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1 INTRODUCTION & PURPOSE OF THIS DOCUMENT

A new scientific frontier opened in 2009 when the world’s first X-Ray free-electron laser (XFEL), the LCLS facility, began operations at SLAC National Accelerator Laboratory. The scientific start of LCLS has arguably been one of the most vigorous and successful of any new research facility, with a dramatic effect on a broad cross-section of scientific 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 total publications (828 papers to date associated with LCLS) and the number in high-impact journals (162 to date). There have been 441 full-scale user experiments (2009-2016), plus 177 in-house experiments and 20 blocks of protein crystal-screening. As such, the scientific productivity of the facility is incredibly high. The scientific output and impact of LCLS during the first five years are summarized in a recently published overview in Reviews of Modern Physics.

LCLS can provide ultrashort pulses (from a few-femtoseconds (fs) to >100 fs), with unprecedented peak brightness in SASE or seeded-mode operation, over an energy range from ~250 to ~12,800 eV, at 120 Hz. It now regularly provides dual-pulses with relatively arbitrary separation in time, with the option of dual color (typically 1% separation), and variable linear/circular polarization.

Details of 6 of the current suite of 7 instruments have recently been published, with the 7th instrument brought into operation in August 2016 (Macromolecular Femtosecond Xtallography, MFX). The scientific output from these instruments can be viewed on the LCLS website.

This success has helped drive the rapid development of a number of new hard-X-Ray free-electron laser facilities around the world, including SACLA (Japan), the European XFEL (Germany), PAL-XFEL (Republic of Korea), Swiss-FEL (Switzerland), as well as soft X-Ray facilities such as FLASH (Germany) and Fermi@Elettra (Italy), and a number of other possible facilities under consideration in other countries.

Looking to the future, SLAC and the US Department of Energy (DOE) Office of Science are pursuing a vigorous and well-coordinated series of developments to keep the LCLS facility in a preeminent state. The LCLS-II Project represents over a billion dollars investment to provide a new, 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 current operation at 120 pulses per second). This project will also extend the range of X-Ray energies the existing accelerator can produce from an upper limit of approximately

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2 Typically $10^{22}$ ph/s/mm^2/mrad^2/0.1% BW
5 See: https://portal.slac.stanford.edu/sites/lcls_public/Pages/Publications.aspx
12.8 keV currently to approximately 25 keV (and substantially higher using the third harmonic), providing capabilities unmatched anywhere in the world.

Beyond this, an extension to higher X-Ray energy at high repetition rate has long been requested by the LCLS user community. In response, SLAC has developed the LCLS-II-HE ("High Energy") project. This seeks to double the energy of the superconducting Linac to 8 GeV, which will extend X-Ray energy from a current cutoff of ~5 keV to at least 13 keV and likely up to 20 keV. Such a step is now technically justified on the basis of recent performance demonstrations of the cryo-cavities being assembled by the LCLS-II Project. The LCLS-II-HE proposal achieved approval of Mission Need (Critical Decision 0) in December 2016, following endorsement by BESAC and strong community support expressed at a number of workshops. Ongoing work by SLAC is centered on defining the expected “first experiments” for LCLS-II-HE via a series of workshops planned for 2017, which are informing the detailed design and instrument requirements.

More broadly, a widespread series of developments are underway to prepare for early science on LCLS-II (and subsequently LCLS-II-HE), with a view to maintaining leadership in the field of ultrafast X-Ray science. Our plans integrate theory, simulation and experiments; pursue focused R&D in critical technologies; integrate new approaches to data analysis both onsite and offsite; ensure alignment between the local SLAC science programs and the evolving LCLS facility; and engage the wider user community in an organized series of events leading up to first experiments to exploit the new facility capabilities.

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. This document represents an update to the first draft of this plan published in July 2015. Community feedback is sought.

It is important to note that the range of developments presented in this document will be selected and prioritized according to the available funding, schedule constraints, and resource availability over the next few years. Not all options will be able to be implemented, hence the need for ongoing strategic prioritization and consultation.

The priorities for LCLS development take account of the following Guiding Principles:

1. Ensure early LCLS-II experiments are able to adequately exploit the new source characteristics (e.g. via availability of suitable instruments, detectors, lasers, optics, data systems, and robust operation of the accelerator/FEL).
2. Use ongoing LCLS experiments to refine our 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, and offline developments.
3. Prioritize the exploitation of the unique characteristics of LCLS-II (and subsequently LCLS-II-HE) compared to other XFEL and storage ring facilities (e.g. the use of continuous pulse trains; the use of independently tunable XFEL beams in the soft-, tender, or hard- X-Ray regimes; the ability to probe in the ultrafast domain; and the use of X-Ray beams of unprecedented average power and spectral brightness).
4. Use the unique in-house knowledge gained from LCLS experiments to evaluate future facility configurations, instrument designs, and experimental aspirations, based on real-world experience.

5. Increase community throughput (via new multiplexing schemes; dedicated end-stations; revised operational models, etc)

6. Ensure any near-term investment in LCLS is consistent with subsequent use in the LCLS-II (-HE) context.

7. Develop systems that are highly robust and configured to run without staff intervention in ‘standard modes’, in order to enable greater control of experiments by the users, and to provide scalable, sustainable, and scientifically creative roles for LCLS staff.

The top-level facility response to the science opportunities is outlined in the upcoming sections as follows:

- Section 2 provides a brief recap of key science drivers;
- Section 3 describes the facility development plans for LCLS-II and LCLS-II-HE;
- Section 4 lists Accelerator / FEL development priorities;
- Section 5 lists Photon Science development priorities;
- Section 6 discusses improvements to Experimental Delivery;
- Section 7 describes how we are leveraging the broad scientific and technical capabilities at SLAC and Stanford to drive continued international competitiveness and leadership in the realm of ultrafast X-Ray science;
- Section 8 provides context for next steps and implementation.

For feedback on the content of this document, please contact the LCLS Director.
2  SCIENTIFIC DRIVERS

2.1  Example Scientific Drivers for LCLS-II

LCLS-II will be a transformative tool for energy science, qualitatively changing 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. This facility will provide access to the “tender X-Ray” regime (2 to 5 keV) that is largely inaccessible today, and will use seeding technologies to provide fully coherent X-Rays in a uniformly spaced series of pulses with programmable repetition rate and rapidly tunable photon energies.

In the following, we briefly summarize six broad areas of science in which the unique capabilities of LCLS-II will be essential to address critical knowledge gaps at the new scientific frontiers of matter and energy. A complete description of these science opportunities can be found in the report: New Science Opportunities Enabled by LCLS-II X-Ray Lasers (SLAC-R-1053)6

2.1.1  Fundamental Dynamics of Energy & Charge

Charge migration, redistribution and localization, even in simple molecules, are not well understood at the quantum level. These processes are central to complex processes such as photosynthesis, catalysis, and bond formation/dissolution that govern all chemical reactions. Indirect evidence points to the importance of quantum coherences and coupled evolution of electronic and nuclear wavefunctions in many molecular systems. However, we have not been able to directly observe these processes to date, and they are beyond the description of conventional chemistry models. High-repetition-rate soft X-Rays from LCLS-II will enable new dynamic molecular reaction microscope techniques that will directly map charge distributions and reaction dynamics in the molecular frame. New nonlinear X-Ray spectroscopies offer the potential to map quantum coherences in an element-specific way for the first time.

Experimental Approaches:
• Dynamic molecular reaction microscope
• Time-resolved photoemission spectroscopy
• Time-resolved Hard X-Ray scattering
• New nonlinear X-Ray spectroscopies: stimulated X-Ray Raman, core-hole correlation spectroscopy

2.1.2  Catalysis & Photo-catalysis

Understanding catalysis and photo-catalysis is essential for directed design of new systems for chemical transformation and solar energy conversion that are efficient, chemically selective, robust, and based on earth-abundant elements. LCLS-II will reveal the critical

(and often rare) transient events in these multi-step processes, from light harvesting, to charge separation, to charge migration and subsequent accumulation at catalytically active sites. Time-resolved, high-sensitivity, element-specific spectroscopy enabled by LCLS-II will provide the first direct view of charge dynamics and chemical processes 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. Such approaches will capture rare chemical events in operating catalytic systems across multiple time and length scales. The unique LCLS-II 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.

**Experimental Approaches:**
- Time-resolved X-Ray absorption and emission spectroscopy
- Time-resolved resonant inelastic X-Ray scattering
- Time-resolved X-Ray photoelectron spectroscopy
- Simultaneous soft X-Rays (spectroscopy) and hard X-Rays (scattering)
- X-Ray photon correlation spectroscopy
- New nonlinear X-Ray spectroscopies

### 2.1.3 Emergent Phenomena in Quantum Materials

There is an urgent technology need to understand and ultimately control the exotic 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.

**Experimental Approaches:**
- Time-resolved and high-resolution resonant inelastic X-Ray scattering
- Time-resolved X-Ray dichroism
- Coherent X-Ray scattering and imaging of domain dynamics
- Time- and spin-resolved hard X-Ray photoemission
- X-Ray photon correlation spectroscopy

### 2.1.4 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. 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, while coherent hard X-Ray scattering will provide...
unprecedented spatial resolution of material structure, its evolution, and relationship to functionality under operating conditions.

