaches to harness solar energy to drive chemical transformations to create fuels from renewable sources. A second general example is the broad class of biological catalysts, enzymes, that accelerate chemical reactions and thereby sustain life. Enzymes achieve remarkable reaction rates and selectivity, while operating at ambient temperatures and exploiting earth-abundant elements. A much deeper understanding of how enzymes function will inform design principles for synthetic catalysts that are efficient, chemically selective, and use earth-abundant elements to drive chemical transformations for clean energy.

Sustainability

Pressing challenges in the area of sustainability include addressing a wide range of extractive, environmentally harmful, and energy-intensive industrial processes. Examples are the need to electrify and decarbonize the production of concrete, steel, and ammonia; mitigate and ameliorate climate-altering atmospheric methane and CO_2; address the pollution and waste remediation of industrial chemical and nuclear processes; and invent new processes for scalable desalination of cleanup of water supplies.

The LCLS strategy is to contribute fundamental new knowledge on the structural dynamics of chemical reaction pathways, and to explore how they can be directed toward desired outcomes. Ultrafast X-rays are a powerful tool for instantaneously capturing this information with element specificity, atomic resolution and under operating conditions - at sufficient precision to inform the development of new theory and simulation methods for a predictive understanding of chemical transformations. One key example is the study of catalysts that are simultaneously energy efficient, chemically selective (desired without unwanted waste products), durable (robust or reusable over millions of cycles), and scalable (based on earth-abundant elements).

A long-standing goal in this area is to direct chemical transformations in molecular and material systems driven far from equilibrium. Key examples include the chemistry of living systems, the flow of gasses and liquids through catalytic media at high temperatures and pressures, and light-driven photochemical processes for solar fuels and chemical synthesis.

Microelectronics, Computing and Communications

The 20th century revolution in computing, communications, and microelectronics is largely based on our mastery of semiconductor technology, based on foundational models of single-electron band structure. As we rapidly approach the fundamental limits of semiconductor technology (e.g. in speed, size, thermal power density, etc.), the most promising basis for 21st century technology applications are quantum materials – which exhibit powerful “emergent” properties such as high-temperature superconductivity, colossal magnetoresistivity, and topologically protected phases. Such properties are referred to as emergent because they cannot be understood or predicted based on a reductionist approach that considers only the constituent particles. Rather, we must also account for the strong coupling between these particles at the quantum level, and this extra complexity pushes the limits of our understanding. This knowledge gap prevents us from fully harnessing the emergent properties of quantum materials in order to address the technology applications that are at the frontier of modern electronics: from quantum information processing, to superconducting electrical grids, to nano-device engineering, and the transition from GHz-rate technologies to THz and even PHz levels.

The LCLS strategy is focused on transforming our fundamental understanding of quantum materials systems and processes, and to develop methods to provide directed control to sculpt desired behaviors. This is to be achieved by making use of the XFEL’s coherence and time-resolution to directly measure the formation, fluctuations and evolution of emergent systems; to make use of the unprecedented spectral flux of LCLS-II and -HE to provide unambiguous information on the interactions between spin, charge, orbital and lattice modes; and to couple the XFEL to ultrafast laser sources (e.g., THz) to drive tailored responses.

An additional area of focus is to use the unprecedented time-averaged X-ray flux of LCLS-II-HE to greatly reduce the time required to obtain nm-resolution 3D tomographic images of semiconductor devices - potentially shortening the time from months to hours for key systems.

Human Health

U.S. national health priorities for bio-preparedness, understanding and prevention of disease, and the development of precision medical therapies all rely on a much deeper understanding of how biological complexes and systems interact and function under physiological conditions. A complete understanding of the function of biological systems requires methods and investigations spanning many orders of magnitude in length-scales and time-scales: from top-down systems-biology approaches to bottom-up structural and molecular biology methods.

A major historical focus of structural and molecular biology has been to investigate the static (equilibrium) atomic-scale structures of biological macromolecules, typically from cryogenically-cooled crystalline samples, in order to infer function. However, living systems operate far from equilibrium, and the function of biological systems are profoundly influenced by changes in molecular conformation that span many decades in time (~psec to msec), and are triggered by subtle changes in local environment or molecular interactions.

The LCLS strategy is to target important knowledge gaps that limit our ability to understand, predict, and manipulate biological systems for crucial applications in human health, such as:

How do structural and molecular dynamics enable the remarkable function of biological systems?

How can we capture and characterize these dynamics at high fidelity (without damage) and in near-physiological conditions?

How are the structural dynamics triggered or mediated by the local chemical environment, temperature, pH, or interaction with small molecules or other external stimuli?

How can we link structural dynamics (and relevant rare events) to biological function in a quantitative way to drive the development of predictive models of therapeutics for human health, bio-energy applications, and environmental sustainability?

Goal 2: Drive step-changes in source and facility performance

The objectives of this strategic goal are to derive and deliver the facility performance requirements and the step-changes in capability needed with LCLS-II, HE and MEC-U to achieve the scientific goals declared above. This focuses on the major projects (Objective 2.1) and the associated capabilities to provide a world-leading user facility (Objective 2.2)

2.1 Design and deliver major facility upgrades to transform the XFEL field

2.1.1 LCLS-II: Deliver kHz-MHz CW capabilities

The LCLS-II Project (2013-2023) responds to the above scientific drivers by:

- Increasing the repetition rate from 120 Hz to 1 MHz (by adding a 4 GeV superconducting linac, capable of supporting a continuous stream of X-rays with variable repetition rate).
- Providing two tunable sources of X-rays (via two new variable gap undulators).
- Enabling access to an intermediate X-ray energy range (2 – 5 keV) for studies of strategically important new materials, chemical catalysis and biological processes.
- Supporting the latest seeding technologies to provide fully coherent X-rays (at the spatial diffraction limit and near the temporal transform limit).
- Maintaining the original copper-based warm linac to extend the operating range of the facility from its prior limit of ~12.8 keV to ~25 keV (at 120 Hz).
- Allowing a factor ~2 increase in experimental capacity.
- Partnering with LCLS Operations to deliver a suite of new instruments and associated experimental systems, as described in Appendix 2.

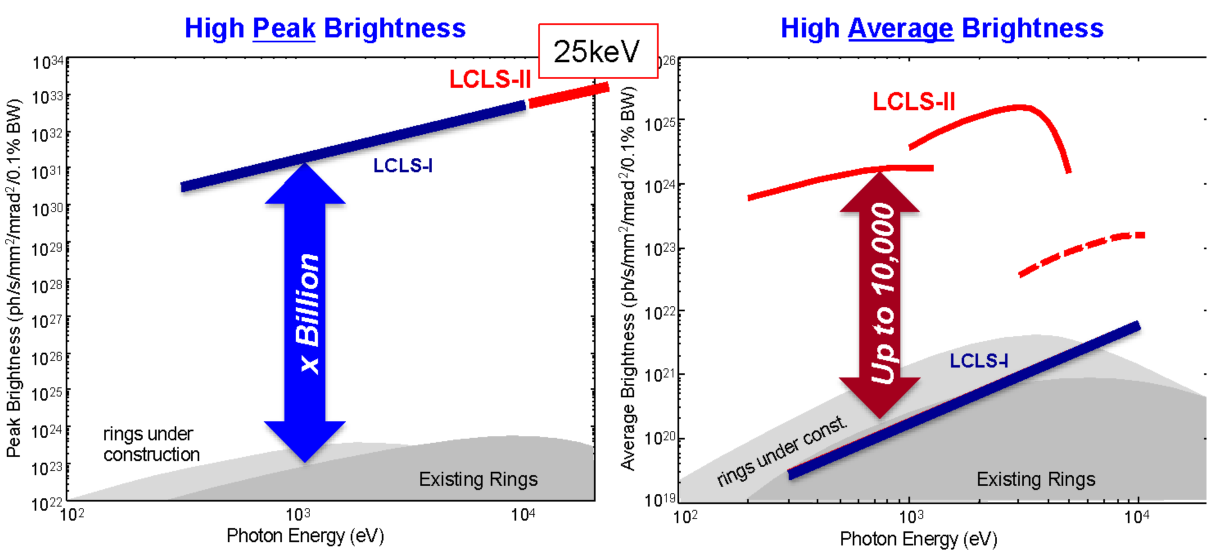


Figure 9 Performance of the LCLS-II upgrade, comparing prior performance (in blue) with the enhanced capabilities (in red; with the 3rd harmonic shown as a dotted line)

The LCLS-II Project was led by SLAC in collaboration with four other DOE national laboratories: Argonne, Berkeley Lab, Fermilab, Jefferson Lab, and Cornell University, and with substantial technical input and advice from international colleagues at DESY, European XFEL and CEA. Commissioning of the fully integrated facility started in mid-2023, with initial operation to the instruments at 33 kHz, rising to full performance over the subsequent years (Figure 9).

2.1.2 LCLS-II-HE: Extend the CW capabilities into the hard X-ray regime

LCLS-II-HE will provide a qualitatively new capability, delivering ultrafast atomic resolution at high average power. The project extends operation of the high-repetition-rate beam into the critically important "hard X-ray" regime (>5 keV) that has been used in more than 75% of LCLS experiments to date, providing a major leap in performance to the broadest cross-section of the user community. The energy reach of LCLS-II-HE, shown in Figure 10, will enable the study of atomic-scale dynamics with the penetrating power and pulse structure needed for *in situ* and *operando* studies of real-world materials, functioning assemblies, and biological systems.

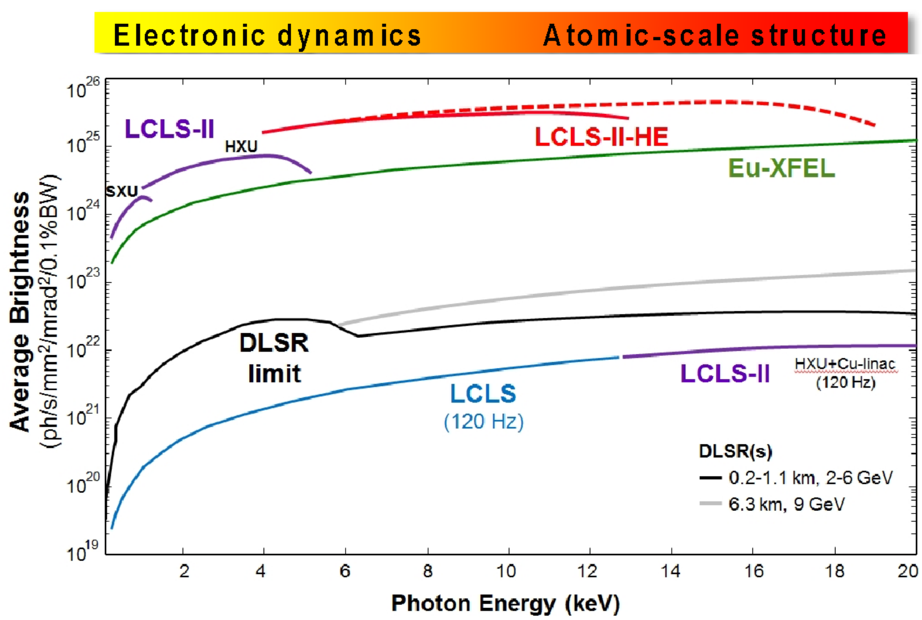


Figure 10 The predicted performance of LCLS-II-HE is shown in red, with the solid line based on a beam with present-day emittance, and the dotted line for expected improvements.

LCLS-II-HE will:

- Deliver two to three orders of magnitude increase in average spectral brightness beyond any proposed or envisioned diffraction-limited storage ring (DLSR).
- Provide temporal coherence for high-resolution spectroscopy near the Fourier transform limit with more than 300-fold increase in average spectral flux (ph/s/meV) for high-resolution studies beyond any DLSR.
- Generate ultrafast hard X-ray pulses in a uniform (or programmable) time structure at a repetition rate of up to 1 MHz – a qualitative advance beyond the burst-mode nature of

the European-XFEL, and a 100,000-fold improvement in temporal resolution compared to storage ring sources.

- Enable the buildout of a new and upgraded suite of instruments to take advantage of these new source characteristics.

To achieve this, the LCLS-II-HE project will add 23 cryomodules with enhanced performance, doubling the electron beam energy from the superconducting accelerator to 8 GeV and making use of the existing cryogenic cooling capacity and space within the linac tunnel. It will upgrade the soft X-ray undulator to enable operation at 8 GeV alongside the hard X-ray undulator, and will add the option of a new superconducting gun to provide low emittance for the highest energy reach. Over this period, LCLS will upgrade or replace 5 X-ray instruments to take full advantage of the new source from the earliest opportunity (see below).

The facility will take advantage of the myriad beam-sculpting techniques developed on LCLS, including bandwidth control via seeding, multi-pulse operation, and delivery of the 3^{rd} harmonic (opening up new areas of science in the energy range 20 to 50 keV).

The scientific impact of LCLS-II-HE is enabled by a suite of unmatched technical attributes:

I. **Access to the energy regime above 5 keV**: This allows analysis of key Earth-abundant elements in addition to providing atomic resolution, as needed for large-scale deployment of photocatalysts for electricity and fuel production; it allows study of strong spin-orbit coupling that underpins many aspects of quantum materials; and it reaches the biologically important selenium K-edge.

II. **High repetition rate, ultrafast hard X-rays** will reveal coupled atomic and electronic dynamics in unprecedented detail. Advanced X-ray techniques will simultaneously measure electronic structure and subtle nuclear displacements at the atomic scale, on fundamental timescales (femtosecond and longer), and in operating environments that require the penetrating capabilities of hard X-rays and the sensitivity provided by high repetition rate.

III. **Temporal resolution**: LCLS-II-HE will deliver coherent X-rays on the fastest timescales, opening up experimental opportunities that were previously unattainable due to low signal-to- noise from LCLS (at 120 Hz) and that are simply not possible on non-laser sources. The typical limit for synchrotron sources is ~100 ps (100,000 fs), whereas the performance of LCLS has progressed from initial pulse durations of 300 fs down to 0.5 fs, coupled to the capability for double pulses with independent control of energy, bandwidth, and timing.

IV. **Temporal coherence**: Control over the XFEL bandwidth will be a major advance for high- resolution inelastic X-ray scattering and spectroscopy in the hard X-ray range (RIXS and IXS). The present scientific impact of RIXS and IXS is substantially limited by the available spectral flux (ph/s/meV) from temporally incoherent synchrotron sources. LCLS-II-HE will provide more than a 300-fold increase in average spectral flux compared to synchrotron sources, opening new areas of science and exploiting high energy resolution and dynamics near the Fourier transform limit.

V. **Spatial coherence**: The high average coherent power of LCLS-II-HE in the hard X-ray range, with programmable pulses at high repetition rate, will enable studies of spontaneous ground-state fluctuations and heterogeneity at the atomic scale from μs (or longer) down to fundamental femtosecond timescales using powerful time-domain approaches such as X-ray photon correlation spectroscopy (XPCS). LCLS-II-HE capabilities will further provide a qualitative advance for understanding non-equilibrium dynamics and fluctuations via time-domain inelastic X-ray scattering (FT-IXS) and X-ray Fourier-transform spectroscopy approaches using Bragg crystal interferometers.

VI. **Structural dynamics and complete time sequences**: LCLS achieved early success in the determination of high-resolution structures of biological systems and nanoscale matter before the onset of damage. X-ray scattering with ultrashort pulses represents a step-change in the field of protein crystallography. An important scientific challenge is to understand function as determined by structural dynamics – at the atomic scale (requiring ~1Å resolution) and under operating conditions or in physiologically relevant environments (e.g. aqueous, room temperature). The potential of dynamic pump-probe structure studies has been demonstrated in model systems, but the much higher repetition rates of LCLS-II-HE are needed in order to extract complete time sequences from biologically relevant complexes. Here, small differential scattering signals that originate from dilute concentrations of active sites and low photolysis levels are essential in order to provide interpretable results.

VII. **Heterogeneous sample ensembles and rare event**s: The high repetition rate and uniform time structure of LCLS-II-HE provide a transformational capability to collect 10^8–10^{10} scattering patterns (or spectra) per day with sample replacement between pulses. By exploiting revolutionary advances in data science (e.g. Bayesian analysis, pattern recognition, manifold maps, or machine learning algorithms) it will be possible to characterize heterogeneous ensembles of particles or identify and extract new information about rare transient events from comprehensive data sets.

2.1.3 MEC-Upgrade: Deliver a revolutionary HED plasma science platform

The field of fusion science and High Energy Density (HED) plasma science performed at the Matter in Extreme Conditions (MEC) instrument requires high pulse energy and high peak power lasers. The current MEC instrument has two mid-scale laser systems: a temporally-shaped, nanosecond laser system that fires at one shot per few minutes with a pulse energy of 100 J / 10ns; and a Ti:S, high intensity, femtosecond laser system delivering 30-100 TW peak power at 5 Hz.

LCLS engaged in extensive community outreach through workshops and direct interactions to identify the areas of scientific opportunity and the corresponding “flagship experiments” that are desired to be performed over the coming decade and beyond. This has demonstrated a broad-based need for an upgrade that combines three sets of beams: a high-power short pulse laser (1 Petawatt at ~150J / 150fs / 10 Hz); a kilojoule-scale shaped long-pulse laser, and the LCLS X-ray laser. Some of the driving areas of science are listed in the table below.

Category	Key Science	Experimental Configuration
Relativistic Laser-Matter Interactions	Relativistic collisionless shocks; plasma instabilities; ion acceleration mechanisms; relativistic transparency; Gbar plasmas	$>10^{21}$ W/cm^2 target irradiation
	Plasma mixing, ion stopping, atomic physics. Secondary radiation sources to enable fusion material studies (damage cascades / accumulation).	X-rays probe plasma conditions; Secondary sources enable fusion material science on secondary targets
HED Laser Plasmas	Re-shock instabilities; microphysics in turbulence; magnetic interactions; HED plasma flows and turbulence	SPL drives target directly, ion source, or magnetic coil 1 kJ laser transverse to X-rays
Compressed matter	Phase transition kinetics; void collapse; microstructure; planetary interior conditions; ICF ablators	SPL from side 1 kJ laser along X-ray direction;
	Equation of state of WDM; dense plasma atomic physics	High repetition rate 200 J @ 2ω for faint signal accumulation

High-peak-power and high energy laser facilities provide a versatile set of tools for creating plasmas under extreme conditions. When focused to a small spot, ultrashort laser pulses with Petawatt (PW) power deliver light pressure in the gigabar regime and create electric fields high enough to strongly ionize matter and drive electrons to ultra-relativistic speeds. These interactions can also be harnessed to produce bright pulses of particles that can be used to volumetrically heat matter to dense, strongly coupled plasma states, or to produce radiation damage in materials of interest. A tailored high-energy laser can drive shocks in materials to access densities much higher than solid. While creation of such conditions can be achieved today at a handful of laser facilities around the world, the high-energy-density states they generate are difficult to characterize in a quantitative manner using the tools available to them.

To address this, a laser facility with high-power, high-intensity beam parameters that is co-located with hard X-ray laser probing capabilities (i.e. with an X-ray wavelength that allows atomic resolution) will provide the required diagnostic capabilities for fusion discovery science and related fields, with representative areas listed in the table below. This co-location enables novel pump-probe experiments with the potential to dramatically improve our understanding of the ultrafast response of materials in extreme conditions, e.g., found in the environment of fusion plasmas, astrophysical objects, and highly stressed engineering materials.

Recent work at LCLS has also demonstrated exquisite ultrafast measurements of the material structural response to radiation, but higher flux sources of deuterons, neutrons and gamma rays are needed to properly emulate the environment and physics processes that occur in materials next to fusion plasmas. An upgrade to PW- and kJ-scale laser systems holds the potential to validate inter-atomic potentials in molecular dynamics simulations of materials to enable long-term predictions of the material behavior in fusion facilities.

The ‘mission need’ (Critical Decision 0) for this type of facility was approved by DOE Office of Fusion Energy Sciences (FES) in January 2019. To meet this mission need, an entirely new facility will be constructed, as shown in Figure 11, to deliver the following key characteristics:

- Independent underground cavern east of the FEH
- Laser systems
  - High rep-rate short pulse: 10 Hz, 150 J, 150 fs, 1 PW
  - High rep-rate long pulse: 10 Hz, 200 J @ 2ω @ 10ns; programmable pulse shape
  - High energy long pulse: > 1 kJ @ 2ω or 3ω @ 10ns; programmable pulse shape
  - LCLS XFEL (5 to 45 keV)
- X-ray + laser target chamber
  - Beam delivery for a combination of the above laser systems and X-rays
  - Optimized to serve a broad plasma physics community (high throughput, rapid reconfiguration, range of illumination geometries and diagnostics)

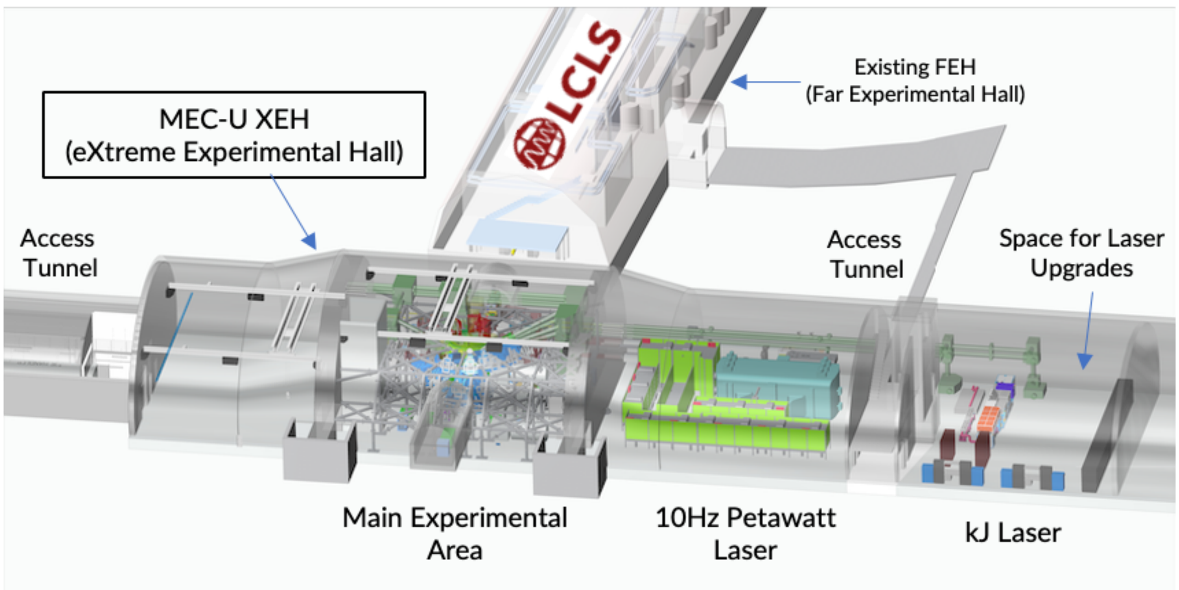


Figure 11 Schematic of the design concept for the upgraded MEC facility, showing two target chambers in a new experimental cavern to the east of the Far Experimental Hall

2.2 Develop and deliver transformative capabilities for the MHz XFEL era

A primary hallmark of the LCLS strategy is to ensure balanced and self-consistent development of the component technologies that make up the integrated user facility - driving investment where needed to ensure that the boundaries of facility performance are optimally advanced. This section outlines the strategy for each major technical area, with the cadence of delivery set by the integrated needs of the facility to deliver to the science drivers listed above and emerging priorities from the user community. At a high level, there is particular strategic focus on development and integration of the following:

- Delivery of new instrumentation to take advantage of the leap to kHz-MHz rates with LCLS-II and subsequently LCLS-II-HE.
- Instantiation of new XFEL modes, such as attosecond timescale pulses, dual-pulse / multicolor delivery, and next generation modes such as cavity-based amplifiers.
- Optimization of accelerator and beamline performance via detailed Start-2-End modeling and AI/ML models to provide timely feedback
- Co-design of detectors, intelligent data reduction, and real-time analysis to cope with the leap to high repetition rate that results in near-TB/s data velocity.
- Development of differentiating sample synthesis, delivery and environmental controls.
- Effective use of the existing hard X-ray instrument suite (XPP, XCS, MFX, CXI, MEC) and the MeV-UED instrument in the period leading up to LCLS-II-HE and MEC-U.

2.2.1 Instruments and experimental techniques for LCLS-II

Details are provided in Appendix 2 of the new instrument suite for LCLS-II (TMO, qRIXS, ChemRIXS and TXI). These are now largely designed and either in service or in an advanced state of delivery. As such, the strategy is set and the task now turns to the tactics of delivery and integration into the user program.

2.2.2 Instruments and experimental techniques for LCLS-II-HE

The instrument development program to meet the scientific goals for LCLS-II-HE is under active development, with recent progress and future ideas discussed at community workshops[8]. The plans are to introduce:

- **DXS-HE**: A dynamic X-ray scattering instrument to transform our understanding of classical and quantum materials, condensed matter chemistry and amorphous materials, studying:
  - Characterization of collective modes of metastable materials phases (e.g. via laser/field manipulations & other transient stimuli)
  - Characterization of complex materials in the critical energy resolution range ~2-25 meV (~kT)
  - Materials heterogeneity and spontaneous fluctuations

[8] See, for example: https://portal.slac.stanford.edu/sites/conf_public/lclsiihe2018/Pages/default.aspx and https://events.bizzabo.com/SLAC-UsersMeeting-2020/agenda/session/332876

- **MFX-HE**: A high throughput instrument for biological structural dynamics, to study:
  - Dynamics / kinetics of biological systems in physiologically relevant conditions (~room temperature, solvated, damage free), including fast mixing systems, enzymology and optogenetics.
  - Measurements of conformational heterogeneity and evolution over near-equilibrium dynamic landscapes.
  - Mapping of rare events and transient states.
- **CXI-HE**: A versatile tool for high sensitivity dynamics, to study:
  - Gas phase photochemistry for excited state systems on the fastest timescales.
  - Chemical and structural dynamics of key (bio)chemical systems, small unit-cell materials, and weakly-scattering proteins.
- **XPP-HE**: An upgrade to make the leap to 100 kHz pump/probe studies, enabling:
  - Incorporation of currently unattainable measurements such as RIXS, REXS, femtosecond ultrafast microscopy, and coherent scattering and imaging.
  - Flexibility and versatility to serve as a test bed for developing new methodologies, technologies, and applications.
- **TXI-HE**: An extension of the LCLS-II capability to expand the photon energy reach from tender to hard X-rays, enabling:
  - Spectroscopy, coherent scattering, nonlinear X-ray science, and a unique combination of soft and hard X-ray FELs for a wide range of dual-beam studies.

The strategy for this instrument suite is to ensure flexibility to emerging lessons from the early LCLS-II era; design for ambitious performance expectations; optimize the instrument design and layout of the Far Experimental Hall based on the extensive experience of the first LCLS era; and deliver in as timely a manner as possible after first light from LCLS-II-HE.

2.2.3 Ultrafast Electron Diffraction (UED)

The MeV-UED instrument, part of the LCLS User Facility, is a powerful "electron camera" for the study of time-resolved, ultrafast atomic & molecular dynamics in chemical and solid-state systems. This instrument has demonstrated the following properties: high spatial resolution (< 0.5 Å), large momentum-transfer range (0.5 to 12 Å-1), high elastic scattering cross sections, high temporal resolution (< 150 fs FWHM), with the additional benefits of relatively large penetration depths (> 100 nm) and negligible sample damage. Its specifications are being actively developed. MeV-UED can field a gas-phase endstation (Figure 12) or a solid-state materials / warm dense matter endstation. An upgrade to kHz operation is planned for 2024.

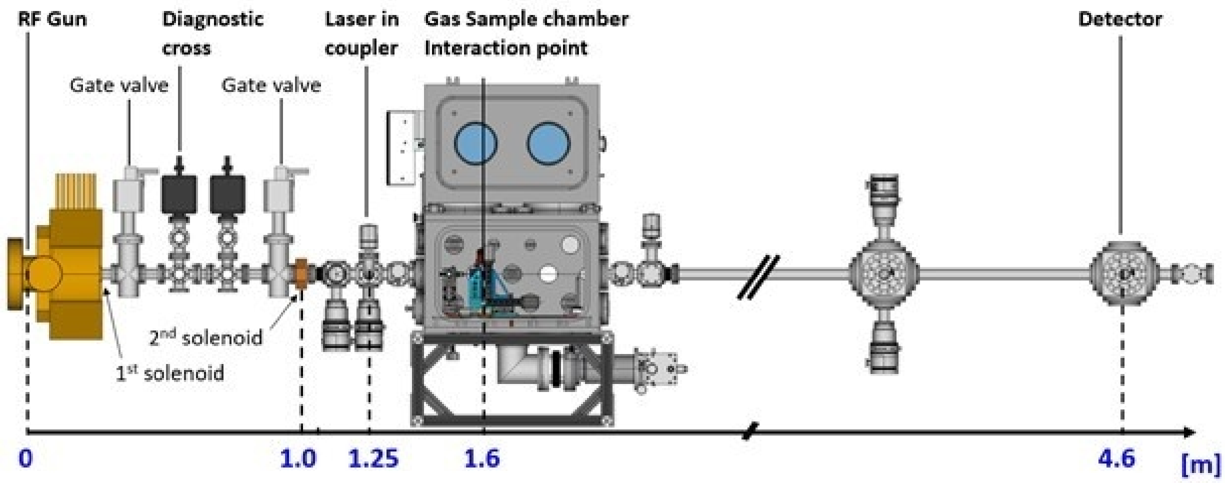


Figure 12 Schematic of the LCLS MeV-UED instrument with gas phase endstation.

The near-term strategy for UED is for a phased R&D approach that includes development of a higher brightness electron source to allow for substantial near-term improvements in time and momentum-space resolution, and preparing for a second user beam line.

User workshops in September 2022 and March 2023 identified three key areas for improvement to keep MeV-UED at the scientific forefront:

1. Improve the instrument sensitivity via increased electron flux and single electron detection.
2. Reduce the instrument time resolution below 150 fs towards a goal of 50 fs.
3. Lower the transverse beam emittance to enable both micro focus and to reach a momentum resolution of $\Delta q = 0.01\ A^{-1}$.

These improvements in the sensitivity – time operation boundary (see Figure 13) would enable hydrogen dynamics to be tracked in photochemistry, both for dissociative reactions and for intramolecular hydrogen transfer. Similarly in microelectronics, enhanced time resolution and sensitivity would allow new understanding of the ultrafast processes governing bi-layer conductivity where processes such as charge transfer are enabled by phonon emission in <100fs timescales. The improvements in transverse emittance would allow access to longer-range electron correlations in quantum materials, going beyond the current 3 nm range, to open new areas such as dynamic Moiré lattice physics in 2D materials. Improved transverse emittance would also enable micro-probe UED allowing the isolation of micron-sized homogeneous regions within complex heterogeneous real-world materials.

Long-range UED strategy

The existing MeV-UED instrument is multi-purpose, with solid state, gas phase, and soon liquid-phase experiment capabilities on offer to users. However, due to the need to swap out instruments and chambers, a single beam line can only accommodate one of these science areas per user run. Upgrades to the existing facility are limited in scope to improvements that are compatible with maintaining a rigorous experiment schedule with high scientific output. The current schedule of user experiments, R&D, and facility maintenance represents a maximal use of the existing single electron source delivery point. Extending substantially beyond this will require one or more additional beam lines operating in parallel with an appropriate diversification of measurement capabilities to better cover a broader array of science drivers. Commissioning of one additional beam line would afford substantial opportunities to include more expansive capabilities that address the scientific needs outlined above.

Finally, incorporation of a superconducting or normal-conducting MHz rep rate RF gun on one or more of these beam lines would leverage ongoing development for LCLS-II-HE while enabling high probe rates with ultra-bright low emittance and low energy spread beams.

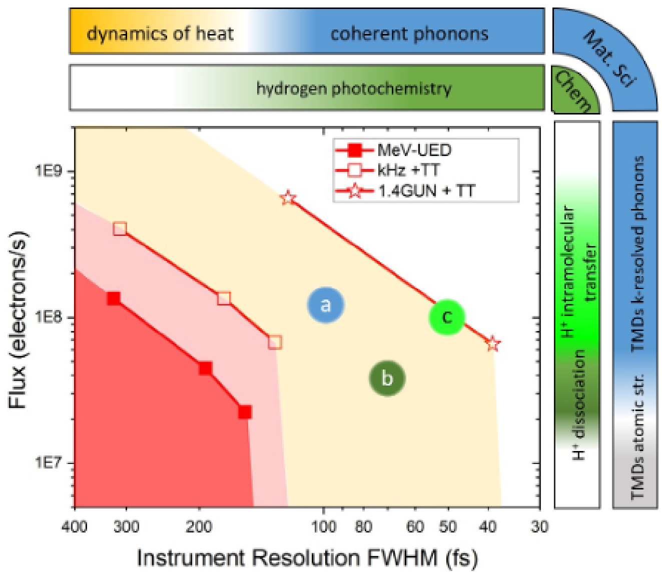


Figure 13 Solid squares & red region show the current MeV-UED flux/time operation boundary. Open squares & light-red region show the projected performance of MeV-UED with 1 kHz operation and a first generation time tool. Open stars & yellow region show the performance of a proposed 1.4 cell gun together with a time tool and pump laser compression.

2.2.4 LCLS Accelerator and FEL systems development

The performance of LCLS has been greatly extended since its initial operation, with an overview provided in a FAQ and performance table. This has been achieved thanks to a vigorous R&D program targeting different areas: from the generation of the shortest possible pulses, to high-brightness seeding modes to basic accelerator developments aiming at improving the electron beam quality.

LCLS can now provide ultrashort pulses (from ~200 attoseconds (as) to >100 femtoseconds (fs)), with unprecedented peak brightness, in SASE or seeded-mode operation, over an energy range from ~250 to ~25,000 eV, at 120 Hz.

Recent highlights include:

- Extension of two-color pump/probe spectroscopy to the sub-fs regime.
- Optimization of GHz multibunch operation with ultrafast kickers.
- Demonstration of the performance of a cold X-ray cavity for future application to a regenerative amplifier and oscillator XFEL modes.

- Generation of sub-fs pulses with a peak power of ~ 1 TW using superradiant cascaded amplification.
- Design of a laser-shaping system to improve the peak brightness of LCLS-II operation and enable pulse duration control down to the sub-fs level.
- Design of a long-period wiggler for the generation of high-power THz pulses.

A core element of the LCLS facility strategy is to maintain the development and deployment of leading-edge capabilities, with rapid transition to the user program. Focus areas are readiness of advanced capabilities for LCLS-II, development of advanced hard X-ray capabilities for LCLS-II-HE, and the development of underpinning technologies for LCLS-X.

A set of strategic drivers defines the various types of development projects**:**

- Projects with immediate relevance to the user science program
- Longer-term high-risk / high-reward R&D
- Conceptual studies for future capabilities
- Basic accelerator and FEL physics to build fundamental understanding and inspire new concepts

The guiding principle of the accelerator R&D program to maximize the scientific productivity of LCLS. This can be realized by projects that have a transformative impact on specific areas of science (e.g. attosecond capabilities) or projects with a broad impact on the science program (e.g. improvements to the beam stability and brightness, seeding schemes etc.).

The conception, prioritization and execution of R&D projects is done in close collaboration with the LCLS Scientific Research Division and the wider FEL user community. Similarly, our accelerator physicists are strongly involved with the LCLS science program and have played leading roles in inhouse and user experiments.

As a result, FEL R&D projects have a strong and measurable impact on the LCLS user science program, with a large fraction of beamtimes taking advantage of advanced R&D capabilities through collaborations between accelerator physicists, instrumentation scientists and users.

The FEL R&D program also offers key opportunities for **education and training** of young staff. The involvement of three Stanford faculty members has led to active and sustained participation of graduate students in our program, with students who have moved on to successful careers in research (both in the DOE system and in the private sector). The DOE SULI program and the LCLS Intern program have provided opportunities for undergraduate students from all over the US to participate in LCLS R&D, with several students moving on to graduate careers in the field.

A description of the strategic research directions for accelerator/ FEL systems is in Appendix 3.

2.2.5 Scientific capabilities for the LCLS user program

In many ways, the most important focus for the LCLS strategy is to ensure a self-consistent approach to the design, development and delivery of the integrated suite of component technology areas - so that optimum use is made of their combination. There is no point having a kHz to MHz XFEL if it cannot be adequately exploited scientifically.

A crucial early step in the facility's strategic planning cycle was to form a single evaluation and prioritization committee for all potential investments using LCLS Operations funds. This "Projects Executive Committee" (PEC) assembles the senior staff from the SLAC Accelerator and LCLS Directorates, with input from the major projects and others as needed. Meeting monthly, the PEC assesses the needs of all developments to deliver a balanced portfolio to support sustainable operations and growth for the facility. This approach grew from the Guiding Principle to "*Treat LCLS as an integrated facility when allocating funding, irrespective of where people sit in the SLAC organization, taking a system-level, facility-wide view of priorities*." The list of project program areas is:

- X-ray Improvement projects (XIP)
- Strategic instrument projects (e.g., L2S-I)
- Accelerator Improvement Projects (AIP)
- Accelerator Small Projects (ASP)
- Operational Improvement Projects (OIP)
- Scientific Initiative Projects (SIP)
- Detector Research and Development (DET)
- Photon Science R&D
- Accelerator Science R&D
- Facilities Infrastructure (FAC)

The details of individual technical strategies are described in Appendix 4 as follows:

1. High power 'optical' (UV to THz) laser systems
2. X-ray optics
3. Sample delivery systems
4. X-ray detectors
5. Real-time automated controls
6. Massive-scale, streaming data systems
7. AI/ML tools

2.3 Plan for a major upgrade to create a third generation XFEL (LCLS-X)

The LCLS ten year anniversary provided the opportunity to assess what aspects of XFEL performance were most impactful, indicating where there was substantial potential for future scientific growth. Alongside this, extensive work has been undertaken to develop the science opportunities for LCLS-II, -HE and MEC-U, drawing from the X-ray and ultrafast communities and from external groups via ‘use-inspired workshops’, DOE PI meetings, and broad outreach.

Many of these scientific drivers need extensive experimental access over a multi-year period to address their ambitious goals. This fact, coupled to the factor 4 to 5 oversubscription for access to LCLS highlights a foundational shortcoming in the nature of the facility - that it is constrained to deliver to just 2 or 3 instruments at a time. Consultation with the user community has shown that the scientific impact of XFELs is heavily affected by scarce and unpredictable access, which also acts to demotivate access by new user groups. The number of potential users far exceeds the worldwide capacity offered by XFEL facilities, even with the recent commissioning of European-XFEL, SwissFEL and PAL-XFEL.

LCLS scientific delivery to date

The mode of operation of LCLS to date has been the deployment of flexible instruments, adapted on a daily to monthly basis, with targeted experiments conducted every few days on a largely one-off basis. This has driven the development of some transformational new experimental techniques, and has led to many high impact ‘proof of principle’ results, but there has only been limited exploitation in the beamtime available (with some exceptions that have a more dedicated configuration, such as structural biology and AMO science).

Recently, the scientific productivity of LCLS was enhanced through the use of ‘standard configurations’, in which multiple user groups can make successive use of an instrument set up in a particular mode. Combined with increased beam multiplexing, the number of experiments increased by ~70% over 2 years. However, the breadth of science that can be performed is inherently limited by the presence of just a single (now dual) undulator source.