**Experimental Approaches:**
- X-Ray photon correlation spectroscopy
- Time-resolved X-Ray scattering

### 2.1.5 Revealing Biological Function

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 comprised 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 portents 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, at the sub-nanometer scale, the conformational dynamics of heterogeneous ensembles of macromolecules — both spontaneous fluctuations of isolated complexes and conformational changes that may be initiated by the presence of specific molecules, environmental changes, or by other stimuli. The unique LCLS-II capability for generating two-color hard X-Ray pulses will enable entirely new phasing schemes for nano-crystallography, and will resolve atomic-scale structural dynamics of biochemical processes that are often the first step leading to larger-scale protein motions.

**Experimental Approaches:**
- Time-resolved X-Ray scattering
- Time-resolved resonant inelastic X-Ray scattering/spectroscopy

### 2.2 Example Scientific Drivers for LCLS-II-HE (“High Energy”)

LCLS-II-HE will provide the U.S. with a true “discovery science” facility that greatly extends our ability to address the scientific challenges listed above. In particular, 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 in the latest report from BESAC\(^3\), by providing detailed insight into the behavior of complex matter in real-world heterogeneous samples on fundamental scales of energy, time, and length.

We highlight seven broad classes of science for which LCLS-II-HE will uniquely address critical knowledge gaps:
i. **Coupled Dynamics Of Energy And Charge In Atoms And Molecules**

Flows of energy and charge in molecules are the fundamental processes that drive chemical reactions and store or release energy. They are central to energy processes 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, and conventional chemistry models are inadequate to fully describe this. Sharper experimental tools are needed to probe these processes simultaneously at the atomic level and on natural (femtosecond) time scales. 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. The combination of hard X-Rays with high peak power and high average power will enable new nonlinear spectroscopies that promise important new insights into reactive chemical flows in complex chemical environments such as combustion.

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

ii. **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-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-HE will provide the first direct view of atomic-scale chemical dynamics at interfaces. The penetrating capability of hard X-Rays will probe operating catalytic systems across multiple time and length scales. The unique LCLS-II-HE 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
iii. Imaging Biological Function And Dynamics

LCLS-II-HE is the ideal, much-desired upgrade to LCLS-II that the structural biology community requires. The combination of high spatial and time resolution with a high repetition rate will make LCLS-II-HE a revolutionary machine for many biological science fields. At high repetition rates, serial femtosecond crystallography (SFX) will advance from successful demonstration experiments to addressing 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

iv. Materials Heterogeneity, Fluctuations, And Dynamics

Heterogeneity and fluctuations of atoms and charge-carriers – spanning the range from the atomic scale to the mesoscale – underlie the performance and energy efficiency of functional materials and hierarchical devices. Conventional models of ideal materials often break down when trying to describe the properties that arise from these complex, nonequilibrium 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 nonequilibrium 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. 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

v. Quantum Materials And Emergent Properties
There is an urgent technological need to understand and ultimately control the exotic quantum-based properties of new materials – ranging from superconductivity to ferroelectricity 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. 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 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-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

vi. Materials In Extreme Environments
LCLS-II-HE studies of extreme materials will be important for fusion and fission materials applications and could lead to important insights into planetary physics and geoscience. The unique combination of capabilities from LCLS-II-HE will enable high-resolution spectroscopic and structural characterization of matter in extreme states that is far beyond what is achievable today. 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
vii. Nonlinear X-Ray matter interactions

A few seminal experiments on the first generation of X-Ray free-electron lasers, LCLS and SACLA, have demonstrated new fundamental nonlinear hard X-Ray-matter interactions, including phase-matched sum frequency generation, second harmonic generation, and two-photon Compton scattering. While nonlinear X-Ray optics is still in the discovery-based science phase, advances in our understanding of these fundamental interactions will lead to powerful new tools for atomic and molecular physics, chemistry, materials science, and biology via measurement of valence charge density at atomic resolution and on the attosecond-to-femtosecond timescale of electron motion. The combination of high repetition rate and high peak intensity pulses from LCLS-II-HE will enable high-sensitivity measurements that exploit subtle nonlinear effects. This will transform the nonlinear X-Ray optics field from demonstration experiments to real measurements that utilize the nonlinear interactions of “photon-in, photon-out” to simultaneously access transient spectroscopic and structural information from real materials.

Grand-challenge science areas addressed:

- Control Matter at the Level of Electrons
- Emergent Properties from Complex Electronic and Atomic Correlations
3 MAJOR FACILITY DEVELOPMENT

3.1 LCLS-II Project

Working closely with DOE’s Office of Science, the LCLS-II Project has been configured to meet a series of requirements laid out by the Basic Energy Sciences Advisory Committee (BESAC), in response to the above scientific drivers.

The LCLS-II design:

- Adds a new, 4 GeV superconducting linac in an existing SLAC tunnel, avoiding the need for excavation.
- Increases the repetition rate from 120 pulses per second to 1 million per second. It will be the world’s only X-Ray free-electron laser capable of supplying a uniformly-spaced train of pulses with programmable repetition rate.
- Provides a tunable source of X-Rays, by replacing the existing undulator (used to generate X-Ray laser pulses) with two new ones. This ability to tune the X-Ray energy on demand will enable scientists to scan across a wide spectrum – opening up new experimental techniques and making efficient use of the valuable beam time.
- Provides access to an intermediate X-Ray energy range (2 – 5 keV) that is currently inaccessible with LCLS, but which is likely critical for studies of new materials, chemical catalysis and biology.
- Supports the latest seeding technologies to provide fully coherent X-Rays (at the spatial diffraction limit and near the temporal transform limit).
- Maintains the existing copper-based warm linac and upgrades parts of the existing research infrastructure to take advantage of the new configuration.
- Extends the operating range of the facility from its current limit of ~12.8 keV X-Rays to ~25 keV using the existing 120 Hz accelerator.
- Provides for a factor ~2 increase in experimental capacity, addressing a principal limiting factor of LCLS (wherein only ~20-25% of proposals can be scheduled).

The detailed scientific potential of the upgraded LCLS facility was explored in a number of consultations with the user community, culminating in a series of user workshops\(^7\) and a summary of the science opportunities for the next decade\(^8\).

The LCLS-II Project is being led by the SLAC National Accelerator Laboratory in collaboration with four other DOE national laboratories: Argonne, Berkeley Lab, Fermilab, Jefferson Lab, and Cornell University (See Figure 1).

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\(^7\) See: [https://portal.slac.stanford.edu/sites/conf_public/LCLS2ScienceFeb15/Pages/default.aspx](https://portal.slac.stanford.edu/sites/conf_public/LCLS2ScienceFeb15/Pages/default.aspx)

\(^8\) See: [https://portal.slac.stanford.edu/sites/lcls_public/lcls_ii/Pages/science.aspx](https://portal.slac.stanford.edu/sites/lcls_public/lcls_ii/Pages/science.aspx)
The LCLS-II project requires two extended periods to modify infrastructure and install new hardware in areas where the LCLS beam is operating. Work in these areas precludes LCLS beams and so LCLS user operations must be suspended. In the project baseline, a 6-month and a 12-month down period are scheduled to begin mid-December 2016 and June 2018 respectively (see Figure 2). Modifications to the Near Experimental Hall (NEH) and some instrument installation activities are expected to occur during these periods.

The new LCLS-II superconducting (SC) linac is expected to begin commissioning in summer 2019, near the completion of the 12-month downtime. The HXR undulator will be commissioned with the Cu linac after the shutdown is complete, at around the same time the SC linac commissioning begins. The HXR and SXR undulators are scheduled to be commissioned with the SC linac in early 2020. The availability of the SC linac is expected to
ramp up over 5 years to the target availability of 95% with 4500 scheduled user hours. Following commissioning, the HXR will be able to be driven alternately by the Cu or SC linac with corresponding high-energy experiments or high repetition rate experiments, while the SXR will continue to be driven from the SC linac. The SC linac beam performance will also ramp up to final performance specifications over the first few years. Ramped commissioning is essential since the undulators can be permanently damaged in minutes if the electron losses are not carefully limited at full beam power. Therefore the beam power allowed in each undulator will be closely controlled and ramped up slowly while undulator magnets are regularly characterized and electron beam losses are carefully monitored and minimized.

Similar to the initial start up years of LCLS, the experimental areas/instruments will be commissioned in a phased approach. The details of the commissioning order and timeline are shown in the following section.

3.2 Instrument Development for LCLS-II

Many options exist for the LCLS facility to adapt its current suite of instruments to the opportunities presented by the LCLS-II upgrade. Over the long term this could include the commissioning of new experimental halls, given the ability of the superconducting accelerator to feed up to 8 or 10 undulators. This would greatly relieve the capacity limitations of the current facility, and allow optimized beamlines for each spectral region and/or experimental technique.

In the near term, it is obviously important to ensure that best use is made of the upgraded capabilities, to take full advantage of the high repetition-rate and extended spectral coverage, and to explore the emergent techniques for this new class of X-Ray FEL.

Adaptation of the hard X-Ray instruments is straightforward for use of the existing Cu Linac with the new undulator. New optics are required to ensure high quality throughput, extension to 25 keV, and improved beam-splitting options.

Adaptation of the soft X-Ray instruments is more involved, as is the extension to tender X-Ray coverage (~2-5 keV). An approach to optimize the Near Experimental Hall (NEH) has been determined following extensive consultation with the user community. An outline is presented here, and further details can be found on the LCLS website.9

The top-level design principles being applied to the new instrument area are as follows:

i. Maximize the time spent on scientific data production.
   • Automated alignment of the beam and end-stations where possible.
   • Quantitative goals for the time and effort required for changes in configuration (aiming for changes in “minutes & hours”, not “days and weeks”), along with % availability of beam-on-sample in data–taking mode.

ii. Deliver a design that allows the role of Instrument Scientists and design engineers to focus on the innovative development of their scientific/technical field, so that they can provide LCLS with a greater competitive edge in science delivery.

9 See: https://sites.google.com/a/stanford.edu/l2si/
iii. Use the high rep-rate beam as the primary driver for experimental prioritization and facility design.

iv. At the earliest stage of design, ensure integration of the instrument designs with the required next-generation detectors, pump/probe requirements, in-situ beam diagnostics, etc.

v. Determine an explicit path to move from "First Experiments" to "mature" and "stretch" goals.

vi. Diagonalize the science objectives at a facility level – not at an instrument level – to allow flexibility in design response.

vii. Assume LCLS-II-HE is implemented to come online shortly after LCLS-II

The solution to-date accommodates four X-Ray branch lines from the soft X-Ray undulator (SXU), and preserves the current suite of five hard X-Ray instruments (XPP, XCS, MFX, CXI, MEC). One of the SXU lines is combined with a branch-line from the hard X-Ray undulator into a multi-purpose tender X-Ray instrument.

The SXU branch lines are created via reflective and grating optics located in the front end enclosure (FEE). They distribute the X-Ray beam to four hutsches (NEH 1.1, NEH 1.2, NEH 2.1, NEH 2.2). As part of this, a new tender X-Ray branch line is created that also operates on the hard X-Ray undulator (HXU) and delivers beam to NEH 1.2. This solution involves substantial modifications to the Near Experimental Hall (NEH) to allow the construction of:

- Two new X-Ray hutsches on the NEH first (upper) floor level.
- Modified X-Ray hutsches on the NEH sub-basement level (replacing AMO and SXR)
- Optical laser laboratories in close proximity to the X-Ray instruments
- Dedicated control rooms for each instrument
- An expanded data/server room

An overview of the revised instrument layout is provided in Figure 3, and a schematic model of the modified NEH subbasement and 1st floor is displayed in Figure 4.

For NEH-1.1, the branch-line is designed with a minimalist approach to maximize the optical throughput.

NEH-1.2 can accept beam from either the SXU and/or the HXU source. Two independent distribution mirror pairs are used to deflect the beams into NEH 1.2 where the beams cross. This configuration allows users to not only take advantage of the specific properties of each undulator source, but to use both sources simultaneously for X-Ray pump/X-Ray probe studies.

For NEH-2.1 and NEH-2.2, a variable resolution grating monochromator is used to direct soft X-Rays (0.25-1.2 keV) to the two experimental areas 1st floor. This system employs multiple gratings and a bendable mirror to create a variable resolution/throughput. The bifurcation of the NEH 2.1 and 2.2 lines is achieved via an insertable horizontal focusing mirror that deflects the beam to NEH 2.1 with an associated ~10 µm focal beam size.
Figure 3 Revised instrument layout, as fed from the 2 new undulators from the LCLS-II Project, covering the soft X-Ray (SXU) and tender/hard X-Ray (HXU) regime.

Figure 4 Schematic model of the modified NEH lower, sub-basement floor (top image) and the upper, 1st floor (lower image).
The hard X-Ray FEE distribution mirrors will be modified to improve their performance in terms of transverse acceptance and harmonic rejection. This will be accomplished by increasing the incidence angle and partially coating the Si substrates with a metallic coating (e.g. Cr). The Cr coating would be used for the 15 – 25 keV photon energy range. The reflectivity of these mirrors drops dramatically above 25 keV and thus harmonics are greatly suppressed. The Si substrate will be used for photon energies below 15 keV, where harmonics greater than 15 keV are suppressed.

The nominal phased delivery schedule for the 4 new instrument areas (dependent on funding and resource availability) is:

- NEH 1.1 Jan 2020
- NEH 2.2 June 2020
- NEH 1.2 Jan 2022
- NEH 2.1 Jan 2023

It is important to note that the detailed design of these instruments is rapidly evolving. Please refer to the LCLS website for up-to-date information. This provides details of the scientific fields being served; the experimental approaches being adopted; source characteristics; beamline and endstation designs; and detector/laser system specifications.

### 3.3 LCLS-II-HE Project

LCLS-II-HE will provide a qualitatively new capability, unique in the world, delivering ultrafast atomic resolution at high average power. The project is a natural extension to LCLS-II, adding known technology and using existing infrastructure. It will extend 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 Basic Energy Sciences Advisory Committee (BESAC) assessed this project in 2016, and concluded that “... the LCLS-II-HE project is considered to be ‘absolutely central to contribute to world leading science’ and ‘ready to initiate construction’”. Subsequent action by DOE led to Mission Need (Critical Decision 0) being approved in December 2016.

The energy reach of LCLS-II-HE (stretching from 5 keV to at least 13 keV and likely up to 20 keV) 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.
The performance of LCLS-II-HE will allow access to the ‘hard X-Ray’ regime, providing atomic resolution capability, with an average brightness roughly 300 times the ultimate capability of a diffraction-limited storage ring (DLSR). Self-seeding will further increase the average brightness of the XFEL facilities by an additional factor of 20 to 50.

The facility will:

- Deliver **two to three orders of magnitude increase in average spectral brightness beyond** any proposed or envisioned diffraction-limited storage ring (DLSR), exceeding the anticipated performance of the European-XFEL.
- 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 proposed or envisioned 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.
- Combine **three independent accelerators** into a single facility, representing an unprecedented level of flexibility for the user community (a new 8 GeV superconducting linac; a separately tunable 3.6 GeV line for the LCLS-II instruments; and the existing 15 GeV Cu-linac). **No other facility in the world will have this capability.**

To achieve this, the LCLS-II-HE project will add 19 cryomodules of the type already being manufactured for LCLS-II, 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.

Therefore, this solution represents a low-risk path with dramatic scientific impact. It will incorporate a linac bypass line to allow simultaneous operation of the soft X-Ray and hard X-Ray undulator sources with optimum electron beam energies, coupled with myriad beam-sculpting techniques developed on LCLS, including bandwidth control via seeding, multi-pulse operation, and delivery of the 3rd harmonic (opening up new areas of science in the energy range 20 to 50 keV).

LCLS-II-HE will lead to significant scientific impact, enabled by a suite of unmatched technical attributes:

I. **Access to the energy regime above 5 keV**: This is particularly important because it allows analysis of key chemical elements in addition to providing atomic resolution. For example, this regime encompasses Earth-abundant elements that will be 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, used for protein crystallography. This is illustrated in Figure 7.

![Figure 7](image)

**Figure 7** The spectral region above 5 keV (the design limit of LCLS-II) is a critical area for many types of measurements. Access to Ångström wavelength (~12.4 keV) X-Rays is a major enabling step for atomic-scale studies, while the ability to probe Earth-abundant elements and access experimental regimes central to biological structure determination and quantum materials studies will provide a fundamentally new capability for discovery science.

II. **High repetition rate, ultrafast hard X-Rays** from LCLS-II-HE 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 5 fs, coupled to the capability for double pulses with independent control of energy, bandwidth, and timing. Ongoing development programs offer the potential for 0.5 fs pulses.

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 events:** 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.

4 **PHOTON SYSTEM DEVELOPMENT**

4.1 **Scientific Technique Development for LCLS-II**

The distinguishing capabilities of the LCLS-II upgrade (high repetition rate ultrafast X-Ray pulses with both longitudinal and transverse coherence, along with two new tunable undulators) will enable entirely new X-Ray techniques that will be important for many areas of science, and will significantly advance X-Ray techniques that have been pioneered at the LCLS facility to date.

This section outlines the development plans for 5 ambitious new X-Ray techniques (focusing on the key instrumentation-related components), and maps them onto the new suite of beamlines. Where appropriate, time will be made available on the existing facility and/or during early operation of LCLS-II to explore these emerging techniques and inform their future potential:

- Fluctuation X-Ray scattering – *interacting complexes and assemblies in natural environments*
- Stimulated X-Ray Raman spectroscopy – *ultrafast charge-transfer dynamics*
- Core-hole correlation spectroscopy – *quantum coupling of valence charge states*
- Single-particle imaging – *toward atomic resolution*
- Dynamic multi-view tomography – *chemical mapping of reactive flows*

4.1.1 **Fluctuation X-Ray Scattering - interacting complexes and assemblies in natural environments**

Fluctuation X-Ray scattering (fSAXS) is a promising route for 3-D imaging of anisotropic ensembles of interacting complexes in natural (solution) environments. fSAXS is an extension of well-developed SAX/WAX techniques, but in a regime in which the X-Ray exposure is much shorter than rotational diffusion times. This gives rise to anisotropic scattering patterns (with annular correlations or fluctuations) which contain $\sim$100 times greater information content than typical isotropic SAX/WAX patterns, thus enabling the reconstruction of 3-D objects.