Alongside this, a range of new modes of XFEL operation continue to be developed that can provide important leaps in performance, but which would greatly benefit from a dedicated beamline setup. Examples are DELTA (polarization control), XLEAP (attoseconds), RAFEL (high power), XFELO (extreme spectral brightness), superconducting undulators (very hard X-rays).

LCLS-X Facility Concept

Extensive analysis of this strategic context has been undertaken, including many iterative consultations with the LCLS SAC and UEC, the Strategic Programs/Technology Committee (SPC/STC) at Stanford/SLAC, an externally-led review of options in 2019. This was informed by a set of SLAC-funded projects to assemble the primary scientific drivers and potential technical solutions that can deliver multiple dedicated beamline and instrument configurations.

What emerged is a concept known as “LCLS-X”. This takes advantage of the design of the LCLS-II-HE accelerator which has sufficient power to feed up to 10 undulators, each running at the optimum rate of 100 kHz, and which could drive a suite of 20 or more experiments to run simultaneously. A schematic of LCLS-X is shown in Figure 14.

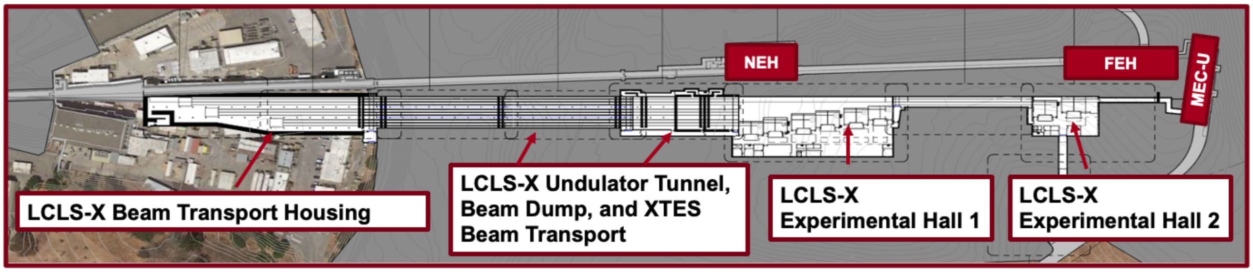


Figure 14 Preconceptual layout of a representative LCLS-X facility in which a suite of X-ray undulators are populated in a newly constructed tunnel to feed a series of new instruments.

LCLS-X would deliver a step-change in XFEL science – a suite of optimized beamlines and instruments (with examples shown in Figure 15(a)) provided to a large user community, allowing full exploitation of each scientific area. This would allow different communities to push instrumentation relevant to their field rather than forced to make compromises. The increased capacity would further permit more innovative experiments, which are not accepted by the proposal panels today because outcome can't be guaranteed.

Operationally, the population of the full set of undulators enabled by LCLS-II will bring XFEL science into a synchrotron-like mode, with a large number of parallel experiments that support a broad critical mass of PI's across the community, and with an associated reduction in cost per experiment - as outlined in Figure 15(b).

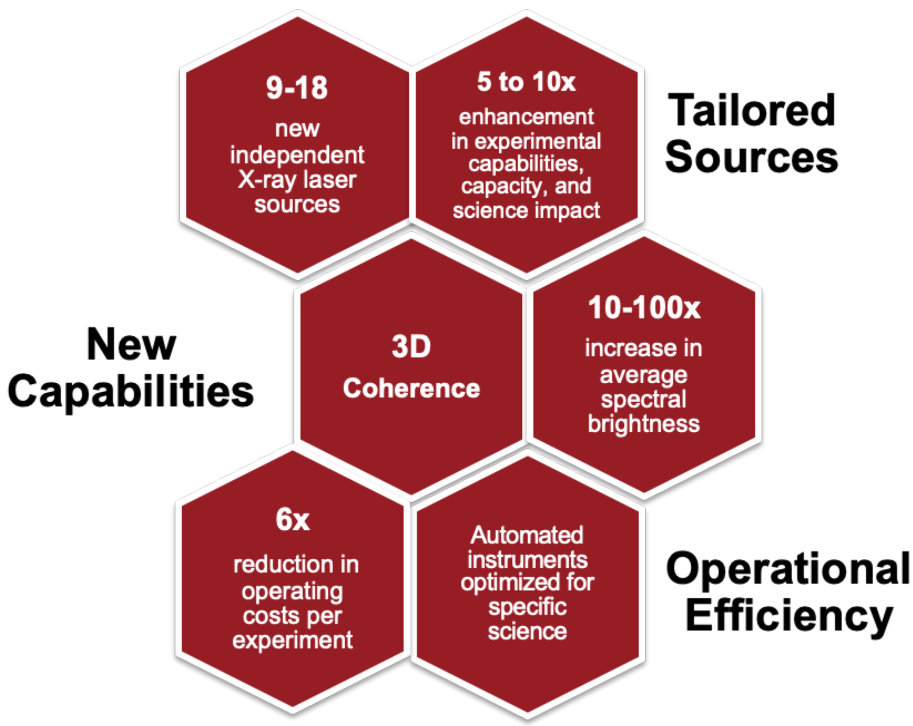


Figure 15(a) Characteristics of the LCLS-X facility and its operational impact on the ability of the user community to access the facility

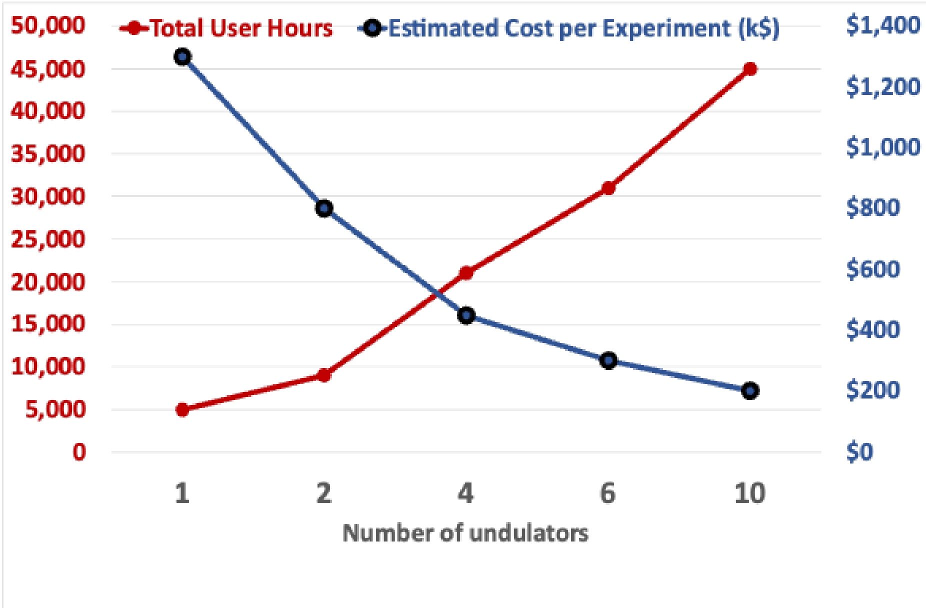


Figure 15(b) Indicative cost scaling for the operation of LCLS-X

Timeliness of design and delivery

LCLS-II is in its early operation phase, with LCLS-II-HE in its procurement and delivery phase. As such, there is a robust understanding of how these systems can be used as a platform for future needs. Internationally, the focus for XFEL-enabled science is shifting from source development to scientific exploitation– pairing dedicated sources with optimized instrumentation at the European XFEL (Germany) and SHINE (China).

Importantly, construction of LCLS-X can be performed alongside operation in the LCLS-II-HE era, since the accelerator platform will already be in place. What is now needed are the additional beamlines and experimental areas, incorporating new FEL capabilities as needed.

With these drivers, the set of strategic goals to motivate and realize LCLS-X are:

(1) Establish a transformative science case and societal impact case for LCLS-X

- This activity builds from the extensive user community engagement to date, from which a subset of ideas were used to define the scientific basis for LCLS-II/HE and MEC-U.
- Many ideas were precluded that required a dedicated beamline and instrumentation, which was inconsistent with the need to retain broad flexibility with the limited number of instruments (and only 2 beamlines) to date. LCLS-X provides the opportunity to address these scientific objectives and so meet the declared needs of the community.
- **A key next task** is to assemble an updated science case - ideally in the context of the broader set of needs for other complementary facilities - to allow a balanced portfolio approach at the DOE level.
- In addition to extensions of the fundamental science and key national priority drivers discussed above, this science case needs to include the wide range of industrially-focused applications for next-generation XFEL facilities. Examples of recently identified industrial impact areas including the following:

(i) Imaging semiconductor chips to detect anomalies and hidden functions
- Enabled by: Unprecedented average flux
- Specialized method: 3D chip-scanning laminography
- Dedicated beamline impact: Extreme stability and ability for continuous scans

(ii) Characterizing and controlling novel functional devices (e.g. sensors, switching)
- Enabled by: Extreme spectral resolution and transform-limited pulses
- Specialized method: Time-resolved IXS for characterization and control of emergent phenomena
- Dedicated beamline impact: In-situ synthesis tools and environmental controls (e.g. cryo, THz, …)

(iii) Understanding and optimizing the fundamentals of industrial chemical synthesis
- Enabled by: High rep rate to sample entire ensembles of nano-catalyst particles
- Specialized method: Combined scattering and spectroscopy
- Dedicated beamline impact: Study industrially relevant samples, which have billions of variants

(iv) Capturing the instant a material fails
- Enabled by: Continuous (CW) pulses (scanning before, during and after failure)
- Specialized method: Coherent scattering (e.g. XPCS)
- Dedicated beamline impact: Time to study unpredictable events such as fracture / failure / breakdown

(v) Directed design of pharmaceuticals
- Enabled by: Extreme brilliance, coupled to high repetition rate
- Specialized method: Coherent diffractive imaging
- Dedicated beamline impact: Rapid-turnaround of new drug targets

(2) Identify the key technical concepts required to deliver LCLS-X

○ **Preconceptual layout options** need to be assessed to identify potential show- stopper barriers, quantify the technical approach and scope, and provide an outline cost and schedule, along with options for the order of construction that enable phasing and best-value. An integrated “point design” is needed that describes a self-consistent layout of electron beam trajectories, FEL sources, beam dumps and instrument areas.

○ **An R&D program** is needed over the next few years that enables timely progress in the design and prototyping of transformative beamline technologies. This includes cavity based regenerative amplifiers (RAFEL), XFEL oscillators (XFELO), superconducting undulators for higher energy, cooled optics for kW-class X-ray beams, and the broad suite of enabling technologies for experimental exploitation (see Goal 2).

○ **The supply chain** needs detailed assessment, particularly where there are domestic supply challenges such as with X-ray mirrors, diffractive optics (particularly diamond crystals), high power lasers, and superconducting technology.

(3) Deliver effective communications on the need for LCLS-X

○ Continued focus is needed to ensure alignment with overall DOE and Congressional priorities, working with BESAC, the LCLS Users Community, and broader national and international perspectives from the National Academies and professional societies.

- Given the pace of change at comparable facilities around the world, timely action is needed to stay consistent with the recommendations of the BESAC International Benchmarking report, "Can the US Compete in Basic Energy Sciences?" A key driver is shown in Figure 16, which maps a substantial emerging disparity in the scale of XFEL capabilities in the US compared to the rest of the world.

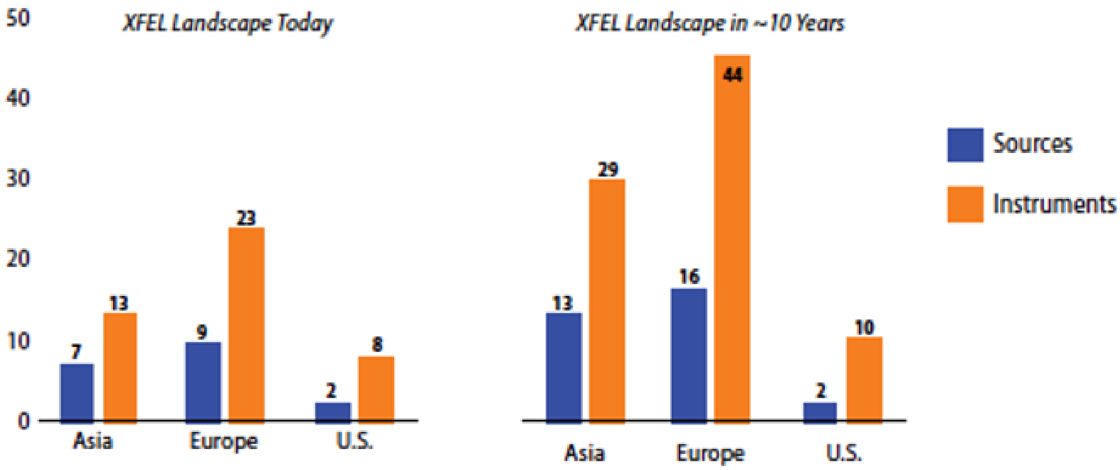


Figure 16 Comparison of the number of independent XFEL sources and instruments at the present time and in ~10 years based on announced projects (from BESAC).

Goal 3: Ensure Mission Success through Operational Excellence

3.1 Maintain safe and secure operations

3.1.1 Implement and update safety policies and practices to meet evolving needs

An overarching guiding principle for LCLS operations is to ensure the safety, health, and mental wellbeing of staff and users. Details of implementation are described elsewhere - in the SLAC Conduct of Accelerator Facility Operations (CAFO), the Accelerator Safety Envelope (ASE), the SLAC Environment Safety and Health (ESH) manual, and derivative documents. At a laboratory level, there are intensive site-wide initiatives to review and improve many policies and procedures for safe working - learning lessons from recent incidents at SLAC and elsewhere, along with a more formalized approach to “high risk / high consequence” activities.

Strategically for LCLS, there is a focus on the integrated approach involving staff and users, given the wide range of hazards, the 24/7 nature of operations, the transient presence of personnel in some areas, and the intensity of time-limited experiments. This drives a proactive approach to continually assess and improve practices, with highlights that include:

- Introduction of “pre-start” reviews ahead of experiments and major activities to solicit input from all team members on the individual and collective readiness to proceed safely. This provides time for all to stop, think, discuss, update, learn and reflect.
- Expansion of the independent safety assurance arm of the LCLS organization to provide enhanced oversight and expertise.
- Allocation of beamtime for formal training and safety pauses in each experimental area on a regular cadence.
- Reduction in the workload on individual staff to help ensure focus and sustainability.
- Emphasis on supervisor and expert presence at the workplace, to lower the barrier for less experienced staff to ask questions, and to rapidly identify off-normal conditions.
- Changes to the LCLS schedule to reduce the number of setup changes and introduce schedule buffers to increase the ability to respond to emerging issues.

3.1.2 Deliver effective capabilities for secure research in targeted areas

LCLS operates in a highly competitive research environment, delivering transformative data to user groups that can often redefine our understanding of the field. As such, it is crucially important to protect access to these data to just the groups authorized by the relevant Principal Investigator. Similarly, data need to be protected for the limited periods where LCLS is used for proprietary industrial access, or potential future research that has other commercial or agency-specific sensitivities. With the transition to LCLS-II, HE and MEC-U, many new user groups will engage, and so it is strategically important to show to these communities that their intellectual property is being protected. LCLS partners with the other BES Light Sources to deliver a consistent approach to this topic, responsive to the relevant DOE Orders.

3.1.3 Promote an open, learning-based culture that engages all staff and the wider community

Core to a culture that fosters open exchange of ideas and concerns is the establishment of a psychologically safe working environment, coupled to building a common understanding of shared values, acting with mutual respect, and enabling the ability to speak out for each other. Psychological safety and respect in the workplace are fundamental to LCLS as a facility and as a community. They are foundations that allow people to feel comfortable to be themselves and communicate openly with their teams, managers, leaders, colleagues and users.

LCLS can present a high stress environment; running 24 hours a day with complex deadlines and priorities. Coupled to this, LCLS as a facility is a large and matrixed organization, bringing together people from all over the world as staff and users. As such, it's inevitable that there will be difficult times, miscommunications, and differences of opinion and approach.

In response, the LCLS strategy has driven the implementation of a series of activities to assess and improve the ability to develop and sustain a welcoming, inclusive, respectful and mutually-supportive culture. LCLS aspires to be the best place in the world to develop as individuals and as a team.

A first step was gathering of data from the staff and users - via workshops, anonymous polls, focus groups (e.g., for women of color at LCLS), and consultations with the Users Executive Committee and others. From this, a prioritized plan has been developed.

In the immediate term, a series of workshops engaging all LCLS staff is underway to discuss SLAC's Core Values and Respectful Workplace commitment and assess how best to translate these into the LCLS workplace - both from the perspective of individuals and as an organization.

These workshops are being designed to help ensure everyone can have a rewarding career in which staff can enjoy and be enriched and enlivened by their time at LCLS. A team of LCLS Culture Champions has been formed to help develop the content and act as a confidential conduit for feedback to/from team members.

This work is coupled to ongoing mechanisms to solicit feedback from users at the level of individual PI's, elected representatives, and in topical meetings (see 3.2.1).

It is also complemented by LCLS support of employee resource groups and community activities, with a focus on "Visibility for All", such as the recent examples of Pride at LCLS:

3.2 Provide world-class user services

3.2.1 Measure and optimize user access and support to maximize scientific impact

LCLS seeks to foster a vibrant research ecosystem, taking advantage of our unified structure within SLAC/Stanford and across the DOE complex. Substantial emphasis is placed on delivery of a "full-service science facility" – with transformative staff input at each stage of the research lifecycle from research ideation to experimental definition to instrument operation, data analysis and interpretation. User beamtime is typically provided for an average of 5 days/week in two 12-hour shifts per day, with up to 5000 hours of user facility access time per year.

The strategy for user access to LCLS is to provide many different modes that are responsive to the evolving demands of an increasingly broad and sophisticated set of user groups:

- **Regular Proposals**: This is the primary access mode, based on investigator-led submission of experiments. Facility time is allocated on a pro-rata basis of the different research fields (subject to facility logistics), with ranking via a set of independent peer review panels. Access calls are typically made every 6-9 months.
- **Rapid Access**: To enable access outside of the usual Run cycle where there is a compelling need for fast turnaround.
- **Data Set Collections**: For limited duration access (typically 1 to 2 shifts) to complete a dataset from a prior experiment, or to take a full set of data for a less complex setup.
- **Protein Crystal Screening**: To assess the viability of using LCLS for new samples.
- **Proprietary**: For confidential industrial access.
- **Scientific Campaigns**: For extensive research programs requiring a series of beamtimes over multiple years, targeting areas where there is great potential for scientific impact from the unique capabilities of LCLS. The topical areas are chosen by the LCLS facility in consultation with its Scientific Advisory Committee, with beamtime limited to 10-15% of the overall time. Campaigns need to be proposed and conducted by a comprehensive research team of experts (e.g. synthesis, experiment, theory, etc.).
- **Director's Discretionary time**: A small fraction (typically 5%, and no more than 10%) of the access time is allocated by the Director to explore high risk/high reward ideas, to open up access to new community, and/or to address potential inequities with regard to community balance and individual circumstances.

Machine Development (MD) Time: Substantial beamtime (typically 1 day / week) is allocated to maintaining peak performance, commissioning new FEL capabilities, preparing complex setups for users, or undertaking exploratory studies in support of accelerator and FEL R&D.

Maintenance: Periods of 2-3 days are allocated each month for preventative and responsive maintenance and installation of new equipment in the accelerator areas in support of a primary DOE metric to run the accelerator with >90% and typically ~95% availability to users.

Complementary facilities: Alongside LCLS beamtime, the strategy calls for coordinated use to be made of the co-located facilities at SLAC (SSRL, UED, Cryo-EM). This includes access to offline science labs, such as in the Arrillaga Science Center (ASC) where LCLS is investing in a suite of ultrafast laser-based beamlines and endstations to provide THz to XUV beams for exploratory studies and sample/technique testing prior to access to LCLS (see Appendix 4.1). This will allow staff and users to make best use of valuable LCLS beamtime, and lower the barrier to entry to XFELs by the table-top laser community. The strategy for the ASC labs is to:

- Allow LCLS staff scientists to remain at the forefront of their fields through collaborations with the external user community;
- Develop new experimental methods, technical capabilities (laser, sample delivery, data, etc.), and instrumentation with clear potential to enhance the science impact;
- Perform demonstration experiments to attract a new user community and/or establish a new area of science where LCLS or MeV-UED will have a significant impact.