LCLS-II instruments NEH 1.1 and NEH 1.2 will enable the full development of fSAXS as a powerful scientific tool. The requirements (and development road map) are quite similar to
those for single particle imaging as described above, with the following differences and additional requirements:

- Adjustable X-Ray focus from ~1 µm to ~50 µm (depending on sample concentration etc.)
- Photon energy range: both tender X-Rays (2-8 keV\textsuperscript{10}) and soft X-Rays (0.3-1.2 keV) are needed for different applications, and to exploit larger scattering cross sections, resonant scattering, and transmission in the water-window.
- Moderate initial resolution goal >1 nm
- High repetition rate (limited by detector read out) to exploit the highest average X-Ray flux.

In the fSAXS approach, annular correlations from many scattering patterns (at modest S/N) can be summed. Thus, fSAXS will exploit the high repetition rate of LCLS-II (limited by detector read out) to achieve the highest average X-Ray flux. This will be complemented by the development of fSAXS at 120 Hz using the maximum flux/pulse to provide individual scattering patterns with high S/N.

### 4.1.2 Stimulated X-Ray Raman Spectroscopy (SXRS)

Stimulated X-Ray Raman spectroscopy represents a broad class of nonlinear X-Ray processes that are anticipated to have significant scientific impact, and are uniquely enabled by the capabilities of LCLS-II. Here we development plans and basic requirements for 3 of the most important examples of SXRS: stimulated X-Ray emission, coherent X-Ray Raman, and X-Ray coherent anti-Stokes Raman spectroscopy (XCARS):

**Stimulated X-Ray emission** is a potentially powerful complement to spontaneous X-Ray emission (XES or RIXS) processes for probing excited-state valence charge dynamics. Three key advantages are (1) weak emission processes can be enhanced by the stimulating photon, effectively competing with Auger and other relaxation channels, (2) the emitted signal of interest is directional, allowing for efficient 0-D detectors in place of collection optics which cover only a small fraction of the 4π spontaneous emission, and (3) the resolution is determined by the bandwidth of the stimulating pulse, eliminating the need for complex (and inefficient) spectrograph optics. Following are some of the key requirements for developing and exploiting this process:

- Two-color pulses with energy spacing tunable within ~100 eV (XANES region)
- Small energy spacing (~10 eV or ~2%) may exploit the two-bunch FEL approach with ~±35 fs relative time delay
- Larger energy spacing (and larger relative delay range) may exploit the split undulator approach
- <10 fs pulse duration (comparable to the Auger lifetime), ideally close to transform limit
- Photon energy tunable over the soft X-Ray range from 0.25-1.2 keV to access lighter elements (C, O, N, ...) and the transition-metal L-edges, and in general to exploit larger cross-sections in the soft X-Ray range.

\textsuperscript{10} Experiments at high repetition rate with energy > 5keV will require LCLS-II-HE
• ~1 µm focus (adjustable) to optimize X-Ray nonlinearity (possible line focus for spatial resolution)

The above parameters can be met at instruments NEH 1.1 and NEH 1.2, and the latter provides greater flexibility to accommodate specialized endstations to detect and develop stimulated X-Ray emission for science applications.

**Coherent X-Ray Raman Spectroscopy (CXRS)** is a nonlinear (2-photon) X-Ray interaction, closely related to the stimulated emission process described above, but configured to create a non-stationary electronic wavepacket in a molecule (or extended solid) that is localized at an atom of interest, based on an X-Ray core transition resonance. The wavepacket consists of an exited manifold of valence states, and is a potentially very powerful new means for understanding charge flow in matter (e.g. light harvesting complexes, photo-catalysts, etc.). Following are some of the key requirements for developing and exploiting this process:

- Broad coherent bandwidth (2-5 eV) to couple to a manifold of valence excited states
- <10 fs pulse duration (comparable to the Auger lifetime), ideally close to transform limit
- Photon energy tunable over the soft X-Ray range from 0.25-1.2 keV to access lighter elements (C, O, N,...) and the transition-metal L-edges, and in general to exploit larger cross-sections in the soft X-Ray range.
- Based on typical transition cross-sections, the “threshold” for nonlinear interaction is estimated to be \( \sim 10^{17}-10^{18} \) photons/cm\(^2\). This corresponds to \( \sim 10^9-10^{10} \) photons/pulse in a 1 µm focus (\( \sim 10^{16} \text{W/cm}^2 \) at 500 eV).
- ~1 µm focus (adjustable) to optimize X-Ray nonlinearity

The above parameters can be met at instruments NEH 1.1 and NEH 1.2. These also support a range of endstations capabilities (e.g. photo-electron and ion spectroscopy, XAS etc.) for characterizing the electronic wavepacket and associated dynamics. Ultimately we will exploit the two-color capabilities of LCLS-II to apply CXRS at one atomic site as an excitation, and a second CXRS process at a second atomic site as a probe.

**X-Ray Coherent Anti-Stokes Raman Spectroscopy (XCARS)** is a variant of stimulated X-Ray emission (as described above), but configured to probe dynamics of low-Z elements within a dense media (e.g. aerosols in ambient gas pressures, or chemistry in a combustion environment) with chemical/element specificity. Following are some of the key requirements for developing and exploiting this process:

- Two-color pulses with \( \Delta E \sim 280 \) eV (carbon edge)
- Tender X-Ray energies for penetration of dense media (gas at atmospheric pressure, aerosols etc.)
- <10 fs pulse duration (comparable to the Auger lifetime), ideally close to transform limit
- ~1 µm focus (adjustable) to optimize X-Ray nonlinearity (possible line focus for spatial resolution)

The above parameters may be met at NEH 1.2 using 3 keV photons from the HXU driven by the SCRF and 2.7 keV from the SXU (e.g. \( 3\omega \times 900 \) eV) similarly driven by a second delayed
bunch from the SCRF. Compensation of the delay (~10 ns inter-bunch spacing) may be accomplished via Bragg optics. NEH 1.2 provides access for optimized (roll-up) endstations to detect and develop XCARS for a range of science applications.

4.1.3 X-Ray Core-hole Correlation Spectroscopy

This a two-pulse, two-color multidimensional X-Ray technique that is a promising approach to reveal the quantum coupling between excited valence electronic states in molecules (e.g. light harvesting complexes). Following are some of the essential parameters to develop and exploit this process:

- Two-color pulses with >100 eV energy spacing tunable over the soft X-Ray range from 0.25-1.2 keV to access different atomic species: e.g. C (280 eV), N (410 eV), O (535 eV), Fe L-edge (710 eV), Cu L-edge (910 eV)
- Split undulator approach for large energy spacing
- Relative pulse delay ~±35 fs from FEL
- <10 fs pulse duration (comparable to the Auger lifetime), ideally close to transform limit
- 0.1-1 µm focus to enhance X-Ray nonlinearity

The above parameters can be met at instruments NEH 1.1 (or NEH 1.2 with larger focus) with the caveat that the small focus will likely require the incorporation of a compact KB mirror pair within the endstation chamber (close to the sample).

4.1.4 Single-particle imaging – toward atomic resolution

LCLS and the scientific community have developed a comprehensive road map to advance the development of single particle imaging (coherent diffractive imaging), with a goal of reaching 3 Å resolution of biological objects\(^\text{11}\). Key X-Ray source requirement identified in this road map include:

- Target photon energy range: 3-8 keV
- Pulse duration <20 fs with maximum flux/pulse
- Clean X-Ray focus of 100-200 nm (minimize beamline scattering)

LCLS-II instruments NEH 1.1 and NEH 1.2 will be developed toward meeting as many of these objectives as possible. In addition, an extension of scope to allow the warm Cu linac in combination with the SXU will generate X-Rays with >5 mJ/pulse at 120 Hz. Beamline optics will deliver pulses to either NEH 1.1 (0.25-3 keV) or NEH 1.2 (0.4-3 keV), with KB mirrors to provide a clean ~500 nm focus.

Detector development for single particle imaging will focus on:

- Optimum quantum efficiency in the tender X-Ray range
- Single photon counting at high-q and sub-Poisson noise elsewhere
- ~10^4 dynamics range, <100 µm pixel size
- High read out rates (>1 kHz)

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In addition to the development of high-intensity single-shot X-Ray imaging in the tender X-Ray regime, LCLS-II will enable the development of new approaches to biological imaging from large data sets of relatively low-contrast scattering patterns collected at high repetition rate (limited by the detector read out). High repetition rate X-Rays from the SCRF linac will be available at both NEH 1.1 and NEH 1.2 instruments.

4.1.5 Dynamic multi-view tomography – chemical mapping of reactive flows

The high repetition rate of the LCLS-II lends itself to imaging dynamic chemical processes in-situ or under operating conditions. The ability to image in 3-D chaotic real time processes such as turbulent flame combustion, liquid jet breakup, fracture propagation in materials, and self-ordering in crystallization provides important new insight and allows for the validation of computational models.

The general theme of 3-D dynamic tomography is the simultaneous view of the sample from multiple directions. Newly developed iterative reconstruction routines allow for only a few views and the additional constraints imposed by motion-tracking optical flow algorithms, gradient approaches, and spatiotemporal analysis constraint the individual images, improving reconstruction and reducing noise. Various optical schemes can be devised to optimize for a particular X-Ray energy range of interest.