Metrics and Assessment

Commentary on the health of the user program is undertaken at an individual experiment level (via “end of run” summaries prepared by each Principal Investigator, and by “shift summaries” prepared by the responsible member of LCLS staff), in which all aspects of the experiment are evaluated - from facility readiness to performance, robustness of the technical and support systems, arising problems and errors, and an assessment of the overall user experience. Statistics are gathered at an aggregate level each year with regards to access time, publications, demographics, financials, scientific use, safety, and user satisfaction. These data are actively reviewed to inform future areas of investment and facility focus.

Input on the health of the user proposal and evaluation processes is undertaken in a feedback session at the end of each Proposal Review Panel (PRP) meeting.

Feedback on the health of the user facility and its interaction with the community is formally undertaken each month via meetings between the LCLS management and the Users Executive Committee, which is an elected body of representative users. There is an annual users meeting, including a Town Hall to field questions from the wider community.

Input from staff is via topical workshops (ranging from major project scope, to operations, to culture), safety pauses, training sessions, and conventional line management feedback.

New metrics are under development in coordination with the other BES Light Sources to better quantify facility operations, user delivery performance, and financial sensitivities. These metrics seek to take account of a range of emerging factors, including: (i) inflation and supply chain cost increases, (ii) the need for enhanced support for hybrid and fully remote operations, (iii) the addition of new and significantly upgraded capabilities, and (iv) the need to address deferred refurbishment and maintenance tasks.

One key new metric being explored is “Utilization”, defined as the ratio of beamtime devoted to user operations and facility commissioning compared to a total that also includes potential beamtime that went unused due to insufficient resources.

3.2.2 Ensure the LCLS review processes are fair and equitable, supported by effective systems

LCLS has put in place a suite of external review activities to help guide and drive the use and development of the LCLS facility. Major elements include the following, ultimately accountable to the LCLS Director:

Strategic scientific and technical programs:

(i) The LCLS **Scientific Advisory Committee** (SAC) and **Users Executive Committee** (UEC) are formally consulted on the identification, selection, and time-phasing of desired capabilities such as new endstations, coupled to strategic advice on new scientific directions (e.g. Campaigns), major facility development projects (e.g. LCLS-II-HE), and key enablers (e.g. data systems and remote access);

(ii) The LCLS SAC performs 6-monthly reviews of whether our R&D programs are suitably prioritized and well matched to enabling high-impact science on LCLS, and whether the approaches being taken are technically sound;

(iii) Specialized sub-committees such as the **LCLS Detector Advisory Committee** (LDAC) provide advice and broad perspective on the development of specific areas;

(iv) Rolling external reviews of each science area and its associated instrumentation ("**Science and Instrumentation Reviews**") are held such that each area is reviewed every 3 years. The reviews are 25% retrospective and 75% prospective, involving existing users and experts from outside the XFEL community;

(v) **Instrument Advisory Panels** (IAPs) for each new endstation are tasked with identifying an appropriate set of scientific requirements and facility performance parameters (akin to KPPs for large projects), along with plans for the early science program and outreach to an appropriate user community.

(vi) Major construction projects (LIC and MIE) have dedicated review processes, consistent with DOE Order 413.3(b), including the use of a **Facility Advisory Committee** (FAC) and **Machine Advisory Committee** (MAC) that review the proposed technical solutions.

Overall strategic direction and fit with DOE and SLAC/Stanford:

(i) Stanford holds a 6-monthly "**science and technology committee** (STC)" review of how LCLS and its associated upgrade projects and scientific research programs are performing, and whether full advantage is being taken of the position of LCLS within SLAC, DOE, and the broader research community;

(ii) DOE-BES runs "**triennial reviews**" of our facility operations, scientific direction and facility development plans. This formal process includes input from our advisory committees and user community as well as from the review team and the DOE program office;

(iii) LCLS seeks community-wide input in the form of regular consultations (e.g. monthly with the Users Executive Committee (UEC) and annually in our users meeting) and informally via annual publication of our facility strategic plan.

Scientific Use of LCLS:

(i) **Proposal Review Panels** (PRP) are held every 6-9 months for prioritization of individual user-defined experiments, involving ~80 experts in 7 topical areas. The PRP is tasked with selecting an appropriate balance of risk, ambition, delivery, new users and breadth of scientific areas. Details of the types of access were provided in section 3.2.1.

(ii) **In-House (staff) access** is prioritized by an internal panel, explicitly balancing career progression opportunities (10% of beamtime) with new capability development (15%).

(iii) **Director's Discretionary beamtime** (~5%), as described above.

Final approval for access is at the discretion of the LCLS Director, based primarily on the peer review input with allocation according to a proposal pro rata model (based on scientific area), coupled to considerations of facility logistics and safe/sustainable operations.

A major task is underway to update the PRP software tools and outreach processes to lower the barrier to entry to new users; underpin efficient and effective external peer review; enable quantitative analysis of each stage of the review process; and ensure traceability of information. A common proposal submission process is being developed by three DOE laboratories (SLAC, Argonne, Brookhaven) and applied to LCLS, APS and NSLS-II.

3.2.3 Deliver effective and impactful internal and external communications

As a relatively new facility with a rapidly-evolving set of capabilities, a growing user community, and major changes in staffing to move into the LCLS-II era, there is a compelling need for targeted and broad-based communications. Key elements of the LCLS comms strategy include:

- **Scientific directions**: Ongoing community engagement via a multi-year, iterative approach to defining and peer-reviewing our priority research directions (see Goal 1).

- **Strategic priorities**: Involvement in DOE (and other agency) workshops and committees to explore how LCLS can contribute to priority topics: via Basic Research Needs, DOE Round Tables, National Academy studies, BESAC/FESAC/ASCAC, etc.

- **User community:** In addition to the wealth of individual and topical contacts, formal mechanisms include:
    - **Monthly meetings** between the LCLS Director and the UEC
    - **Annual Users Meetings**, held jointly with SSRL to maximize engagement, at which there are topical workshops, tutorials for new users, masterclasses, consultations on new instruments, feedback on operations, plenary updates, and Q&A with senior staff.
    - **Town Halls for each User Run**, with the intent to ensure each proposal is well-matched to LCLS capabilities, and to ensure all investigators have access to the same information. These provide information on the latest capabilities, modes of beam operations, constraints, points of contact (especially for new users), and overall Q&A.
    - **3D "Virtual Tours"** of our instrument areas to help experiment planning, design of new equipment, and overall awareness.
    - See 4.1.2 for other mechanisms used to seek expansion of the user community.

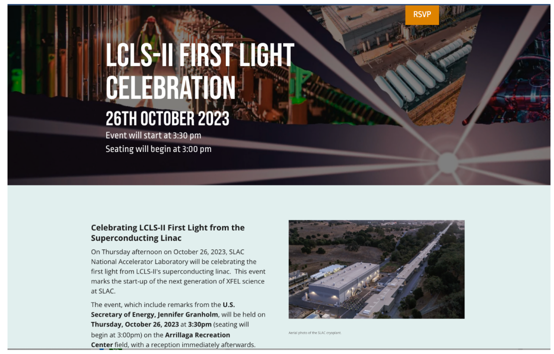
- **Domestic facilities**: Monthly engagement between the 5 Light Sources (see 4.2.1), plus topical contact with other partner facilities such as ESnet, NERSC, LCFs, NSRCs, neutron sources, etc. Extensive participation in each others' reviews and advisory committees.

- **International facilities**: See 4.2.1

- **SLAC/Stanford**: See 4.2.2

- **Pipeline**: See 4.1.2 / 4.1.3 (from high school to undergraduates, graduates, staff and users)
- **Public understanding of science**: Via outreach lectures, "Science at SLAC", engagement in local science festivals, school visits, partnerships and board membership, etc.
- **Congress / government**: Hosting VIP visits, preparing reference material, exhibiting at Congressional events, and responding to staff/member enquiries.
- **Local community**: As a flagship facility, LCLS provides access to regular public tours and community events, with a selection shown below:

- **Staff communications**: Crucial to the effective running of a complex, multi-disciplinary and multi-organization facility like LCLS is an effective flow-down of information and priorities, coupled to efficient feedback mechanisms for staff to raise concerns and suggestions. In addition to the usual line management processes and All Hands meetings, LCLS has driven active use of democratized communication channels (such as SLACK), focus groups, culture workshops, safety pauses, and professional development via engineering schools and on-the-job training days.
- **Celebrating success**: A key element in the LCLS comms strategy is to mark major events with staff and partner celebrations, with examples below of the 10-year event, LCLS-II, and stages in the transformation of the new instrument suite.



- **Social events**: Another purposeful element of the strategy is to arrange regular social interactions to offset the high-intensity, 24/7 nature of LCLS operations and delivery.

3.3 Deliver infrastructure for sustainable operations and growth

Conventional infrastructure resilience: LCLS relies on a diverse suite of infrastructure to operate, which is mostly in the purview of the host laboratory (SLAC) and so is not detailed here. The strategic need is to ensure key utilities' resilience to failures to maintain sustainable operations. This includes high voltage, process gases, cooling systems, HVAC, etc. The fundamental changes in the nature of LCLS operation (e.g., the transition to cryogenic super-conducting systems) has necessitated major investments at a laboratory level via programs such as the DOE Strategic Laboratory Infrastructure (SLI) fund and internal SLAC and Stanford resources. The primary impact on LCLS strategic planning is to ensure timely quantification of requirements, priorities, and the risks and consequences of failure to deliver or maintain these systems. Within LCLS, a dedicated “Facilities Infrastructure” program has been established that prioritizes program-specific investments with a multi-year planning horizon, as described next.

Normal Conducting Linac infrastructure: The LCLS Cu Linac is over 50 years old, with many systems that are obsolete, and a design that introduces substantial operational jitter and sub-optimum performance compared to comparable modern linacs (e.g., at PAL-FEL or SwissFEL). The LCLS strategy calls for targeted investment in preventative maintenance, spares, and upgrades in the period leading up to operation of LCLS-II-HE (when the majority of experiments will be fielded by the superconducting linac). A tradeoff analysis needs to be performed for the subsequent period (2028 onwards) when only selected programs will require use of this linac.

Superconducting Linac Infrastructure: The LCLS-II cryoplant needs to run continuously in order to maintain the operating temperature of the linac and retain the helium inventory. Extended loss of power (~2 days) can lead to substantial losses, with no credible option for full-system generator power. Mitigation includes retaining an onsite spare helium inventory, upgrading the electrical supply to minimize the probability of failure, procuring key spares, and installing a 1.5MW generator and additional recovery compressors to minimize helium losses.

Collaborative space: One of the hallmarks of the LCLS-II era is the need for collaboration space for scientific programs to meet and co-develop innovative science both internally and externally, temporarily and permanently. This requires space for visiting scientific user groups to collaborate with staff, and for the different internal groups to work together. Crucially, there needs to be a focus on the development of massive-scale data analytics methods, and associated machine learning solutions for large datasets. To meet this strategic need, LCLS has taken a lead role in defining a new SLAC facility called the “Large Scale Collaboration Center” (LSCC), which has been funded $66M by the DOE SLI program.

Support labs: A major limitation at many labs, including SLAC, is the availability of high quality lab space to develop new technologies to meet the staff and users' research needs, including prototyping, and performing ongoing calibration, maintenance and testing of deployed systems. This strategy calls for substantial effort on the build-out of such labs, with examples including:

- **Nano-X**: Diffractive X-ray optics and nano-fabricated components
- **Detector Lab**: For calibration and testing
- **Metrology Labs**: For X-ray distribution and focusing systems
- **Laser Labs**: As described in Appendix 4, along with dedicated laser development areas

- **Biology Labs**: For bio-sample preparation and manipulation, up to BSL-2
- **Sample Characterization Labs**: For chemical and biological samples
- **Injector Characterization Lab**: For offline testing of liquid-phase injectors, including an all-optical endstation that mimics aspects of LCLS experimental sample environments.
- **Maker Space**: Mechanical setup area for testing and prototyping
- **Assembly Areas**: For construction, baking, alignment and offline testing of endstations
- **Controls Test Labs**: For offline build and test of controls equipment

3.4 Secure supply chains for critical systems and components

The ability to support ongoing operations and timely development of new capabilities for LCLS rests on deep partnerships with other DOE/NNSA national laboratories, industry, and academia. Focused attention is needed for the LCLS strategy to identify likely gaps in the supply chain, from which 4 principal actions arise:

1. **Modernize systems to reduce dependency on outdated or isolated components:**
   - Addressing obsolescence is a focus for ongoing maintenance of the Cu linac, as described in section 3.3.
   - Another key task is to engineer sub-system redundancy, providing fallback solutions for when a key system fails that would compromise operations (e.g., injector laser)
2. **Develop in-house expertise and capabilities in targeted areas**
   - This objective seeks to ameliorate the challenges of obtaining equipment from sole-source suppliers, or where there is time-urgency and mission-criticality for which the regular vendor base is unable to respond satisfactorily.
   - Examples underway (of many) are development of nano-scale X-ray optics, advanced modes of operation of high power lasers, X-ray 2D detectors, high power RF systems, and specialist controls, data and network systems.
   - Examples where this remains highly problematic are: meter-scale X-ray mirrors (sole supplier in Japan), diamond crystal optics (prior reliance on Russian sources), and advanced electronics (extraordinarily long lead times).
3. **Foster the development of domestic suppliers**
   - Other mechanisms to address the challenges of specialist supply include:
     i. Partnership with industry (e.g., via SBIR/STTR programs)
     ii. Licensing of in-house technology (e.g., microfluidic sample delivery)
     iii. Increasing domestic supply capabilities (e.g., via the new DOE ARDAP office)
4. **Maintain critical spares for accelerator and beamlines**
   - The impact of even short (hour-timescale) downtimes on LCLS operations can mean the difference between success and failure of an experiment. Understanding the potential failure modes of the system is crucial - calling for expert-based FMEA and quantitative assessment of reliability, availability, maintainability and inspectability (RAMI) at the component and subsystem levels. Along with information on likely lead-times from vendors (or in-house), this informs the priorities for spares inventory.
   - The introduction of large-scale cryogenic systems to LCLS, with the ability to compromise the operation of the entire SCRF facility, is a particularly acute case - demanding procurement of backup helium and critical spares for the cryoplant.

Goal 4: Empower Societal & Economic Impact

4.1 Cultivate & attract a talented, diverse workforce and user communities

LCLS was the first Hard X-Ray FEL in the world, and has attracted high quality staff that have gained unique experience in the design, operation and optimization of XFELs and associated science. With the recent commissioning of 3 new XFEL facilities (European-XFEL, SwissFEL, PAL-FEL) in addition to SACLA, FERMI, FLASH and emerging FEL sources such as SXFEL and SHINE (China), there is high and increasing interest in recruiting LCLS staff from all areas of the facility. This is exacerbated by the broad international makeup of our local staff. Alongside this, Silicon Valley has a highly competitive job market, particularly for qualified engineers, data/controls experts and other specialist staff, making recruitment and retention challenging.

The existence of ambitious facility upgrades at LCLS provides a counterbalancing attraction, as does the exciting R&D program across all aspects of facility performance, and the compelling societal impact and open-science nature of the research programs. Substantial focus has also been placed on assessing the factors that impact quality of life for facility staff (e.g., in terms of mitigating the demands of 24-hour operations, and the level of support that is needed to execute experiments and deliver major projects). A focused program is underway to develop enhanced levels of automation for LCLS; to pass operational control where appropriate to the users; and to divide out ‘routine’ beamline tasks from those that require dedicated professional input (e.g. from beamline scientists). A major guiding principle is to minimize the need for staff intervention. These actions form part of a wider exercise to identify an attractive “day in the life” paradigm for our staff, and then drive our facility design and operational structure accordingly.

The objectives described in this strategic goal cover the key elements to support staff engagement (4.1.1), build a vibrant and expanding user community (4.1.2), and increase diversity in the workforce and user community (4.1.3).

4.1.1 Foster a welcoming, inclusive, diverse, equitable and sustainable work environment

Strategic actions to protect and develop the LCLS culture of inclusivity and respect were described in section 3.1.3. This section thus focuses on the sustainability of staff careers.

The BESAC International Benchmarking report recommended a need to “*[Strike] a balance between the need to develop world-leading facilities and the need for access to and technical support of existing facilities [to] increase research impact and help retain talented scientists.*”

This manifests at LCLS with a strategic focus on increased deployment of “standard configurations” of instruments to minimize the level of effort to prepare for individual experiments, and lower the barrier to entry for less experienced user groups. This also enhances the ability of early career staff to lead the delivery of user operations, by providing a more stable system on which they can learn their craft. Alongside this, SLAC and LCLS have invested in a range of offline laboratories to provide staff with the ability to access experimental capabilities outside of the mainline User Facility - to the benefit of staff and users alike.

Additionally, this report called for "*Mechanisms for significant financial support of scientific investigators at all career stages [to] create a more sustainable career path that builds on current investments in the development of the scientific workforce — enhancing U.S. competitiveness for talent.*"

At LCLS there are multiple elements in place that support a flexible approach to career development - including options to focus more on technical capability development, delivery of user operations, and/or pursuit of specific scientific goals - with a confidential "augmented CV" evaluation to assess the best path for career and salary progression. These categories of expertise/accomplishment can be summarized as follows, noting that these areas are not mutually exclusive, and staff are encouraged to excel in more than one area.:

- Scientific domain leadership
    - Current or future leaders in one or more fields of science
- Facility development enabling new science
    - Current or future major contributors toward the mission of the facility
    - Providing significant added scientific value to facility users (e.g., in the form of development of new methods, capabilities and/or instrumentation)
    - Engagement and/or development of significant new user communities
- Operational delivery
    - Operational efficiency and effectiveness
    - Providing significant added value to facility users (e.g., actions or expertise that enable and ensure the scientific success of user experiments)
    - Technical or operational advances that cut across scientific areas or instruments (e.g . sample delivery or environment)

To provide flexibility in career progression, a range of funding opportunities exist, including:

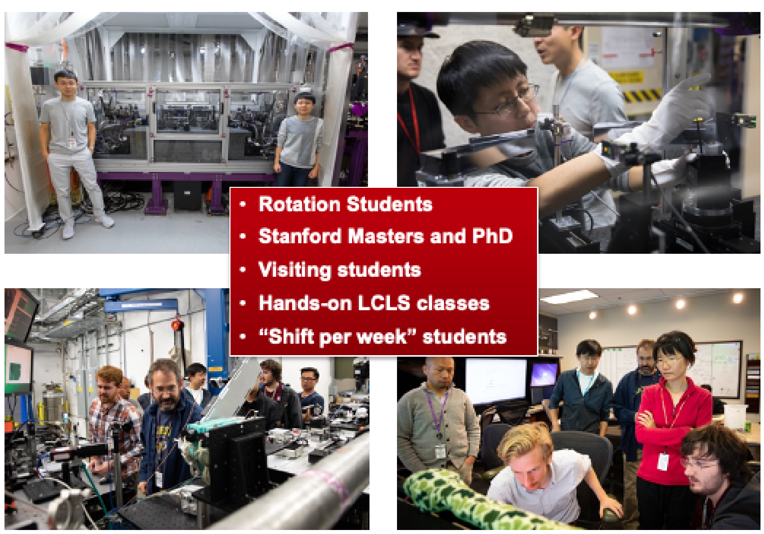
- For beamline scientists and some other user-facing roles, 20% of staff time is set aside for 'personal research' to provide bandwidth for individual career development.
- Staff can take on joint appointments with Stanford Institutes such as PULSE (for ultrafast AMOS research), SIMES (for materials science), SUNCAT (for catalysis) and KiPAC (for astrophysics) - including opportunities to co-supervise graduate students and postdocs.
- All staff can apply to mentor interns funded directly by LCLS, which often provides an opportunity for staff to experience direct supervision of others for the first time. Similarly, the presence of Stanford faculty within the organization allows for shared supervision of graduate students and postdoctoral scholars.
- A "Scientific Initiatives Program (SIP)" has been created to fund individual ideas for new research directions, including allocation of equipment and time from engineering/controls/technical teams.
- An "Operational Improvements Program (OIP)" funds activities and equipment that will improve the safety, robustness, flexibility, and reliability of LCLS operations.
- A range of major development programs exist for substantial enhancements to the facility in which staff can lead projects at the $0.25M to $5M level, and thus gain experience as Principal Investigators, project managers, and many other roles. This includes: X-ray Improvement Program (XIP), Accelerator Improvement Program (AIP), Accelerator Small

Projects (ASP), Detector R&D, Photon Systems R&D, Accelerator R&D, and strategic initiatives such as the LCLS-II Instruments Program (L2S-I).
- Opportunities exist at the SLAC Laboratory level to become a Principal Investigator on research projects (via the LDRD program) and/or develop potential new directions via the lab's Program Development (PD) program.
- SLAC is an active participant in the DOE's I-Corps program that seeks to develop skills in technology transfer and market-relevant development of intellectual property and ideas.