In the soft X-Ray regime, a transmission grating (or convex grating in conical diffraction geometry) may be used to generate multiple diffraction orders. Multilayer mirrors may then be used to provide multiple instantaneous views of the sample from different angles. In the tender X-Ray regime, crystals may be used in a wave-front splitting geometry to generate multiple beams, with additional crystals to re-direct the beams onto the sample to provide multiple instantaneous views. Following are some of the essential parameters to develop and exploit this process:

- Maximum average flux in the soft and tender X-Ray regimes
- Optical instrumentation for generating and manipulating multiple beams of soft or tender X-Rays
- Fast 2D detectors in the soft and tender X-Ray range
- ~25 µm pixels, 1k×1k, ~10²-10³ ph/pixel/pulse

4.2 X-Ray Optics Development

4.2.1 Optics development for transient grating studies, four wave mixing and multidimensional spectroscopy

The full potential of XFELs will be achieved when they not only provide a lot of X-Rays in a short time, but can be used in the same way that optical lasers are used today for experiments such as transient grating spectroscopy, four wave mixing and multidimensional spectroscopy more generally. Developments at FERMI@Elettra have already demonstrated transient grating experiments in the XUV to soft-X-Ray range, and they are on the brink of commissioning a four wave mixing experiment. The development of all of these spectroscopies will qualitatively impact the science reach of LCLS-II(-HE).
Demonstration experiments can be performed on LCLS-I today, and will benefit from targeted development of the component optics and underlying theory.

4.2.2 Distribution and focusing mirrors

To preserve the source characteristics, in particular to preserve the wavefront in and out of focus, the demands on mirror shape precision are very high. A shape error of 0.5 nm rms and a radius of curvature larger than several hundred kilometers is needed in most of the energy range. Such precision also needs to be preserved when the mirror is irradiated by the high repetition rate source, with as much as 200 W incident on the mirror. The main difference with respect to Synchrotron Radiation mirrors is the challenge of implementing liquid nitrogen cooling (due to contamination and vibration issues) and the fact that the footprint on the mirror changes considerably with the photon energy. In fact, a beam footprint smaller than the mirror length (as in the case of LCLS-II for certain energies) induces a significant temperature variation in the tangential direction. The resulting thermal 'bump' around the beam footprint is not spherical and is therefore difficult to correct with a bender.

To face such challenges, LCLS is developing a new scheme for active shape control, which combines variable cooling with applied auxiliary heating, and is tailored to the spatial distribution of the incident thermal load. These developments are funded in part directly by DOE-BES via the REAL project, involving a partnership with BNL, ANL and LBNL. The underpinning approach, known as “Thermal Portrait Mirror Figure Control” (TPMFC), may achieve sub-nanometer surface figure error control. An initial finite-element study suggests that TPMFC can reduce surface height errors by more than 10x, compared to traditional, full-length cooling.

4.2.3 Variable resolution beamline for RIXS experiments

A RIXS endstation is planned for the upper floor of the NEH, designed to cover the energy range 250 eV to 1500 eV.

To deliver the beam upstairs, it is necessary to tilt the beam to quite a large angle, namely 7.1°, while ensuring any single angle of incidence is kept below 1.6° in order to reach 1500 eV and to avoid mirror and grating ablation. The initial concept is to use a first mirror (M1) with fixed incidence angle and use the monochromator system, Grating-M2, to deflect (or diffract) further (Figure 8).

To obtain variable resolution (from <3,000 to >50,000) it is necessary to both use a few gratings (three minimum) and to change the working configuration of the grating (Figure 9). This is achieved through the use of a bendable first mirror. This can produce a virtual focus behind the grating to reduce the resolving power when needed, preserving the total deflection onto the monochromator. To continue to focus the beam into the fixed exit slit, the angle of incidence on the grating shall be increased when the source becomes negative (e.g. when the beam is focused by mirror M1). This preserves the angle of diffraction by reducing the number of illuminated lines and the angle of diffraction. Both effects reduce the resolving power. A maximum safe angle of incidence shall be preserved to avoid ablation on the grating. The grating will have a variable groove density. The resolution can be changed by focusing the beam with M1, to change its shape from flat (e.g. no source distance alteration) to a minimum of 3 km of radius of curvature for low resolution.
Figure 8 Scheme of the Variable resolution beamline. M1 is a bendable mirror deflecting the beam upward by 2.2° (full angle). The grating-M2 deflects the beam up by further 4.9° and the following two mirrors, one flat and one focusing, bring the beam again parallel to the ground. A sixth mirror is used to focus the beam horizontally.

Figure 9 Resolving power for 300 eV (red curves) and 1,000 eV (black curves) as a function of the groove densities; 50 l/mm solid fat line, 100 l/mm dash lines, 400 l/mm thin solid lines and 1200 l/mm dotted line.

Considering all the mirrors and the grating efficiency, optimized for flux rather than for high harmonic suppression, the photons per second delivered to the sample can be as high as $10^{15}$ even for a resolution of 50,000. This large number of photons is mainly due to the high repetition rate of the source. This gives several orders of magnitude of flux enhancement delivered to the sample with respect the most advanced synchrotron beamlines with comparable resolving power.
**RIXS spectrometer**

The RIXS spectrometer for NEH2.1 is based on a spherical VLS grating with fixed angle of incidence and to achieve a resolving power of 30,000 or higher across the photon energy range. The distance between sample and grating is set to be 1 m and the maximum detector distance from the sample will be below 6 m (Figure 10).

**Figure 10** Scheme of the proposed 6 m RIXS spectrometer

The expected resolving power is calculated considering a 10µm vertical spot on the sample and 10µm spatial resolution for the detector (Figure 11). A resolving power in excess of 30,000 is expected up to 900 eV, while it is larger than 20,000 over the entire range. At the maximum resolution, a count rate as high as 100,000 counts/sec are expected for standard RIXS spectrum peaks. This is roughly three orders of magnitude higher than the achievable levels on synchrotron sources with lower resolution.

**Figure 11** Expected resolving power for the 1800 l/mm grating. A 10 µm spot size and 10 µm spatial resolution for the detector are considered in the simulation.
4.3 Advanced Detector Systems

This section provides a very brief overview of the LCLS Detector Strategy. A more comprehensive detector strategy has been detailed separately.

The most taxing requirements are to provide area detectors for soft and tender X-Rays at a readout speed of few kHz for the initial period of LCLS-II operations, scaling to tens of kHz thereafter. Similar performance will be required in the Hard X-Ray regime for LCLS-II. In addition, SLAC is pursuing the development Transition Edge Sensor (TES) technology to enable spectroscopy at very high repetition rates with sub-eV resolution. More conventional spectroscopy and detection systems employing 1D readout are already available, able to function at the full (1MHz) repetition rate.

To achieve these goals, multiple pathways are being developed in parallel, to reduce the risk to delivery in time for LCLS-II.

A very-fast CCD is being developed in collaboration with LBNL. This 1 Mpixel area detector will provide high quantum efficiency in the 250-1200 eV energy range with very low noise and kHz frame rate. To achieve this readout speed, a fully column-parallel CCD together with its corresponding readout and data acquisition system has to be developed. The main difference with conventional CCDs consists in eliminating completely the output transistors (typical source-follower configuration) to directly couple the charge into a low impedance preamplifier, implemented in a readout chip. Each readout channel is then directly wire-bonded to a CCD column. To achieve high quantum efficiency at low photon energy the detector entrance window has to be very thin. A low temperature contact created by molecular beam epitaxy (MBE) will be used to provide good soft X-Ray quantum efficiency.

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. This class of detectors is currently able to provide a readout speed matching the LCLS repetition rate (120 Hz) 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, while maintaining low noise and high maximum signal (10,000 8 keV photons equivalent). Extension to 10’s kHz operation is also under development, for deployment in the mid-2020s. Thanks to the intrinsic scalability of hybrid pixel array detectors, large areas can be covered and maintained in a sustainable way. Specifically, two major development projects are underway: ePix-M (based on CMOS technology for the soft X-Ray regime), and ePix-HR (as an extension to the current ePix-100 and ePix-10k systems for the tender/hard-ray regime).

The current versions of these ePix detectors can be modified to use different sensor materials, such as Ge or GaAs, to increase the quantum efficiency at higher photon energy (25 keV).

To provide an alternative pathway to very high repetition rates (>10 kHz), SLAC has partnered with Fermilab to develop a novel detector, FLORA (Fermilab-LCLS CMOS 3D-integRated detector with Autogain), with the objective to deliver very low noise, high dynamic range and fast readout suitable for imaging experiments using soft-X-Rays with LCLS-II. Funded by DOE-BES, this system aims to provide small pixels (~50 µm), adaptive gain (leading to handling up to 1,000 photons per pixel per frame with a single photon
resolution), high quantum efficiency in the energy range between 250 eV and 2 keV), and tileable to cover large areas (solid angle).

Transition Edge Sensor (TES) micro-calorimeters can provide a unique combination of spectral resolution and efficiency. Superconducting detectors are intrinsically capable of very high energy resolution. The challenges with such detectors have been the small number of pixels possible in an array, the low readout rate, a low fill factor (active/total area), and the need for sub-Kelvin cooling. Recent advances in each of these aspects makes TES spectrometers a very interesting alternative to standard grating spectrometers. Ongoing R&D aims to provide spectrometers for pulsed sources with multi-kHz frame rates and ~0.5 eV resolution at 1 keV, with initial (lower specification) operation in time for first science on LCLS-II.

To address high field physics applications, a detector is needed that is capable of measuring the 3d momentum for hundreds of particles per laser shot in coincidence at very high pulse repetition rates. A prototype ‘Tixel’ detector is under development at SLAC to meet this need. A prototype is already capable of 2kHz frame readout rate, with potential to extend to upwards of 10kHz. With the implementation of an on-chip zero suppression / sparse data readout, the design should be able to operate at 100 kHz. If successful, this detector will also have huge impact on multiple other experimental techniques and will replace the delay-line detectors in COLTRIMS and coincidence spectrometers (while removing the number-of-hits-per-shot limitation), phosphor-based velocity-map-imaging detectors (removing the rep rate limitation), and supersede most other position-sensitive particle detector.

4.4 Data Systems Strategy

The high repetition rate (1 MHz) and, above all, the potentially very high data throughput (100GB/s) capable of being generated by LCLS-II will require a major upgrade of the data acquisition and storage system and increased data processing and data management capabilities. The main challenge will be developing high density, high-throughput, petabyte scale storage systems that allow concurrent access from thousands of jobs.

Another critical feature is the deployment of a trigger/veto system to veto the readout process for uninteresting events, thus reducing the data throughput. Development of such a system requires in-depth consultation for each class of experiments, to arrive at a practicable balance between data throughput and subsequent data mining capability. This is currently underway, working with the LCLS Users Executive Committee (UEC) and individual user groups to determine the most appropriate solutions for this Data Reduction Pipeline (DRP).

This strategy is motivated by the following aspects:

i. **LCLS-II Upgrade**: The high repetition rate (1-MHz) and, above all, the potentially very high data throughput (100GB/s) generated by LCLS-II will require a major upgrade of the data acquisition system and increased data processing capabilities [2], [3].

ii. **Fast feedback**: Experience has shown that a capable real-time analysis is critical to the users’ ability to make informed decisions during an LCLS experiment. Powerful fast feedback (~ minute or faster timescales) capabilities reduce the time required to complete the experiment, improve the overall quality of the data, and increase the success rate of the experiments.

iii. **Time to science**: Sophisticated analysis frameworks can significantly reduce the time between experiment and publication, improving the overall productivity of the LCLS science community.

iv. **No user left behind**: Most of the advanced algorithms for analysis of the LCLS science data have been developed by external groups with enough resources to dedicate to a leading edge 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 forced into collaborations with larger groups. LCLS support for externally developed algorithms and the development of in-house algorithms for some specific science domains, would alleviate this problem.

This strategy is organized into a three-pronged approach aligned with the following areas:

i. **Infrastructure**: This area includes the systems for processing and managing the LCLS data: computing farm, disk and tape storage, network, data movers, experiment portal.

ii. **Tools**: This area includes all the core software needed by the LCLS users to access and analyse their data: build tools, documentation tools, version control, visualization, calibration, data persistency, and basic data analysis algorithms like fitting and filtering.

iii. **Algorithms**: This area includes the adoption, development and support of advanced algorithms specific to the various LCLS scientific areas: hit finding, indexing, diffraction patterns integration, macromolecular structure determination, etc.

Where possible, LCLS will pursue partnerships with other facilities and make every effort to leverage the work and expertise of the community to solve common problems. LCLS personnel will encourage the collaboration between software engineers, instrument scientists and users to ensure that code and algorithms are shared. Open source tools will be used where feasible, and shared repositories will be used to store and distribute code to users. LCLS personnel will work closely with the users and scientific staff to provide resources to install, understand, and use the analysis software. By participating in the development of these algorithms and actively communicating with users, LCLS staff can ensure that these algorithms are portable and reusable around the world.

We envision an evolution of the LCLS data system where the fast feedback storage layer is built on flash memory and where the offline processing and storage capabilities can be
offloaded to multiple facilities, such as NERSC. See the data strategy referenced above for further details.

LCLS recognizes the central role advanced algorithms and computing have in x-ray science and facility operations. The facility, however, does not have adequate resources to maintain a fully staffed in-house research team. Our strategy will be to maintain a core set of personnel who will perform three functions:

- Remain aware – at an expert level – of algorithmic advances that could expand the scientific capabilities of the facility and work to ensure that these advances are available in usable software to the entire LCLS user base.
- Work with users and scientific staff to understand problems facing the user community that could be addressed by computational advances, and communicate these to the broader computational community, for example academic computer science departments.
- Build and maintain relationships with outside research organizations in computational science whose interests and expertise overlap with the computational challenges facing LCLS.

This strategy aims to ensure that first, novel algorithms and software that enable new science are distributed as quickly and broadly to the user community as possible, and second that academically interesting computing problems facing LCLS are rapidly communicated to research communities with the expertise and resources to develop solutions to those problems. A simplified flow of these interactions is shown in Figure 12.

**Figure 12** The approach to data systems development engages partners at other labs and the user community in a tight feedback loop.
The Need for Advanced Algorithms

Historically, algorithmic and mathematical advances have enabled new x-ray science: phase retrieval, computed tomography (slice theorem), and auto-indexing are canonical examples. Each enables a new experimental mode – coherent lensless imaging, 3D x-ray microscopy, and serial crystallography – that would not have been possible or even conceivable before algorithmically demonstrated. We expect further algorithmic advances will enable new science at the LCLS, and we will position the facility to maximize the yield from these advances.

Additionally, we will work to develop advanced algorithms for operational improvement, including data triage, reduction, and fast feedback as we look towards the LCLS-II upgrade. LCLS-II will result in a data rate increase outpacing standard Moore’s law hardware improvements, meaning it will be increasingly expensive to rely on hardware alone to handle the increased data rate. Streaming algorithms, for instance, capable of providing reliable vetoes or pulling data of particular interest for fast feedback, could significantly reduce the data rate burden. We will aim to prototype these algorithms now on LCLS, where they can impact current operations in a positive but modest manner, for use when LCLS-II sees first light where they may be an essential component of data collection and analysis.

The academic scientific model provides strong incentives for the development of novel algorithms, but not for the wide distribution of technology to other academic groups. Distribution often involves many tasks not typically considered in the scientific domain: writing production-quality software, documentation, tests, and tutorials. In order to maximize the impact of algorithmic advances on LCLS experiments, we will commit resources to translating published computational research into software that the entire LCLS user base can employ. We believe facility-provided and maintained codes implementing the latest algorithmic advances will result in a reduced lag between experiment and publication and ensure no user is at a disadvantage due to limited computational expertise or resources.

4.5 Laser Systems

Approximately 75 percent of all experiments at the LCLS require optical laser excitation to initiate a reaction or state within the sample under investigation. The vast majority of the physical phenomena under investigation by pump/probe techniques occur on a timescale of picoseconds to femtoseconds, requiring both optical and X-ray sources to have femtosecond pulse duration and a well-defined and controllable temporal separation. LCLS-II will present challenges for optical lasers primarily in two broad areas: (1) increasing the repetition rate of the lasers to match that of the LCLS-II X-ray beam (up to ~1 MHz) with suitable pulse energy, (2) maintaining low temporal jitter and drift relative to the X-ray beam. Related challenges will include managing high average power beams with robust personnel and machine safety systems, producing sufficient pulse energy at wavelengths of interest where the conversion efficiency is low (e.g., THz, deep-UV), and producing and maintaining increasingly shorter pulse durations to take full advantage of the high time fidelity of the X-rays and optical beams for experiments on extremely short
time scales. Alongside this, new opportunities in high energy density (HED) science will drive demand for increased optical laser intensity and very high per-pulse energy.

4.5.1 Lasers for LCLS-II

In the baseline design for the LCLS-II superconducting accelerator, the maximum repetition rate for electron bunches (and therefore X-ray pulses) is ~1 MHz. While specific experiments may be limited by the rep-rate of detectors, sample refresh rates, or related considerations, the majority of science opportunities will require lasers for pump-probe measurements at THz to EUV frequencies and high average power. Pump-probe systems of this scale have a major impact on the overall facility layout, requiring extensive tradeoff analyses and close integration throughout the design process.

LCLS has initiated an R&D program to develop a 100 W average power (1 mJ at 100 kHz or 0.1 mJ at 1 MHz) laser system to assess the feasibility of applying this technology to LCLS-II. Based on Optical Parametric Chirped Pulse Amplification (OPCPA), a target specification of ≥1 mJ was selected to provide sufficient peak power to drive low-efficiency wavelength conversion processes such as THz generation by optical rectification, which has a ~10⁻⁵ conversion efficiency. Other targeted baseline performance parameters include 15 fs FWHM pulse duration (scalable to <10μm), broad spectral tunability, and timing synchronization jitter ≤20 fs RMS from 0.01 to 1 MHz.

This system is based on a commercial oscillator for seeding the amplifier and the pump laser for passive synchronization, a commercial Yb-fiber pre-amplifier, and several stages of OPCPA pumped by a commercial Yb:YAG amplifier producing >1 kW average power with a few picosecond pulse duration.