At a personal level, the financial compensation options offered to staff are set by Stanford University, with a range of incentive packages. Affordability in the San Francisco Bay Area is a crucial driver, with institutional-level commitment to address this to the degree possible. Local LCLS actions include offering remote- and hybrid- work arrangements where practical, with flexibility in working hours and a focus on the lived experience of team members.

An additional major contributor to a healthy work environment is cultivating a diverse pipeline (see 4.1.3) and easing the path to entry into this field for early career researchers. Key actions are as follows (with some examples captured in the image below):

- Sponsorship of 'rotation students' for one or two quarters of the academic year, in which early-stage Stanford graduate students can work in LCLS labs and programs to assess their interest in pursuing their PhD in this field. Conversely, existing staff can gain valuable mentorship experience.
- This extends to full-term PhD and Masters students, under the supervision of local faculty.
- Hosting of visiting students, postdocs, staff and faculty from across the user community - which can help enrich the breadth of innovation and contribute to the staff pipeline.
- Provision of LCLS beamtime for Stanford student courses.
- Financial support to students to perform a "shift per week" at the facility, to gain knowledge of how LCLS operates and to provide their skills to the team.
- Support of LCLS staff to engage in postgraduate courses, including pursuit of masters and PhD courses.
- Support of joint fellowships - e.g., recently with the Stanford Institute for Materials and Energy Sciences (SIMES), and often with the PULSE Institute.



4.1.2 Stimulate continued innovation and expansion in the user community

These are still early days for XFEL-enabled science, with much of the early operations period focused on how to adapt to the factor-billion leap in X-ray brightness and factor thousand- to million reduction in pulse duration from prior sources. Many expert groups have emerged across a broad range of scientific fields, but there is the potential for substantial expansion in the depth and breadth of impact for XFELs. This will benefit not only the current research goals, but can also identify unanticipated grand challenges for which XFELs can offer meaningful insight.

The LCLS approach is represented as a 12-point plan:

(i) **Identification of new directions** by positioning LCLS as a key area of topical debate in strategically driven DOE collaborations (e.g. via Stanford joint institutes and new initiatives in areas such as QIS, microelectronics, biopreparedness, and sustainability), and by leading community groups (e.g. the Liquid Sunlight Alliance (LiSA) and relevant EFRCs and EERCs).

(ii) **Engage a broad community** of X-ray users via strengthened ties to SSRL, enabled by targeted development of 'cross-over' beamlines and techniques that provide a scientific and instrumentation bridge. Similar approaches are underway with the Cryo-EM data analysis team.

(iii) **Initiate Scientific Campaigns:** Broad, community-led multi-year strategic programs involving theory, modeling, synthesis, novel data analysis, and experiment design. Campaigns are allocated 10-15% time at LCLS and have already engaged a large number of new groups.

(iv) **Invite near-neighbor experts** to LCLS reviews – both to gain their insight and to attract interest in our capabilities (i.e. recruitment into our PRP, SAC, reviews, etc.). Similarly, invite early career researchers to these panels to inject new perspectives and to avoid stagnation.

(v) **Allocate LCLS Director's "discretionary beamtime"** to target new groups and new ideas (typically 5-10% of LCLS beamtime, selected each Run).

(vi) **Use in-house staff beamtime** and 'early science' programs to build partnerships with new user groups and to pursue ideas with higher technical risk.

(vii) **Issue "seed grants"** to potential new users to explore new directions. Good success with this approach emerged from a trial process with Stanford faculty (with eleven grants from a competitive award process in 2020).

(viii) **Showcase LCLS capabilities** at sponsors' PI meetings and national conferences.

(ix) **Hold a series of bridging workshops** (e.g. solar energy + X-ray science) and tutorials for new groups to help craft new proposals and make best use of beamtime for new users.

(x) **Take advantage of new "remote user capabilities"** to lower the barrier to entry for non-traditional users, partnering them with experienced teams. Remote access is being augmented by a suite of tools, including 'cyborg headsets', mobile robots, 'NoMachine' controls, etc. Such access is a strategic driver for LCLS, calling for considerable effort to enhance hybrid user engagement during beamtimes and ongoing collaborations.

(xi) **Train new and inexperienced users** via summer schools, mock proposal calls with guided feedback, tutorial sessions at user meetings, and dedicated staff time.

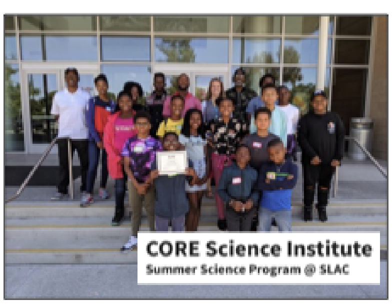
(xii) **Encourage "superuser" groups** to co-opt researchers in allied areas, and coach them through the fielding of samples and analysis of data. This has been successfully trialed in a number of areas, including structural biology and chemical sciences.

4.1.3 Pursue outreach and collaborations with under-represented communities

Consistent with the community broadening approach outlined in the previous section, a key element of the LCLS strategy is to ensure this growth encompasses previously underserved research institutions and demographics. Great opportunity exists here, since LCLS is in a period of major change rather than being in a quasi-steady state mode of operation. As such, there are many actions that can be taken to foster such engagement. Examples of targeted initiatives:

- **LCLS Internship program**: LCLS funds ~40 positions for an 8-12 week summer program for undergraduates (with some high school and graduate participants). This was initiated to address shortfalls in skills and to develop mentoring experience for our staff. All interns are required to present a poster at the end of the summer, and activities are coordinated with other SLAC intern programs (SULI, CCI, GEM, etc.) to create a vibrant experience. Preference is given to candidates from disadvantaged and underrepresented backgrounds
- **CORE Science Institute (CSI)**: A week-long experience for middle- and high- school students from under-represented backgrounds, often in partnership with Greene Scholars.
- **SLAC SAGE Camp**: A week-long onsite camp for female high school students.
- **Visiting faculty programs**: LCLS is active with the Vertically Integrated Projects (VIP) program with Howard University, and in exploration with a number of other institutions.
- **Courses for Undergraduate Research Experience** (CURE): partnering with under-graduate university departments in areas such as biochemistry.
- **Capstone projects**: For example with Chico State University in mechatronics.
- **Local Community College engagement**: LCLS partners with Cañada College in their Photonics And Laser Technology (PALT) program – to train and certify laser technicians, along with exploration of work with biochemical and molecular biology lab techs.
- **Alonzo Ashley Fellowship**: LCLS funds new hires in a variety of disciplines in partnership with this program, with long-standing success in attracting high quality staff.

Partnership with the SLAC DEI Office lies at the heart of all these activities, as does strong encouragement for LCLS staff to participate in - and lead - SLAC Employee Resource Groups.



4.2 Foster a vibrant research ecosystem to underpin innovation and impact

4.2.1 Pursue strategic collaborations with BES light sources and internationally

The LCLS strategy is to provide leadership in the direction and depth of interactions with allied facilities and communities, nurturing an open and collaborative culture that seeks exchange of staff, information and technologies to the greatest extent practical. This is driven in part by the relative immaturity of the field, both technologically and scientifically, such that coordinated development of science, user groups, capabilities and operations is to the great benefit of all. Examples of the types of collaboration are as follows:

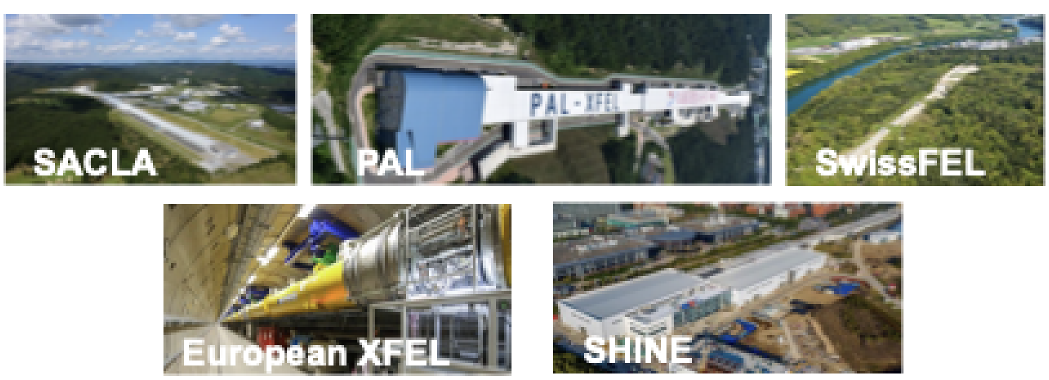
US Light Sources: A key strategic strength of LCLS is its operation as one of five X-ray light sources funded by a single agency (DOE-BES): ALS, APS, LCLS, NSLS-II and SSRL. The resulting close collaboration affords many opportunities for coordinated development of scientific directions, technologies, user communities and for sharing of operational lessons. Regular (~monthly) meetings of the 5 Light Source Directors are held.

Task forces are formed between the 5 Light Sources to address areas of common interest, with examples including: (i) Data systems and computing, (ii) Optics, (iii) Remote access, (iv) Detector development, (v) User proposal systems, (vi) Industry partnerships, (vii) Facility metrics and evaluation, (viii) Supply chain management.

International XFEL Community: There are currently five operational hard-X-ray XFEL facilities (LCLS (USA), SACLA (Japan), PAL-XFEL (Republic of Korea), Swiss-FEL (Switzerland) and European XFEL (Germany)), with a sixth under construction (SHINE (China)) due to turn on in the 2025-27 period. There are periodic (~18 month) in-person meetings to exchange information on operational issues, as well as regular (~monthly) online seminars to share latest advances.

LCLS has benefited greatly from extensive international cooperation in technology (such as on superconducting cavities with DESY and CEA), facility commissioning and operation (with European XFEL and DESY), X-ray optics (with SPring-8 and SACLA and also DESY), sample environment and Start-2-End modeling (DESY / Eu-XFEL), self-seeding (all), and many others.

There are strong scientific links between all facilities, with a heavily overlapped user community that seeks the best performance wherever it can be found. This extends to the XUV / Soft X-ray XFEL facilities, including FLASH (Germany), FERMI (Italy), and SXFEL (China). Together this drives a very healthy collaborative competition on performance, user access, and impact.



4.2.2 Pursue strategic partnerships within SLAC/Stanford and with users

(1) SLAC/Stanford: The integrated nature of the lab's science and technology programs and its major user facilities provides a wealth of opportunities for deep partnership in the definition and execution of priority science programs. This includes joint development of the core strategies for chemical science, materials science, high energy density science, bioscience and more. Regular updates to the strategies for each area are developed for DOE.

The existence of joint Institutes between SLAC and Stanford (PULSE for ultrafast AMOS research, SIMES for materials science, SUNCAT for catalysis, and KiPAC for astrophysics) further augments this partnership approach, providing additional mechanisms for shared staff and development of experimental systems.

More broadly, SLAC has invested in a suite of laboratories, with examples shown in Figure 17, to align activities in areas of shared strategic importance - such as data science.

PULSE
SIMES
Energy solutions through materials science
KIPAC
SUNCAT
CENTER FOR INTERFACE SCIENCE AND CATALYSIS

Arrillaga Science Center laboratory investments
- Diffractive X-ray optics (Nano-X)
- Biolab suite
- Cryo-EM center
- New ultrafast laser labs for R&D and EUV beamline science

Massive Scale Data Analytics and advanced computing
- SRCF-II expansion
- Science Data Facility (S3DF)
- Machine Learning initiative
- Large Scale Collaboration Center (LSCC)
- HPDF (DOE data facility) partnership proposed

New Experimental capabilities
- Quantum materials – momentum microscope endstation (Shen et al)
- Interfacial catalysis and surface science endstation (Heinz et al)
- NNSA applications to MEC-U (new funded program)

Faculty and Staff growth
- Panofsky Fellows, LDRD
- Lab infrastructure for LCLS-II and LCLS-II-HE
- Stanford seed grants
- Graduate Student Initiative
- New Photon Science faculty
- Local and national MSI programs

Figure 17 Overview of some shared facilities and complementary labs at SLAC

(2) User partnerships: A central element of the LCLS strategy, as described earlier, is to further foster deep partnerships with the user community - from individual science programs, to multi-institution Scientific Campaigns (see 3.2.1) and joint development and fielding of user-supplied instrumentation (learning from the examples of CAMP/LAMP and SXR, to implementation of the Surface Science and Momentum Microscope endstations - Appendix 2).

(3) SSRL/LCLS: A cornerstone of the strategic landscape at SLAC is the close partnership between SSRL and LCLS - in which there are countless examples of co-development of science programs, instrumentation, techniques, and support systems - with shared staff and students. Some recent examples are captured in Figure 18.

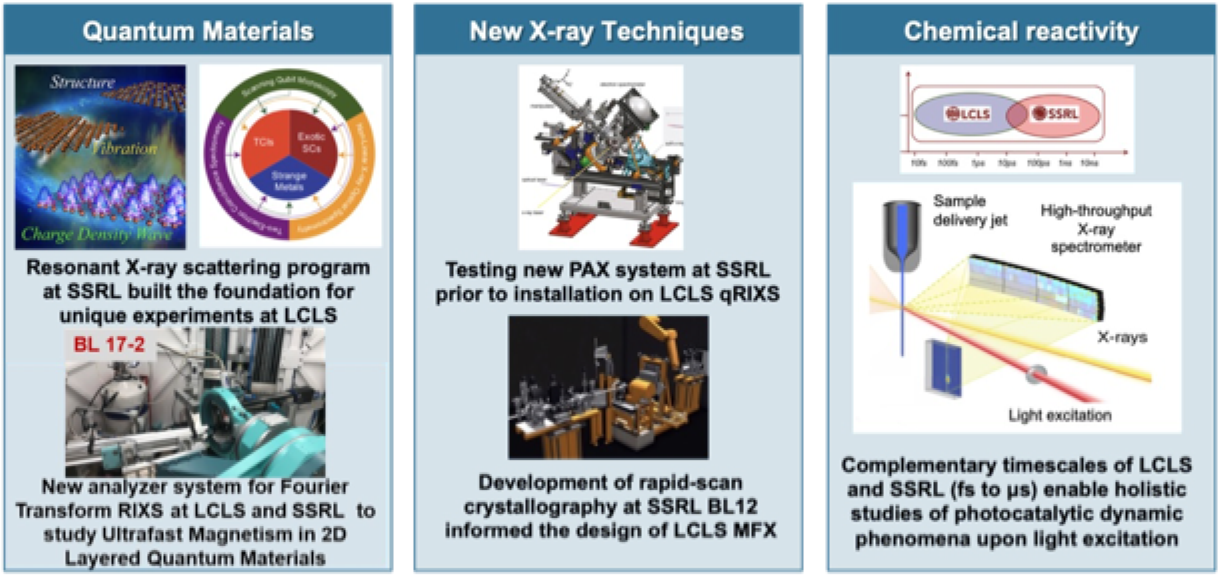


Figure 18 Examples of co-development of research topics between SSRL and LCLS

4.2.3 Support US industry via facility access, joint projects, and tech transfer

As noted by BESAC, there is a need to facilitate interactions "*across the continuum of basic research, use-inspired research, applied research and industrial research [to] accelerate translation of fundamental research to impactful technologies that benefit society*."

The LCLS strategy takes this forward via application of the following objectives:

(1) Promote industrial usage via targeted outreach, collaboration and proprietary access

- While LCLS user experiments are predominantly focused on exploratory, fundamental science, they offer the potential for transformation of our understanding of fields that are key to many industrial areas, as described in the National Priorities section.
- Increasingly, access to XFELs is targeting these types of applications, with recent focus areas across the community in water, pharmaceutical drug design, clean energy technologies, aerospace, and microelectronics to name a few.
- Consequently, LCLS has opened up "rapid access" mechanisms to overcome the ~year-long gap between proposal and experiment that would otherwise deter some industrial studies.
- LCLS has also put in place, and successfully deployed, proprietary access mechanisms to allow confidential information to be secured from beamtime.
- Cross-over workshops are held to bridge between the arcane world of X-ray science, and industrially-focused areas such as solar energy and electrochemistry.

(2) Support US small business through joint SBIR and STTR projects

- LCLS is an active and successful initiator of work with US-based small businesses - with examples ranging from optics to X-ray instrumentation, detectors and sample environment systems.

- Staff time and attention will continue to be encouraged to identify and execute projects under this mechanism, in close partnership with DOE

(3) Pursue tech transfer of inventions from successful R&D to empower US industry

- Working with the Stanford Office of Technology Licensing, and the SLAC technology transfer office, LCLS encourages the development and licensing of ideas by its staff.
- SLAC is an active participant in the DOE's I-Corps program that seeks to develop skills in tech transfer and market-relevant development of intellectual property and ideas.

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LCLS | Linac Coherent Light Source

APPENDIX 1 - Building from the scientific advances of the first XFEL decade

The future strategic directions of LCLS are informed by the results of the first decade of the XFEL era, with a representative selection summarized below to provide examples of where XFELs have made major advances to date, and to inspire new ideas and directions:

Imaging molecular motion. The characteristic LCLS ability to directly image the motions of atoms comprising a molecular reaction on fundamental time scales represents a qualitative advance in our ability to link molecular structure with function and reactivity. Hallmark LCLS studies have focused on the evolving structure and bonding of ring-opening reactions, a fundamental building block of organic chemistry. Comparison with theoretical models revealed dominant reaction trajectories and tested long-held assumptions about the electronic structure changes mediating such reactions. Pioneering LCLS experiments pave the way for a wide range of X-ray studies examining gas phase chemistry and structural dynamics associated with ultrafast chemical reactions.

Coupled dynamics of energy flow. A grand challenge in chemistry is to understand how electronic and nuclear configurations couple in molecules and thus mediate reactivity. This knowledge gap profoundly limits our ability to predict charge separation dynamics, impacting the development of robust, cost-effective systems to convert and store solar energy. LCLS has demonstrated the ability to generate and use X-ray pulses that can track the motion of excited-state charge and spin dynamics with element-specific precision, revealing the coupling to subtle coherent motion of the atomic structure, as well as how to trigger specific molecular responses with targeted light pulses.

Understanding natural multi-electron photo-catalysts. Sunlight-driven oxidation of water by photosystem II (PS-II) has generated most of the dioxygen in the atmosphere, central to life on earth. Detailed understanding of this four-photon four-electron process remains a grand science challenge, and an inspiration for inventing artificial photo-catalysts to convert sunlight to fuels. LCLS studies have provided the first damage-free structure determination of all three intermediate PS-II catalysis cycle intermediate states at room temperature, at unprecedented <2Å resolution. These results reveal important new structural details about substrate water binding and the water oxidation mechanism, resolving key discrepancies and driving the refinement of catalysis cycle theoretical descriptions.

Transition states in heterogeneous catalysis. Significant knowledge gaps in catalysis prevent us from fully exploiting and optimizing the transformation of many chemicals on which modern society depends. Short-lived reactive species mediate catalysis but are extremely difficult to characterize. The ultrafast element-specificity of LCLS X-rays have enabled the first direct observation of a transition state in a model surface catalytic reaction: the oxidation of carbon monoxide on a metal bed. This pioneering work opens new opportunities for element-specific studies of catalysis on fundamental time scales for direct input into the theory of heterogeneous catalysis.

Coherent control of complex materials. Coherent light-matter interactions represent a powerful new approach for controlling emergent material properties and creating novel material phases. One important example is coherent control of multiferroic materials based on manipulating magnetic order with electric fields. The underlying physics, strength, and ultimate speed of magnetoelectric coupling present significant knowledge gaps. Seminal LCLS studies in multiferroic TbMnO3 applied coherent THz excitation of specific magnon modes, while ultrafast resonant X-ray diffraction revealed the coherent spin dynamics. Coherent magnetic switching should be achievable with modest scaling of the THz field. A second important example is coherent excitation of selective lattice modes to manipulate high-case temperature (Tc) superconductivity, such as in yttrium barium copper oxide (YBCO). Comparison of X-ray scattering with density functional theory (DFT) calculations revealed structural changes analogous to directional pressure associated with remarkable enhancement of superconductivity above Tc.

Correlated phenomena in quantum materials. A hallmark of quantum materials is the dominant influence of quantum-level coupling between charge, spin, orbital, and lattice modes in determining the bulk material properties. LCLS has demonstrated its ability to yield extreme precision measurements using such methods as time-stamping at the femtosecond timescale. A prime example is an LCLS study that provided the first direct measure of electron-phonon coupling strength in the superconductor FeSe purely from experiment. This provided a critical test of theoretical predictions, with results nearly 10-fold larger than the classical model. These results prompted a reassessment of the significance of such coupling in superconductivity in these compounds, and provides a powerful new means of assessing the emergent properties of a broad range of quantum materials.

Extreme material and plasma science. LCLS has demonstrated its ability to create and precisely measure new metastable material phases in extreme environments relevant for high energy density science, planetary science, and fusion research. Examples include the verification of “diamond rain,” the calibration of white-dwarf based cosmic clocks, and the laboratory demonstration of Fermi acceleration.

Bioscience. LCLS delivered the first high resolution, room temperature and damage-free atomic structures of biological membrane proteins, used in the targeting of roughly 40 percent of all drugs, along with impact on diseases ranging from Zika to dengue fever, tularemia, African sleeping sickness, hypertension, influenza, and now COVID-19. LCLS has also pioneered the study of biological function by capturing the structural dynamics of biomolecules in action, on timescales ranging from picoseconds to seconds, with key results in systems such as retinal, b-lactamase and RNA riboswitches, resolving long-standing questions for how changes in enzyme structure and dynamics facilitate passage along the reaction coordinate.

APPENDIX 2 - Instruments and experimental techniques for LCLS-II

The new instruments for LCLS-II are housed in a modified Near Experimental Hall (NEH) and Front End Enclosure (FEE). This provides:

- Initially two, and ultimately three new X-ray beamlines from the soft X-ray undulator (SXU) to serve four new instruments (TMO, qRIXS, ChemRIXS and TXI), as well as an open port for user-supplied endstations (SurfSpec, k-Microscope, and others).
- A hard X-ray beamline to serve the current suite of five hard X-ray instruments (XPP, XCS, MFX, CXI, MEC), and jointly to TXI to create a unique 'dual XFEL' instrument.
- Three new hutches (NEH 1.1, 1.2, and 2.2) to accommodate the instruments, and a major new "central laser laboratory" to serve the NEH.
- Dedicated control rooms for each instrument.
- An expanded data/controls capability, consistent with the leap from 120 Hz to 1MHz.

An overview of the new instrument layout is provided in Figure A2.1. A suite of "First Experiments[9]" for these instruments using LCLS-II was developed on the basis of the science drivers to drive the instrument design and implementation. These mark the user-assisted transition from commissioning to open user access.

TMO (NEH-1.1) specializes in atomic and molecular studies in the gas phase. It supports two experimental endstations positioned in tandem. The first endstation location (MBES/MRCO) employs velocity map and angular resolved spectrometers to measure femtosecond and sub-femtosecond excited state dynamics of atoms and molecules. The second endstation, DREAM, delivers coincidence charged particle spectroscopy to yield kinematically complete measurements at each time step of an evolving reaction. This experimental approach, known as a "molecular reaction microscope" will enable the complete spatial reconstruction of the excited-state charge transfer and subsequent dissociation at each time step to visualize a broad range of excited-state molecular dynamics.

TXI (NEH-1.2) is a dual-beam instrument, fed by both the soft and hard X-ray undulators; a feature currently unique among XFEL instruments. The tender x-ray instrument will enable x-ray pump/x-ray probe techniques especially in the emerging field of nonlinear x-ray science, support tender X-ray spectroscopy measurements, and provide a coherent scattering/ forward diffraction instrument for single particle imaging of sub-micron samples. It is designed to accommodate a variety of additional techniques, such as absorption and photoemission spectroscopy, as well as an array of samples from fixed targets to gases, aerosols and liquid jet targets.

A variable resolution grating monochromator directs soft X-rays (0.25-1.2 keV) to a suite of experimental areas on the upper floor (NEH-2.2), designed for moderate resolution (~5,000) and high resolution (~30,000) photon spectroscopy. Multiple instruments can be hosted in series:

[9] See: https://lcls.slac.stanford.edu/instruments/neh-1-1/science-drivers, https://lcls.slac.stanford.edu/instruments/neh-1-2/science-drivers, and https://lcls.slac.stanford.edu/instruments/neh-2-2/science-drivers

qRIXS is designed for high resolution, momentum resolved resonant inelastic x-ray scattering (RIXS) to study bosonic excitations in solid state samples. The spectrometer is designed to achieve a target resolving power of over 30,000 when integrated with the monochromatic beamline performance, with the option for lower resolving power, ~10,000, and higher throughput through the use of a second grating in the spectrometer. The spectrometer arm is also designed to field X-ray Photon Correlation Spectroscopy (XPCS) and REXS experiments.

ChemRIXS is designed to map the energy distribution and evolution of occupied and unoccupied molecular orbitals of model complexes and functional photo-catalysts in operating (liquid) environments, using time-resolved RIXS methods.

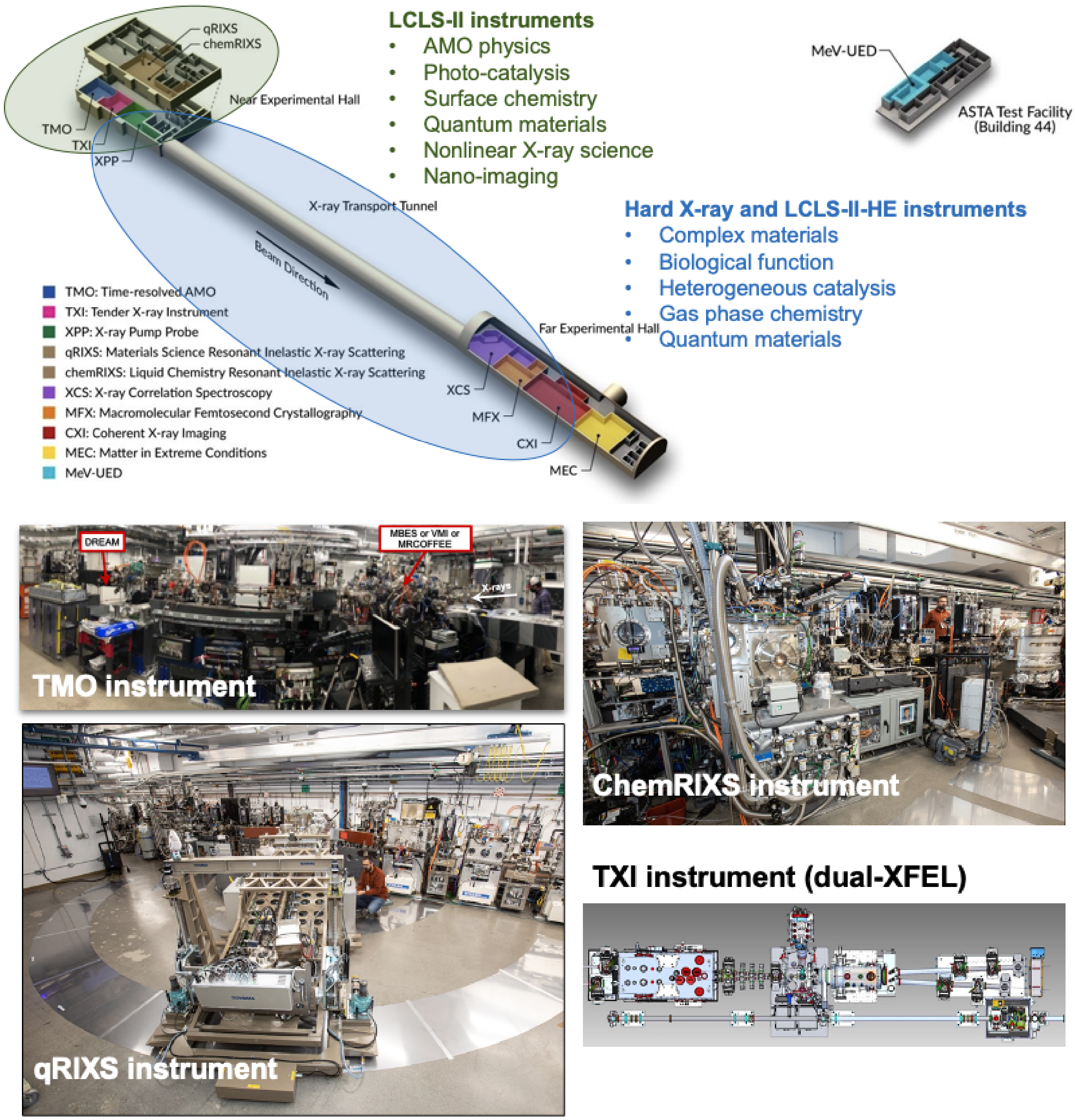


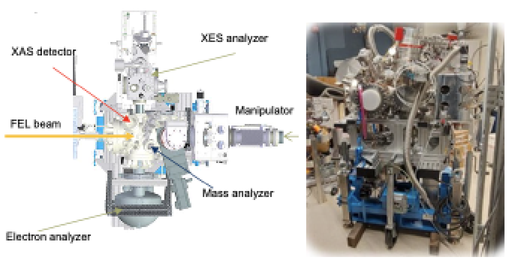
Figure A2.1 LCLS instrument layout and images of the four new instruments for LCLS-II.

In addition to this instrument suite, user consortia are also delivering (see Figure A2.2):

- A momentum microscope, for time-resolved ARPES investigation of quantum materials.
- A surface science endstation for ultrafast chemistry and interfacial catalysis research can be fielded at the open port of this beamline .

Surface Science Endstation

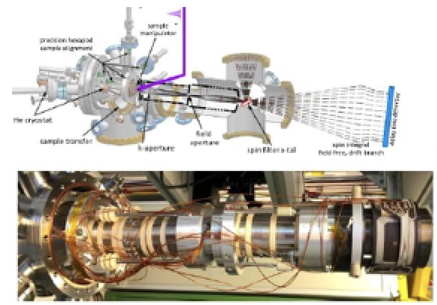
(following ultrafast reaction dynamics and capturing rare intermediates in heterogeneous catalysis)



T. Heinz, A. Nilsson, H. Ogasawara et al.

Momentum Microscope Endstation

(coupled interactions in quantum materials via multi-modal tr-ARPES & element-specific PE diffraction)



Z.X. Shen, K. Rossnagel, G. Schoenhense et al

Figure A2.2 Two endstations supplied by user consortia to be fielded at the open port in NEH2.2

APPENDIX 3 - Accelerator and FEL systems development strategy

Attosecond capabilities

The XLEAP project has delivered isolated sub-fs pulses with tens of uJ of pulse energy. These pulses are more than six orders of magnitude brighter than those generated with table-top high-harmonic sources and have opened a new science direction in nonlinear attosecond spectroscopy. A vigorous R&D effort on attosecond capability is ongoing. Recent developments include the generation of TW-scale pulses and the demonstration of pump/probe experiments with sub-fs resolution.

The focus is now on extending the capabilities for high-repetition rate operation, and improving pump/probe capabilities with the use of optical delay lines for more flexible control.

The use of the electron bunch in pump/probe experiments is also being studied. This capability enables sub-fs stability and pump frequency from the THz to the UV.

Electron beam shaping studies

The LCLS-II accelerator provides a revolutionary improvement in average power and stability. However the new accelerator provides lower peak power due to the lower brightness of the injector and the non-linearity of the compression system.

An R&D program to improve the LCLS-II peak performance was launched in 2019 and produced several new concepts for laser-based beam shaping methods. A dedicated laser system was installed in the LCLS-II injector laser laboratory and will be employed for improvements to the bunch brightness and for shaping the electron beam at the femtosecond and sub-fs level.

Multibunch operation and dual undulator operation

Multi-bunch operation of the LCLS has been demonstrated with trains of up to four electron bunches with sub-ns to >100 ns separation. This experimental capability is important for the time-resolved study of non-reproducible processes and dynamics induced by low repetition rate high-energy lasers. Furthermore, this operation mode will enable the demonstration of cavity-based XFELs with the copper linac (see below). In the recent past we have developed tunable ultrafast kickers to control the orbit of individual bunches in a multi-bunch train, significantly improving the stability and the peak power of multi-bunch operation.

Ultrafast kickers for the LCLS-II linac are also being developed, to feed both undulators with closely spaced bunch pairs. In combination with an X-ray delay line (in development), these kickers will enable simultaneous delivery of pulses from the soft and hard X-ray undulators to the TXI instrument for pump-probe applications and non-linear X-ray experiments.

Self-seeding

Self-seeding is a reliable method to generate narrow-bandwidth pulses from an X-ray free-electron laser without the need of an external seeding system. This can provide very high longitudinal (temporal) coherence, with delivery of pulses near the Fourier transform limit for spectroscopic applications. In a self-seeded XFEL the undulator is divided in two parts: the first part generates a seed pulse that is filtered through a monochromator; the second part is used to amplify the seed pulse to saturation. Self-seeding has been demonstrated in the past at soft

X-ray energies with a grating-based monochromator and at hard X-ray energies with a single-crystal monochromator.

The soft X-ray self-seeding system (SXRSS) has recently been upgraded to operate at high repetition rate for LCLS-II. Additionally, advanced self-seeding methods to generate fully coherent and stable pulses have been proposed and will be explored experimentally by combining the attosecond XLEAP capabilities with the SXRSS system.

An R&D effort on hard X-ray self-seeding (HXRSS) will be launched in FY24 with the aim to study new seeding options for the LCLS-II HE hard X-ray line as well as beam shaping and optimization methods to maximize the peak brightness of self-seeded pulses.

DELTA Polarization Control

Control of X-ray polarization is an important feature in XFEL beamlines. In the hard X-ray regime, quarter wave plates using ‘off Bragg’ diffraction have been very effective.

In the soft X-ray regime, the polarizing "Delta" undulator was tested at the end of the LCLS-I undulator line, providing ~200 uJ of circularly polarized X-rays at a very high degree of polarization (>99%) and tunability. To reach saturation, it is estimated that three DELTAs will be required for the LCLS-II SXR line. The additional length of the DELTA will not only enhance the intensity of the circularly polarized X-rays but also strongly suppress harmonics on axis. These will be real advantages for many spectroscopies enabled by LCLS-II in the soft X-ray range.

Cavity-based X-ray Free-Electron Laser

Funded by DOE-BES, and in partnership with Argonne National Lab and RIKEN (Japan), SLAC is developing the design of a cavity-based X-ray FEL that would direct the X-ray beam around a multi-pass round trip of the X-ray undulator. The initial test will be done with two electron bunches from the Cu-linac. When this scheme is combined with a suitably high rep-rate beam from LCLS-II-HE, it is predicted to result in an enhancement of the XFEL brightness by two to three orders of magnitude and high longitudinal coherence near the Fourier Transform limit, via the periodic FEL amplification and Bragg monochromatization of the X-rays. Recent tests on a 14-meter cold-cavity at LCLS show suitable diamond optics now exist, capable of sustaining the required efficiency. This cavity demonstrates individual optic reflectivity of >99% and can store x-ray pulses for >59 round trips, exceeding the requirement for a regenerative XFEL amplifier (RAFEL). The CBXFEL project at LCLS is currently under construction with major installations and testing in FY24, to inform the deployment of dedicated systems on LCLS-X.

Superconducting Undulators

In the past decade, superconducting undulators (SCU) have been developed and tested at the APS at Argonne. Compared to permanent magnets, SCUs offer a higher magnetic field, a more convenient way to adjust the undulator field, improved resistance to radiation damage, and better vacuum for the electron beam chamber. SLAC and ANL are collaborating to develop SCUs for XFELs. The goal is to demonstrate key technical features such as magnetic field quality, thermo-mechanical properties, beam-based alignment, and FEL gain. Testing of SCUs in the LCLS-II hard X-ray undulator is planned for FY25. The successful demonstration of SCUs on a working XFEL will be a major milestone toward the design and construction of an all-SCU beamline for the next-generation X-ray free-electron lasers such as LCLS-X.

APPENDIX 4 - Strategic plans for scientific capabilities for the LCLS User program

This appendix describes the strategies for individual technical areas in support of LCLS science:

A4.1 High power "optical" (UV to THz) laser systems

Optical laser systems (here meaning those that operate in the UV, visible, IR and THz regimes) are a critical, enabling technology in many areas of the LCLS facility. For example, at the photoinjector, they are used to generate and shape the electron bunch and subsequent X-ray characteristics, while in the hutches they are used to initiate the dynamics in systems under study. In particular, ultrafast lasers generating pulse durations in the femtosecond to picosecond range are required with a wide range of tailored characteristics, tuned to meet the specific needs of the application.

In order to maintain LCLS at the forefront of scientific discovery, strategic development in laser performance is being pursued in several key axes. These include: high repetition rate, ultrashort and tailored pulse duration, increased spectral range, tunable wavelengths, improved stability and reliability, etc. Current, strategically important development areas are described below.

High repetition rate laser sources

To take full advantage of the high repetition rate X-ray source enabled by LCLS-II and HE, a step change in laser technology is required. Laser capabilities that were previously delivered at 120 Hz for LCLS-I[10], must now be provided at repetition rates of 10 kHz to 1 MHz. This 1000x increase requires a transition to a new laser technology at much higher average powers. The initial approach has delivered optical parametric chirped pulse amplification (OPCPA), which uses high power picosecond duration pulses to amplify a chirped, broadband seed laser, subsequently compressed to short pulse durations[11]. Two such OPCPA systems, delivering 35 W, <20 fs, 800 nm pulses at up to 100 kHz are deployed in a newly-constructed Central Laser hall in the NEH (see Figure A4.1) for the first two endstations receiving beam from LCLS-II. Recent developments have shown that the spectral broadening and compression of the very same pump lasers used in the OPCPA system can be used to produce similar pulses to the

[10] Minitti et al "Optical laser systems at the Linac Coherent Light Source", *J. Synchrotron Rad.* **22**, 526-531, (2015)
[11] Mecseki et al. "High average power 88 W OPCPA system for high-repetition-rate experiments at the LCLS x-ray free-electron laser", *Opt. Lett.* **44**, (2019)

OPCPA at 1 µm wavelength, but with much greater efficiency[12]. In addition, this approach is far simpler, gives greater stability, simplicity, reliability, has a smaller footprint and lower cost, with near-term prospects for scaling to 10x higher average power than OPCPA.