The architecture of the system is designed to enable enhanced performance through upgrades or alternative modes of operation. Substantial development is required in terms of characterizing thermal properties of nonlinear optical crystals for OPCPA and modeling the amplification process prior to design and operation of an amplifier.

More broadly, the development of high average power, ultrashort laser systems has developed rapidly over the past few years, both in results from research institutions, and in commercial laser products (e.g. with regard to Ti:Sapphire systems, and fiber lasers that offer breakthrough potential with emerging research on coherent combining techniques and non-linear spectral broadening technology). The choice of laser technologies that will be implemented for LCLS-II experiments will be informed by continued clarification of the scientific requirements for LCLS-II science, continued advancement in the capabilities of commercial lasers, and the knowledge gained as part of the of the above R&D project.

4.5.2 Laser Synchronization and Timing

Taking full advantage of the temporal resolution of femtosecond X-ray pulses and femtosecond optical lasers in pump-probe experiments requires timing measurement and control of the variable delay between the pulses on a timescale from a few tens of fs to sub-fs. At present, LCLS has a pulse-to-pulse timing jitter relative to the accelerator radio-frequency (RF) distribution of approximately 60 fs RMS, integrated over a bandwidth of 0.1 to 100 kHz. Optical lasers must be locked to the accelerator RF distribution with similar or better timing jitter, and drifts in the laser beam path and RF distribution must be controlled
The CW RF drive and high Q of the superconducting accelerator cavities of LCLS-II promises to significantly reduce the timing jitter, possibly to as low as a few fs. This improvement will drive a corresponding demand for improvements in the jitter of the pump-probe lasers and timing distribution systems, particularly in experiments that probe ultrafast dynamics of transient systems.

For LCLS-II an upgraded version of the current RF timing system (based on RF distribution over stabilized coaxial cable) is planned, employing RF-over-fiber.

An R&D project is currently underway to evaluate a second timing distribution system technology based on pulsed femtosecond laser signals over optical fiber utilizing optical balanced cross-correlators for timing detection. In the cited reference, remote two-color optical-to-optical synchronization was demonstrated with 3.3 fs RMS slow drift over 24 hours between a Ti:sapphire oscillator and an Er-doped fiber laser. Similar systems are already in use (DESY/FLASH) or planned (European XFEL and SwissFEL) for precision synchronization of optical laser with FEL X-ray beams.

To complement the stabilized timing system, cross-correlation techniques that provide a pulse-by-pulse measurement of the x-ray/optical synchronization have proven to be highly useful at LCLS to date. Investigations are now underway to study methods of scaling cross-correlation techniques up to the 0.1-1 MHz repetition rate of LCLS-II, and to improve the temporal resolution of the this technique, ideally down to the <10 fs level.

4.5.3 Lasers for High Energy Density Science

The field of High Energy Density (HED) science performed at the Matter in Extreme Conditions (MEC) instrument has laser requirements for high pulse energy and high peak power. The current MEC laser capability is comprised of two laser systems: an Nd:glass, high-energy, temporally-shaped, nanosecond laser system that fires at one shot per few minutes with a pulse energy of 40 J / 10ns; and a Ti:sapphire, high intensity, femtosecond laser system capable of producing 30 TW peak power at 5 Hz. A 100 TW peak power system is currently being commissioned, with repetition rate determined by the high energy pump laser. There are multiple, overlapping pathways for expanding capabilities in these laser systems.

High peak power (>Petawatt)

The unique combination of a petawatt laser and LCLS in the MEC endstation would, for the first time, permit detailed pump-probe studies employing X-ray scattering techniques to measure and uncover the physical mechanisms underlying the interaction of ultra-intense

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laser radiation with matter. Commercial petawatt laser systems are available operating at “low” energy (~30-40 J) and short pulse duration (~30-40 fs) with repetition rates of up to ~1 Hz. Similar systems operating at up to 10 Hz are under development for delivery to the Extreme Light Infrastructure (ELI) projects in the EU. Higher energy (>100 J), longer pulse (>100 fs) systems operating at one shot per few minutes are also commercially available. Higher peak power systems (~10 PW) are also under development for various European projects (such as ELI and ILE-Apollon). Within the user community there are proponents for both “single shot” and “high repetition rate” lasers, depending on the specific scientific objectives. LCLS is engaging in community outreach through workshops and direct interactions to help articulate the case for different types of petawatt laser systems. The compelling science cases will determine the selection of the specific laser technology.

**High pulse energy (>100J)**

To access conditions of relevance to the study of planetary interiors and “warm dense matter”, it is necessary to reach pressures in the multi-Mbar regime with well-defined shock conditions. Currently in MEC, such shocks are driven by the second harmonic of a Nd:glass laser system, producing 20 to 40 J in 10 ns pulses at a repetition-rate of ~0.2 shots/minute.

Due to the relatively low pulse energy of the drive laser, a small laser focus is required to achieve high pressures, whereas higher laser pulse energy would allow for higher pressures to be reached with uniform shocks. One possible upgrade path would be to replace the final glass amplifier rods with a commercially available amplifier, in conjunction with larger aperture LBO crystals, enabling the generation of >100 J in a 10 ns pulse at up to 1 shot/minute. These upgrades would significantly enhance the possibilities for shock physics studies at LCLS-II. The possible extension to high energy pulses (~1kJ) is under exploration.

For all existing systems, and any additions, one overriding priority is to establish a comprehensive suite of beam diagnostics that provide sufficient information to optimize and subsequently interpret the quantitative laser-matter interaction conditions.

### 4.5.4 Upgrades of Existing Laser Systems

The Ti:sapphire laser systems in the NEH are mature, stable, and nearly identical between AMO, SXR, and XPP. The core NEH laser systems are stable and require only routine maintenance and incremental upgrades such as replacing older hardware, e.g. to improve timing jitter performance, and adding new or improved diagnostics. The mid-IR OPA setup on the general use table has been very successful in reducing set-up time and providing consistent output and diagnostics of the mid-IR source. Similar mobile, well-defined configurations will be developed for the optical THz source and for the <10 fs hollow fiber source. Further improvements in THz conversion efficiency by cryogenic cooling of LiNbO3 crystals is being developed by researchers at LCLS, and this will be engineered for deployment in the LCLS hutches. Other R&D activities on THz sources include the development of collinearly-pumped THz using organic crystals, CEP-stabilized mid-IR pulses, and narrow-band, multi-cycle THz sources.
Further planned laser system improvements include: (1) upgrades to accommodate <25 fs laser pulses for higher temporal resolution in pump/probe experiments; (2) dedicated harmonics and OPA configurations for each instrument to reduce time spent moving and aligning shared systems; (3) additional diagnostics for on-line monitoring during experiments; (4) development of extended capabilities in wavelength (XUV, UV, THz) and pulse duration (<10 fs); (5) further development of existing mid-IR and THz techniques and diagnostics.

Space for R&D efforts on optical sources, such as cryo-cooled THz, <10 fs sources, UV and HHG sources, etc. is now available in two LCLS laboratories, housing systems identical to those used for hutch operations. These labs will also provide laser light to users to test samples, detectors and measurement schemes prior to beamtime. The new Arrillaga Science Center laboratory building at SLAC is scheduled for beneficial occupancy in 2018, providing space for laser laboratories to further develop sources and experimental capabilities, working closely with researchers from the PULSE Institute and external groups.

Continued enhancement of pump-probe laser capabilities will be completed in 2017 in the Far Experimental Hall, with the installation of a new 30fs, 6mJ laser system in XCS. This system will provide ultrafast optical pump pulses at wavelengths spanning from the visible to near-infrared, providing similar capabilities to those of XPP in the FEH.

In CXI, an increasing number of experiments require higher pulse energy and changes in wavelength using OPAs, with both at nanosecond and femtosecond lasers. Typically, each of these configurations must be set up from scratch and disassembled after the experiment. To increase operational efficiency, we will develop stable, interchangeable configurations of standard optical setups such as an OPA stage or harmonic conversion. To enhance the laser capabilities and meet user demand, a compact multi-pass amplifier will be added to the existing femtosecond Ti:Sapphire laser system, providing ~20mJ pulse energies for driving shocks in materials and extending wavelength conversion capabilities to the mid-IR and THz.

In the MFX instrument a tunable nanosecond laser system has been installed to generate pump wavelengths spanning 410-2200 nm. It is expected that similar ultrafast laser systems to those in CXI will also be implemented in the hutch, enabling time-resolved experiments on this instrument.
5 ACCELERATOR SYSTEMS DEVELOPMENT

5.1 Accelerator R&D

5.1.1 FEL photon beam diagnostics

From the start of LCLS, development of diagnostics to characterize the FEL beam has been crucial to all aspects of LCLS science. Very significant developments have been made in cross-correlators to provide optical laser FEL arrival times with resolution approaching 10-20 fs on a routine basis. A hard X-Ray spectrometer has been implemented and extended to the range of SASE radiation at LCLS. A transmissive soft X-Ray spectrometer has been developed. A polarization monitor has been tested for the Delta undulator. There have also been developments and deployments of various intensity monitors. All of these efforts have extended the capabilities of the day one diagnostics developed through the LCLS and LUSI projects.