This transition is an enabling step for ultrafast science in all new endstations connected to LCLS-II, HE, and beyond, as well as future developments for UED. The direct compression approach is being implemented at 80 W average power for LCLS-II, with R&D to refine the performance and scale to several hundred Watts of power to enable operation at 1 MHz.

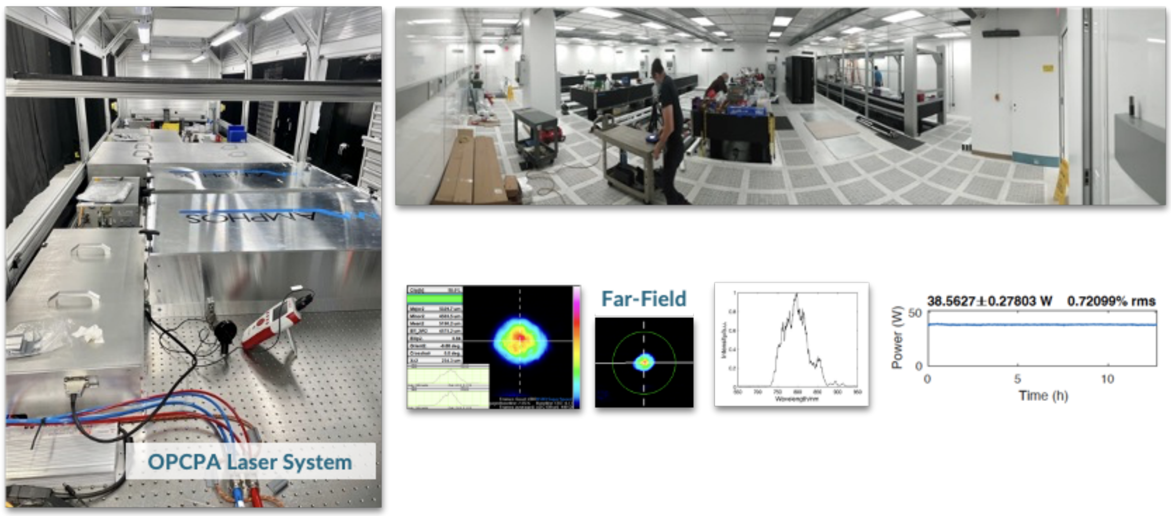


Figure A4.1 Layout of the new central laser hall to serve the Near Experimental Hall instruments

Nonlinear frequency conversion for experiments

The broad range of science served by LCLS requires that we provide laser wavelengths across a broad portion of the spectrum, spanning the UV to THz range. These wavelengths are typically derived from the drive laser described above through single or cascaded nonlinear interactions that generate these new wavelengths.

For example, photoexcitation in the UV and visible is particularly important for electronic excitations, where high temporal resolution, and therefore short laser pulse durations are required. Applications in AMO, chemistry, and materials science require laser pulses < 10 fs in duration, with µJ-level pulse energies and 100 kHz repetition rate. These parameters in the UV-visible range require approaches beyond conventional crystal-based frequency conversion. Gas-based four-wave-mixing, resonant dispersive wave generation[13] and pulse compression in hollow fibers, are being actively pursued in LCLS R&D projects to meet these needs.

Similarly, near- to far-infrared wavelengths and THz radiation are important for accessing both electronic and structural excitations in molecules and materials, as well as providing strong electric fields for streaking photo-electrons in AMO experiments or the electron bunch in UED.

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[12] Kramer et al "Enabling high repetition rate nonlinear THz science with a kilowatt-class sub-100 fs laser source," *Opt. Express* **28**, 16951-16967 (2020)

[13] Travers et al. "High-energy pulse self-compression and ultraviolet generation through soliton dynamics in hollow capillary fibres" *Nat. Photonics* **13**, 547–554 (2019)

Here, tailoring of the laser bandwidth to provide both short duration or, alternatively, narrow bandwidth pulses, is required. The efficiency of conversion to infrared wavelengths is typically very low, and there is a significant gap in the accessible frequency range (the ‘THz gap’), where there is limited coverage from laser-based sources. Scaling of processes such as optical parametric amplification, difference frequency generation, and optical rectification[14], up to higher average power is a key development direction, as is bridging the ‘THz gap’ through either laser-based approaches or accelerator-based approaches[15].

Timing & synchronization

Due to a myriad of factors, there is an inherent jitter between the arrival time of the X-rays and pump-probe laser at the interaction point, which, alongside the duration of the X-ray and laser pulses, is a major contributor to the response function of instruments which is targeted to be <10 fs in some cases. A two-pronged approach is required: to improve synchronization by minimizing sources of timing jitter, and to improve shot-to-shot measurement of the arrival time of laser pulses relative to the X-rays. The former involves the continued development and refinement of RF and optical timing references that distribute a low-noise reference between the accelerator, laser systems and experimental interaction regions. The latter involves the development of new materials and techniques for cross-correlation of the lasers, optical reference and X-ray pulses, that increase accuracy and sensitivity

Higher energy lasers

The Matter in Extreme Conditions upgrade project (MEC-U)[16] aims to combine both a rep-rated petawatt (PW) laser, and a high-energy kilojoule (kJ) laser with LCLS. In addition to the major construction and laser development efforts within the project, there is a need for developments relevant to both the current MEC instrument and MEC-U on topics such as: component validation (damage testing, reflectivity measurement, etc.), beam characterization and manipulation (alignment, timing, intensity, wavefront, contrast, target back reflection, etc.), and other enabling capabilities (high-energy secondary sources, large-aperture optics, etc.)

Offline laboratory laser labs

Successful deployment of the capabilities described above requires laboratory space to conduct development activities on LCLS systems and experimental techniques prior to their integration into the facility. A key strategy is thus to fully equip, staff, and utilize the offline labs to enhance the facility’s ability to deliver impactful science. To this end, LCLS is building a suite of laboratories to act as a hub of research, developments and application of laser sources, instrumentation, controls, and data acquisition systems, without using precious X-ray beamtime. Most notable are the ASC (‘Arrillaga Science Center’) laser laboratories. This will allow staff and users to maximize the effectiveness and impact of laser capabilities when deployed in LCLS beamtimes, provide complementary scientific measurement tools, and will lower the barrier to

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[14] Kramer et al "Enabling high repetition rate nonlinear THz science with a kilowatt-class sub-100 fs laser source," Opt. Express **28**, 16951-16967 (2020)

[15] Zhang et al “A high-power, high-repetition-rate THz source for pump–probe experiments at Linac Coherent Light Source II” *J. Synchrotron Rad.* **27**, 890-901, (2020)

[16] Dyer et al. ”Matter in Extreme Conditions Upgrade (Conceptual Design Report)”, SLAC National Accelerator Laboratory, (2021)

entry to XFELs by the table-top laser community. See Figure A4.2 for layout of the suite of optical, THz and XUV lasers and beamlines being configured in this area.

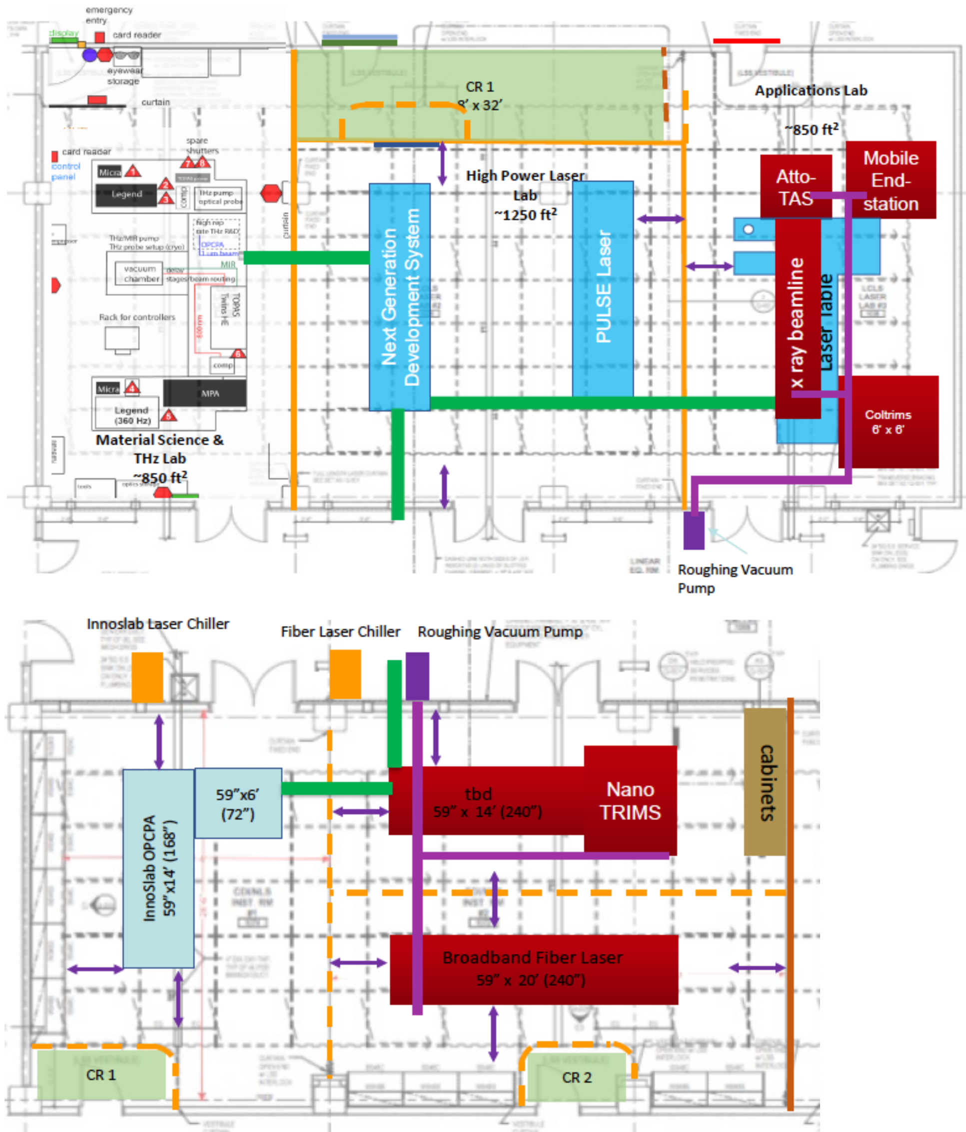

Figure A4.2 Layout of the ASC Laser labs, providing offline development space and XUV beamline capabilities

A4.2 X-ray Optics

Increasing the time-average X-ray beam brightness by orders of magnitude (from <0.5 W to >>100W) imposes challenging requirements on the X-ray optics in terms of survivability, wavefront preservation, and response to the pulsed and intermittent nature of the beam. An underpinning element of the LCLS strategy is to develop detailed modeling tools, validate these where possible on existing facilities, iteratively ramp performance self-consistently with the scientific goals of the experiments on a Run-by-Run basis, and provide start-2-end predictive capability to enable quantitative experiment design, real-time feedback, and analysis.

The three component elements of the X-ray optics deployment strategy are then:

(1) Preservation of wavefront to a figure error of sub-nm RMS for X-ray mirrors and less than 25 pm for crystal monochromators:

- **For monochromator crystals**, nearly two orders of magnitude are needed to reduce the thermal deformation to less than 25 pm [1]. The approach adopted is to use cryocooled silicon crystals combined with a focusing element to compensate second order component of the thermal deformation, and a cooling pad to optimize the effective cooling temperature. Using this approach, the thermal deformation of a high heat-load monochromator crystal can be preserved for a 100 W SASE FEL beam – as needed for the Dynamic X-ray Scattering (DXS) instrument.
- **For reflective X-ray mirrors**, the near-term approach is to combine water cooling and resistive heating (known as Resistive Element Adjustable Length, REAL), as demonstrated in laboratory- and synchrotron-based tests [2,3]. LCLS-specific solutions require optimized cooling pads and power distribution along with UHV-compatible parts and an effective control and feedback solution. LCLS has invested in an Optics Metrology Laboratory to test these systems prior to operational deployment.
- **Pulse-by-pulse transient effects of X-ray optics under high rep-rate FEL power**. Terawatts (TW) of peak power from XFEL pulses induce spikes in temperature, thermal deformation, and acoustic waves, enhancing the X-ray optics' thermal deformation. With LCLS-I, the 8.33 ms between pulses (120 Hz) was long enough that the optics could recover from the spikes. However, with LCLS-II(HE) operating up to 1 MHz, it is unlikely that the optics will have enough time to recover from the spikes in thermal deformation and acoustic waves. Measurements of the damping properties of the optical materials is needed alongside transient modeling of the integrated optical systems.

(2) Design of specific optics:

- **High-Resolution Monochromator** (HRM) for the LCLS-II-HE Dynamic X-ray Scattering (DXS) instrument. This needs to cover a photon energy range of 6 – 25 keV with 2 meV precision, corresponding to 10^{-7} resolution, which is at the forefront of HRM in the X-ray community. An innovative 4f design has been adopted, consisting of multiple sub-components: two channel-cut crystal monochromators, two focusing/defocusing mirrors, a wavelength definition slit, an E_0 diagnostic spectrometer, and diagnostics.
- **Inelastic X-ray Scattering (IXS) Spectrometer**, with energy resolution down to a few meV for studying the time-resolved atomic dynamics of crystalline matter. To meet this resolution, the IXS spectrometer is an extreme engineering design with a long and movable arm. The optics system consists of two long mirrors and two pairs of channels cut crystals precisely aligned and distributed along the spectrometer arm with a tolerance of motion error between tens of nano radians and hundreds of μm. Some of the significant challenges are motion control, repeatability, alignment, and stability.
- **Focusing mirror systems** capable of variable focus sizes from tens of μm down to ~100 nm to enable forward scattering and gas-phase chemistry studies. The mirror design combines a pair of KB mirrors with Wolter-type mirrors.
- **Soft X-ray delay line** to generate two pulses with sub-femtosecond delays possible at experimental stations in soft X-ray beamlines, including crossing time zero.

- **Dual XFEL capability via a delay line** to enable X-ray Pump / X-ray Probe techniques. A 5-ns X-ray delay line on HXR branch is to be implemented, using a cooled channel-cut monochromator combined with a 4-crystal delay line.
- **Automated X-ray beam feedback** to perform rapid alignment of all optical components along the beamline to the global optimum within a tight tolerance. An attractive solution is to employ machine learning-based control to manipulate the many complex optical systems and maintain the nanoradian pointing stability. This requires a mockup system to mimic the optics components combined with simulation and testing to validate the performance of the ML models.
- **X-ray Optics Metrology.** Currently, the LCLS Optics Metrology Laboratory can simultaneously characterize long and bendable optics (up to 1-m long) in both vertical and horizontal configurations. However, the resolution is limited by the reference flat on the Fizeau interferometer. An upgrade will integrate a deformable mirror (known as a bimorph mirror) as the reference mirror to the Fizeau interferometer stitching setup. This can be shaped to demand curvature, even higher-order shapes beyond the conventional mirror figures, to extend the stitching limit and accuracy to measure highly curved mirrors Such an optic solution also enables the deployment of automation and machine learning to control the mirror shape and extend the on-demand shape control to non-conventional and higher-order shapes.

(3) Maintenance of X-ray optics to ensure continuous and successful delivery of the desired beam to the experiment hutches. This incorporates:

- **Spares:** the time-critical turnaround of optics maintenance requires a healthy inventory of spares due to their long lead time.
- **Preventative and in-situ intervention:** An example of preventative maintenance action is a non-invasive in-situ mirror cleaning. This procedure should be carried out in the as-installed mirror system, i.e., costly installation and metrology effort will not be needed. A safe and successful cleaning procedure requires careful consideration and rigorous testing owing to the mixed coating materials on each mirror substrate.
- **Replacement:** An in-house facility is needed for removing bad or contaminated optic coating and to undertake specialist processes where possible to avoid unnecessary shipping and handling.
- **Machine Learning in engineering optimization:** Calculation of the performance of advanced optics such as the 4f-HRM, or future cavity-based XFEL (CBXFEL), requires pulse-by-pulse transient response modeling to define the optical design; their response to different operational parameters; and damage risk factors. To have an adequate picture of this response, the response to a quasi-steady state needs to be calculated in seconds or minutes. This represents a scale up of one million times the current modeling approached. Machine learning can help to shorten the X-ray optics design optimization time by identifying strategic parameters, reduce the number of simulation cases, and automating the post-data processing.

A4.3 Sample delivery systems

Sample delivery capabilities for liquid systems is for the most part common between LCLS instruments. The mechanical systems to position nozzles to deliver samples to the X-ray interaction region differ but the nozzle technology as well as the liquid and gas pressure systems to deliver and monitor flow parameters are common. LCLS maintains, deploys and operates high-performance liquid chromatography (HPLC) pumps, gas pressure regulators, gas mass flow controllers, as well as flowmeters and sample cooling, shaking and switching systems. LCLS supports the operation of Gas Dynamic Virtual Nozzle (GDVN), Double Flow Focusing Nozzles (DFFN), Lipidic Cubic Phase (LCP) and other high viscosity nozzles as well as the Microfluidic Electrokinetic Sample Holder (MESH) and its rapid mixing variants. Several sample environment and delivery themes emerge as priorities for development:

- **Versatility / optimization** for specific needs of bio complexes (buffers, other conditions), as well as different methods such as solution scattering or SPI.
- **Operational efficiency** (robust, reliable, automated, user friendly, low- maintenance).
- **Reduced sample volume** to enable access to precious proteins and the most important bioscience problems, consistent with LCLS science advantages for:
    - Mapping dynamics in near-physiological conditions
    - Exploiting diffract-before-destroy to mitigate radiation effects
    - Higher repetition rates
- **Faster dynamics** by pushing the state-of-the-art for mix/inject

A4.4 X-ray Detectors

Given the unprecedented characteristics and unique needs of LCLS, X-ray detectors have been an integral part of LCLS facility development. The LCLS detector strategy is to foster a balanced portfolio of projects that leveraged commercial detectors, compatible external developments, and internal R&D focused on developing detectors tailored to the unique needs of LCLS.

The first two generations of detectors specifically developed for LCLS (CSPAD and ePix) were tailored to satisfy the resolution and dynamic range requirements at a repetition rate of 120Hz, while maintaining a modular and scalable architecture. With the LCLS-II/HE upgrades, R&D is focused on extending the acquisition rate of ePix detectors to the 25 kHz to 1 MHz range. This was done using a diversified approach tailored to the requirements of the key LCLS science drivers by progressively increasing the detector frame rate, while also adding real-time information extraction capabilities to minimize data rates and volume.

Detector requirements imposed by the key science drivers can be summarized as follows:

- **Imaging non-identical objects**: Requires a 2D detector with a large dynamic range, high QE for tender/hard X-ray energies, capable of operating at rates of up to 100 kHz. Information is contained in the majority of pixels, requiring readout of the entire frame.
- **Stochastic dynamics**: XPCS techniques will benefit from a 2D integrating detector with fine spatial resolution operating at the full MHz pulse rate of the accelerator. Information in these experiments is spatially “sparse” and confined to a limited number of pixels per frame, with each pixel containing a limited number of photons (small dynamic range).

Extracting information using a sparsified readout would allow efficient implementation at MHz rates with contained data volumes.

- **Rare events**: This would benefit from a detector operating at the full 1 MHz rate. Information in rare events is temporally "sparse," so an event-driven triggered detector capable of extracting frames centered on a rare transient event would produce acceptable data rates. Spatially coarse MHz frames could locally generate feature-based triggers via automatic pattern recognition and related machine-learning approaches.
- **Molecular dynamics** (e.g., COLTRIMS): To take full advantage of the timing options of FELs (multi-bunch, multi-polarization, and sub-fs pulses), a highly segmented TOF particle detector accommodating hit rates of 6000/s/cm2, and a time resolution of 100ps is needed.
- **Extreme states**: Fast framing (GHz) imaging detectors are needed to take advantage of the new laser drivers and diagnostics capabilities from LCLS, such as an X-ray pulse train that allows measurements of material dynamics with ultrafast temporal resolution.

Additionally, more conventional spectroscopy and detection systems employing 1D readout functioning at the full (1MHz) repetition rate are required but already available.

The most taxing requirements are to provide area detectors for soft and tender X-rays at a readout speed of a multi-kHz for the initial period of LCLS-II operations, scaling to tens of kHz for full-frame, full-depth readout, and MHz rates for sampled/sparsified readout. Similar performance will be required in the hard X-ray regime for LCLS-II-HE with the additional requirement of high quantum efficiency sensors at high energies.

To achieve these goals, multiple pathways are being developed in parallel to reduce the risk of non-delivery in time for LCLS-II and HE operations. To cover the entire soft-, to tender-, to hard-X-ray regime, hybrid pixel array detectors based on the ePix family are being developed at SLAC, as shown in Figure A4.3. Two parallel development paths have been identified:

- **ePixHR / UHR ("[Ultra] High Rate")**: a platform-based approach extension of the present generation of ePix detector family toward full frame readouts up to 100kHz
- **SparkPix**: dedicated to classes of experiments with "sparse" data characteristics where information extraction in real-time can push operation to 1MHz with optimized performance and with manageable data throughput.

The design and construction of the ePixHR class of detectors have been completed, and currently able to provide full frame readout at 5kHz, and support Region of Interest (ROI) mode for faster readout of a subset of pixels. In the next generation, these cameras will be able to provide multi-kHz readout speed with trigger and veto capabilities implemented at the edge while maintaining low noise and high maximum signal (10,000 8 keV photons equivalent). Prototypes of ePixUHR at 35kHz and 100kHz operation have been successfully implemented, retiring risks for staged deployment in the mid-2020s. Thanks to the intrinsic scalability of hybrid pixel array detectors, large areas can be covered and maintained sustainably. Specifically, two major 5kHz detectors have been designed and will be deployed to the experiments in the next year: ePixM (based on CMOS sensors technology for the soft X-ray regime) and ePixHR_{5kHz} (as an extension to the current ePix10k systems for the tender/hard-ray regime). In parallel, the development of the first generation of detectors for the HE era is underway. This includes an ePixUHR 35kHz version to be deployed in 4Mpix formats for the LCLS-II/HE upgrades of CXI and XPP and a 16MPix version for MFX, together with the first generation of MHz information-extracting detectors named SparkPix (SparkPix-S for XPCS, SparkPix-ED for rare events and SparkPix-T (a.k.a. Tixel) for measuring the 3d momentum for hundreds of particles per laser shot in coincidence at very high pulse repetition rates).

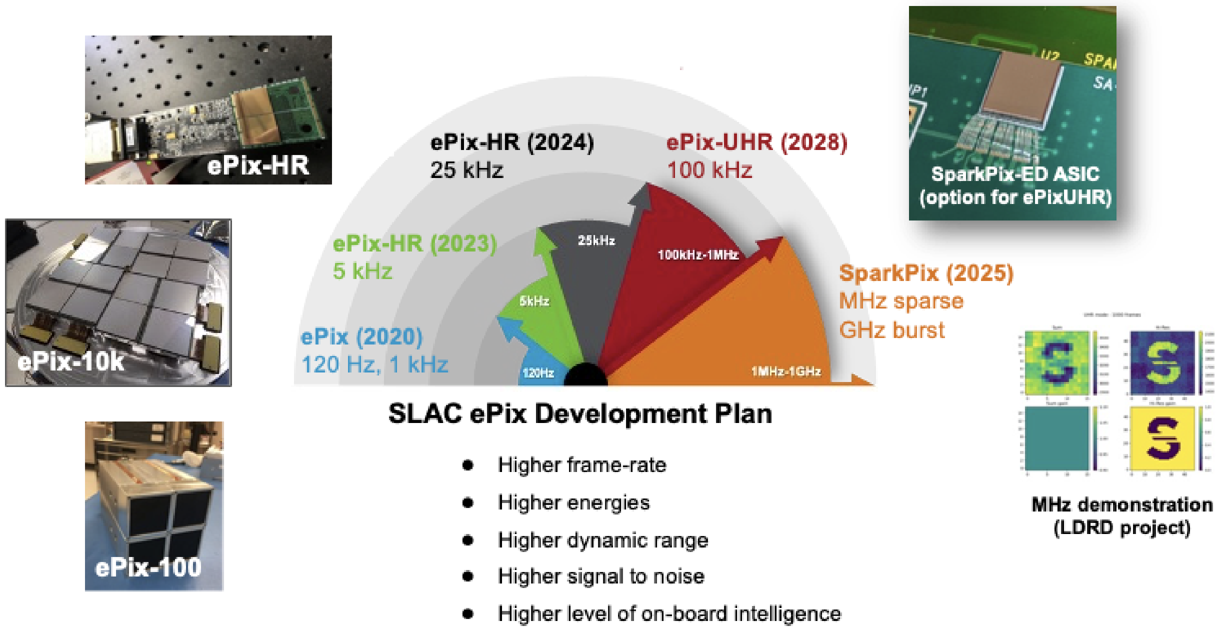

Figure A4.3 Development path at SLAC of 2D X-ray detectors for LCLS.

The current versions of these ePixHR/UHRa and SparkPix detectors can be modified to use different sensor materials, such as Ge or GaAs, to increase the quantum efficiency at higher photon energy (>18 keV) or CMOS sensors and LGADs to extend performance to the soft x-ray regime (~250 eV). A joint effort between SLAC, ANL BNL, and Cornell to develop high-z sensors for high-energy applications has been funded directly by the BES Detector R&D program and is progressing successfully.

To prepare for the next generation of detectors beyond LCLS-II/HE, SLAC will move to data-driven detector architectures with increased intelligence by distributing computing at the edge within the detectors and leveraging AI/ML hardware implementations based on data analysis workflows established for LCLS experiments. It is foreseen that future detectors can revolutionize the way we conduct experiments by providing high degrees of adaptiveness in performance, self-calibration, information extraction, and energy efficiency. To achieve these goals, innovation in microelectronics technologies at the materials and devices level, interconnections, computing architectures, and algorithms are required. These challenges are broadly shared with the microelectronics industry in sectors requiring implementations of networks of sensors and their control (IoT, Automotive, Quantum-Classical Interface).

A4.5 Real-time automated controls

The strategy for LCLS controls systems is to balance **performance** (e.g., new features) with **agility** (responsiveness to emerging user requirements) and **reliability**. This is to be achieved via the adoption of a modular architecture in which individual components can be automatically tested, and allow reversion to a functional baseline. Key elements include:

- **Robust industrial controls**: A new control system was developed and deployed for the LCLS-II instruments, oriented around a unifying platform (Beckhoff and EPICS). A similar system is in production for LCLS-II-HE instruments. A preemptive machine protection system for the high-rate beam is used to optimize beam delivery, with the ability for future offline validation of equipment configurations and to support flexibility in experiment control hardware (including mechatronics plant simulation and testing prior to deployment, and vacuum system simulations).
- **User Interface**: Following extensive consultation, PyDM was chosen as the UI. Typhos was created to automatically generate screens from Python objects; LUCID was created to automatically generate hutch home-screens and provide maximum reconfigurability; and a PMPS diagnostic was adopted that utilizes advanced PyDM features. In the future, user-tailored screens based on personal profiles and UI regression testing are planned.
- **Machine Protection**: High-rate beam parameter management systems are now in use, with multiple attenuator control and optimization for X-ray optics stability.
- **Automation**: The architecture allows for development of real-time automation (e.g., for beam alignment, or for lasers using the MODS/Tiles platform). System observability is achieved via ELK stack, Grafana, and log emitters. An automated Test Execution Framework has been deployed, validating beamline functionality. Next ALarm System (NALMS) is deployed and alarm thresholds and hierarchies implemented. Future development focuses on expanding usability (e.g., the Not A Beamline Scientist, NABS, experiment automation toolkit based on BlueSky), with offline simulation capability and ML and machine vision to provide high-level automation and/or diagnostics.

A4.6 Massive scale data analytics - Achieve the DISCUS vision

Advanced data and computing systems play a vital role in LCLS operation, data interpretation, and overall scientific productivity. As a facility, LCLS provides the infrastructure to acquire very high throughput data, transport the data to disk, manage the data, provide access to sufficient computing resources for analysis, and provide sophisticated analysis frameworks for data access. The increase in repetition rate from 120 Hz to 1 MHz introduces a step change in the size and complexity of data sets and demands a similar advance in computing, algorithms, and analysis to fully exploit the incredibly rich information content contained in this new torrent of data. Recent developments at LCLS and the convergence of new data analysis techniques, advances in hardware architectures, development of AI/ML methods, and improvements in computational capabilities provide an opportunity to accelerate science, leverage large datasets, and optimize the use of oversubscribed beam times.

LCLS seeks to provide seamless access to computing for users, making use of local compute resources as well as ASCR compute and network capabilities when required. These capabilities will provide researchers easier access to data, computing, and analysis tools, and enable the adoption and use of promising but compute- and data-hungry methods, such as AI/ML, to shorten the time between experiment and publication and accelerate science.

Due to common strategic needs, LCLS has partnered with the other DOE-BES X-ray Light Sources (ALS, APS, NSLS-II and SSRL) to develop a 10-year vision for transforming X-ray science that adopts the Integrated Research Infrastructure (IRI) principles laid out by DOE-ASCR. This vision is known as **Distributed Infrastructure for Scientific Computing for User Science (DISCUS)**, and is described further below.

Drivers

The LCLS data analysis strategy is motivated by the very high throughput generated by the LCLS-II and HE upgrades, the need for capable fast feedback, a desire to improve the time to science, and a desire that no user be left behind. The **major increase in the scale and speed of data production** introduces the challenge of producing science information in real-time from massive streaming datasets. A new canonical workflow for LCLS experiments is captured schematically in Figure A4.4. An initial Data Reduction step is mandatory for a suite of experiments, with data rates in the 100-1000 GB/s range. The methodology of this step requires very careful testing, user feedback, and co-development of detector ASIC, edge-computing (e.g., FPGA firmware) and near-edge compute. **Fast feedback** for real-time analysis is critical to the users' ability to make informed decisions during an LCLS experiment. Meaningful feedback in minutes or faster reduces is required to successfully complete an experiment. A tight coupling between analysis, control, and user intent improves the overall quality of the data, and provides actionable feedback that can be used to efficiently adapt data collection and analysis during live experiments and increase their success rate. Sophisticated analysis frameworks can significantly reduce the time between experiment and publication, improving overall productivity and **reducing the time to science**. Most of the advanced algorithms for analysis of LCLS data have been developed by external groups with resources to dedicate to a computing effort. Smaller groups with good ideas may be hindered in their ability to conduct science by not having access to these advanced algorithms or may be forced into collaborations with larger groups due to lack of resources. LCLS support for externally developed algorithms and the development of in-house algorithms for some specific science domains alleviates this problem, ensuring that **no user is left behind**.

The LCLS data strategy requires a three-pronged approach aligned with the following areas:

1. Advanced data analysis workflows that may include on-demand access to HPC while an instrument is collecting massive datasets, ultimately exploiting exascale computers; new experimental methods are also needed involving tighter coupling between analysis and acquisition allowing for machine-assisted and even autonomous experiment control.
2. Transparent data analysis that shields users from increasing complexity of the underlying hardware and software stack.
3. Advanced algorithms and ML methods to extract new scientific insight from massive data sets interpreting data in new ways at higher speeds.

Where possible, LCLS will pursue partnership with other light sources and facilities and make every effort to leverage the work and expertise of the community to solve common problems.

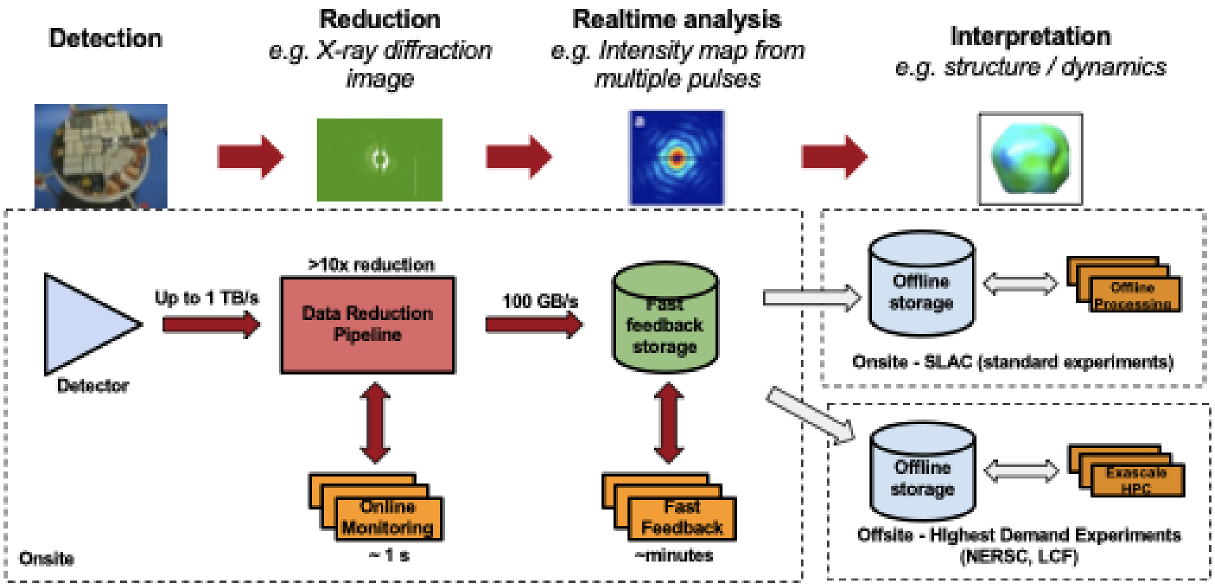

Figure A4.4 High level workflow for massive-scale data extraction and analysis

Key Investments

There are three key investments in computing and data at LCLS that will most benefit the users and science in the next five to ten years: AI/ML (see next section), advanced workflows and visualization, and autonomous experimentation.

- **Advanced data processing workflows** are needed that can mine streaming, high-rate data to select interesting events, reject poor data, and adapt to changing experimental conditions. Real-time and near real-time data analysis can be used to provide curated feedback to the user to inform immediate decisions about data collection or directly to the instrument controls as actionable information to enable self-driving experiments. These workflows must support the seamless coupling of LCLS instruments with edge, local, and ASCR computing resources in heterogeneous pipelines that run data reduction, processing, analysis, interpretation, and visualization tasks.
- **Autonomous experimentation** is a specialized workflow that requires a tighter coupling between data analysis, data acquisition, and controls, taking real-time information produced at the point of collection and using it for the purpose of controlling or steering the experiment. In collaboration with the other light sources, LCLS is developing a framework for building these feedback loops capable of driving experiments, giving scientists a powerful tool to radically accelerate scientific discovery and innovation.

DOE-wide collaboration on data systems

The Distributed Infrastructure for Scientific Computing for User Science (DISCUS) vision seeks to address the challenges of leveraging data across the 5 DOE-BES X-ray Light Sources by using DOE complex-wide computing resources to reduce the time to science, utilizing billions of core hours per year to fully leverage AI/ML and digital twin capabilities, to extract information from complex data, to steer experiments, and to use shared data for ML-driven discovery.

The key elements of the DISCUS plan are as follows, coupled to the ongoing investments in the light sources' instrumentation (see also Figure A4.5):

1. Algorithms, applied math and AI/ML
2. Scalable software library
3. Workflow and orchestration tools
4. Seamless real-time on-demand computing
5. Networking improvements
6. Discoverable data repositories

Unified solutions across the facilities, leveraging efficiencies of scale, can provide users with the ability to manipulate their data easily and transparently, and will better enable new scientific opportunities. AI/ML use by scientists escalates the need to share and move data across facilities and drives the push for more computing and transparent data movement.

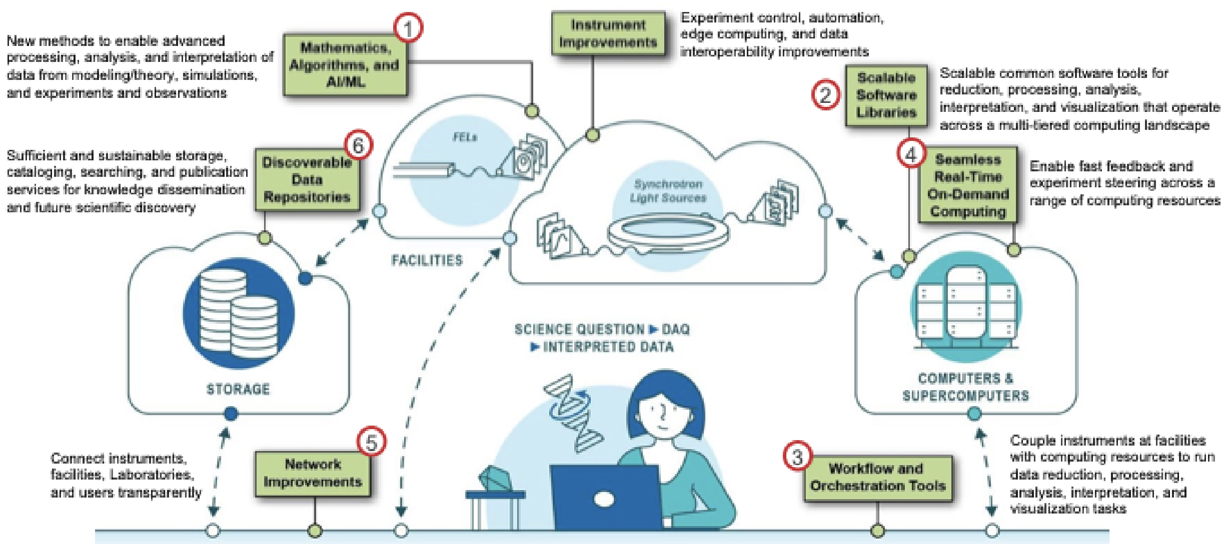

Figure A4.5 An integrated set of computational tools and capabilities are needed

The High Performance Data Facility (HPDF) national program aligns well with the high-level needs outlined in the DISCUS vision and with overall LCLS needs. LCLS seeks to be a pathfinder for new HPDF capabilities as they come online. The HPDF call introduced the idea of a Hub and Spokes. In the LCLS Data Systems view, LCLS, as a data-generating user facility with an onsite compute facility (S3DF) should be viewed as a Spoke that adopts the same interfaces developed for the Hub and participates in the HPDF software ecosystem in order to seamlessly inter-operate with the HPDF Hub and Spokes. This seamless integration will be critical to utilize data from multiple facilities, the coupling of simulations with experiment, digital twins, and ML-driven discovery. Although the urgency of LCLS facility needs may temporarily drive independent development, the LCLS Data Systems strategy is aligned with DISCUS and HPDF to build common tools and infrastructure to enable scientific discovery.

A4.7 Incorporate the transformative impact of AI/ML

At LCLS, AI/ML is used for data reduction, feature extraction, for providing analysis results (both real-time and offline), for supporting decision making during experiments, and for experiment design via the use of digital surrogates. To enable LCLS users to fully leverage AI/ML, LCLS seeks to provide seamless access to computing (GPUs) in its local facility (S3DF, the SLAC Shared Scientific Data Facility) and ASCR compute nodes. It also seeks to enable the publishing of curated “FAIR” datasets, making data findable and reusable, and provide access to algorithms developed by others, and allow easy integration into LCLS workflows. Finally, because the savings in speed and data system capacity are highest when the techniques are applied as far upstream as possible, LCLS will produce this information using accelerated algorithms running at the experiment edge – on devices close to the instrumentation, often on the detector itself – in an intelligent rather than pre-programmed manner to capture anomalous events, track evolving processes to completion, and adapt to dynamic experimental conditions and pass fast, actionable information to feedback mechanisms throughout the readout chain.