There is a continuing need for development of improved diagnostics, and to address the needs of the high repetition rate LCLS-II beamlines:

- Further development of two-color FEL operation beyond the SASE bandwidth requires the design of a hard X-Ray spectrometer that will give the proper relative intensities of the two colors on a pulse-by-pulse basis. The crystal spectrometer is sensitive to the spatial position of the beam, while the development of the hard X-Ray analog to the transmissive soft X-Ray spectrometer (where the photon spectrum is converted to a photoelectron spectrum) would address this issue.

- The development of the existing timing diagnostics has addressed the needs of LCLS operation at 120 Hz. For the SCRF linac, the goal is to be able to reduce the jitter between optical pump and X-Ray to below 20 fs, with the goal of reaching well below 10 fs. In order to reach these levels, development of a cross correlator capable of operating at rates in excess of 10 kHz is required. It will no longer be possible to use the thin Si$_3$N$_4$ film that is at the heart of the present method. Such a cross-correlator could be incorporated into a feedback loop providing the desired timing stability.

- Another important development is an $I_0$ monitor with sufficient accuracy to permit accumulating measurements for the high repetition rate of LCLS-II. Many experiments have the potential to accumulate data from a 'stream' of pulses at high rate as long as the relevant beam parameter jitter is sufficiently small. Solution of the timing issue is thus an important R&D area. As long as the experiment is operating in the linear response regime and there is no sample ‘damage’ during accumulation this approach is extremely appealing as a way to take full advantage of the FEL capabilities.

- Finally, with the scientific drive toward sub-femtosecond pulses, the development of a single pulse diagnostic ideally providing both phase and amplitude is an important requirement.

5.1.2 Polarization Control

Many X-Ray techniques, especially in the soft X-Ray spectral range, require circularly polarized light. In the hard X-Ray regime, quarter wave plates using ‘off Bragg’ diffraction
have been very effective and this is the approach that will be taken for LCLS-II. Test of this approach to ensure its viability is important, and can made use of the existing LCLS facility to develop a robust optical configuration.

In the soft X-Ray regime, one polarizing "Delta" undulator is currently installed at the end of the LCLS-I undulator line, providing ~200 µJ of circularly polarized X-Rays at a very high degree of polarization (>99%). To reach saturation, it is currently estimated that three DELTA undulators 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. Adoption of this “afterburner” configuration will be a high priority for early operation of the upgraded facility.

The current design for the LCLS-II DELTA undulators calls for the magnetic fields to be stronger than the current device to match the higher K values of the regular SXR undulator segments (increased from K=3.50 to K=5.48). They also will require water-cooled vacuum chambers due to the much higher beam current for LCLS-II. Two modest R&D efforts are envisaged to drive the required developments. First, the Delta undulators use a very small round vacuum chamber (6.3/5.0 mm outer/inner diameter). While water cooling is a challenge, initial concepts have been developed to build a prototype that would be used to understand cooling efficiencies and temperature gradients, and to optimize parameters for the final design. Secondly, in order for the SXR Delta undulators to operate at the higher K value, a larger magnet block design is required. Higher K values also mean higher magnetic forces (increased by about a factor 2). The design and prototyping of the magnet blocks, magnet block holders, carriers and drive unit is envisaged.

5.1.3 Two-Pulse (variable delay)

X-Ray pump X-Ray probe experiments open a very broad array of new scientific possibilities. Extensive machine development effort has recently been devoted to developing 2-pulse, 2-color techniques, with notable success. Table 1 provides a snapshot of current capability.

An important advance beyond two pulses with the same energy and variable delay has been two pulses with different colors and variable delay. Accelerator-based techniques have addressed this within a finite parameter space: two colors with separations on order of 1 % have been demonstrated with delays ranging from 50 fs in soft X-Rays to ~150 fs in hard X-Rays. Also, two pulses separated by one or more RF buckets (up to >100ns separation) can be provided with different colors. The challenge is the delay between the 100 fs scale and the few hundred ps to ns scale. Solutions for hard X-Rays using crystal split and delay methods are being implemented, but the soft X-Ray range is challenging.

LCLS-II has an additional advantage compared with the present undulator in that it has a variable gap design. At SACLA they have already demonstrated the production of two well separated pulses, more than a keV, but have not yet reached saturation for either color. Here too the delay from the accelerator is from a magnetic chicane and is of order a few tens of fs. There is the possibility in hard X-Rays again to develop a crystal based split and delay to extend this range.
Table 1: Summary of 2-pulse, 2-color modes of operation. See FAQ for latest information.

Finally, LCLS-II offers a unique potential: to bring the SXR and HXR undulator beams to one experiment with variable delay. The Cu linac and SCRF linac will have relative time jitter of ~100 fs, and with timing diagnostics this can provide high peak power pulses to the experiment again with very different photon energies. This option, of course, would operate at 120 Hz limited by the repetition rate of the Cu linac. One could use a crystal split and delay to vary the HXR arrival time for X-Ray pump probe experiments as an example. There are many variants of this scheme, for example using the SCRF linac for both the SXR and the HXR undulators and ‘combine’ the third harmonic of the SXR undulator with a similar energy HXR undulator pulse at repetition rates in the 100kHz scale.

5.1.4 Sub-femtosecond pulses

An exciting new horizon is the development of methods to routinely deliver sub-femtosecond pulses, ideally close to the Fourier-Transform limit. The recent LCLS-II science workshops also highlighted the advantages of sub-fs pulses with sufficient Fourier-limited bandwidth (3 eV or above) to produce a coherent excitation of two or more electronic states in a molecule.

Perhaps the most promising technique is laser slicing. Such a technique takes advantage of the high field intensities of commercially available lasers to generate a short, high-current spike in an electron bunch via particle/laser interaction in a magnetic undulator.
The short current spike is subsequently used in the FEL undulator to generate a short X-Ray pulse. Numerical studies for LCLS and LCLS-II indicate that pulses as short as a few hundred attoseconds at a photon energy of 1keV can be generated. An experimental program (known as XLEAP) is underway to develop out this approach, with initial tests planned for Run-15 (mid-2017), and the possibility of it being offered to the user program in Run 16 (2018). The expected XLEAP performance is as follows:

- 30-50 uJ per pulse
- 0.5 fs FWHM pulse duration
- 4 to 8 eV FWHM bandwidth

### 5.1.5 High resolution soft X-Ray self-seeding

The system envisioned for self-seeding at high resolution is an upgraded version of the existing soft X-Ray self-seeding scheme. The SXR self-seeding scheme is described extensively elsewhere (Proc. SPIE, vol. 8849, p. 88490A). It is a monochromator inserted into the undulator chain of LCLS that collects the SASE radiation produced by the first 8 undulators, selects a narrower bandwidth, and uses the resulting monochromatic beam to seed the electrons beam into the following undulator section.

The resolving power of the existing system is of the order of 5,000. Since the resolving power is dominated mainly by the diffraction limit contribution of the grating, e.g. the number of illuminated lines, one can increase the resolving power by moving the source point further upstream, e.g. by opening the gap of the last few undulators just before the monochromator.

By opening the gap of the last undulators before the grating, one can increase the resolving power almost arbitrarily. However, one must also increase the power delivered to the grating, to preserve the power required to seed the electron beam. Within the projected damage limit of the grating, a resolving power of the order of 30,000 or slightly higher is expected. It is possible that with further R&D (ongoing) the resolving power can be increased at the lower photon energy.

### 5.1.6 Self-seeding at the highest X-Ray energies

The advantages of the self-seeded beam are many-fold, as already demonstrated in a variety of LCLS experiments. The simple single crystal approach however has difficulty at X-Ray energies in the tender regime, or much beyond 10 keV. The most obvious approach is to use two bunch concepts letting the first bunch provide the seed for the second bunch. This requires development of a chicane with sufficient delay and optimization of the location due to the reduced seed power compared with the single crystal approach.

### 5.1.7 External seeding

A significant number of science opportunities require exquisite control of the FEL bandwidth, and utilization of a well-defined spectral spike. This will be particularly powerful for spectroscopic methods such as time-resolved RIXS. The potential for creating large coherent spectral bandwidth, and pulse durations ~1 fs or less will enable non-linear X-Ray spectroscopies in a similar manner to what has been achieved for optical non-linear spectroscopy.
While self-seeding has provided much-needed capability, the development of an external seeding system would provide far greater flexibility, if it can be realized. There are presently a variety of potential methods under investigation in the community, including High Gain Harmonic Generation (HGHG), Echo-Enabled Harmonic Generation (EEHG), and direct High Harmonic Generation (HHG) injection schemes. Alongside this, there are other options to produce narrow bandwidth pulses, including harmonic lasing, pSASE and iSASE. There is no clearly preferred solution for LCLS, and so the immediate task is to undertake a quantitative tradeoff analysis; learn from recent experience at Fermi@Elettra, FLASH, and SACLA; and from the internal Echo-75 program at SLAC. Following this assessment, a prototype project will be launched.

5.2 FEL Performance Improvement

5.2.1 High Peak Power and Extended Energy for LCLS-II

Driving the LCLS-II soft X-Ray undulator with the high-energy electron beam from the warm copper SLAC linac would generate pulses with very high energy (>5 mJ) in the tender (2-5 keV) X-Ray regime at 120 Hz. The peak power levels from this source are calculated to exceed the TW level, opening up new capabilities for single particle imaging.

Such a modification to the beam switchyard (allowing either accelerator to feed either undulator) would also have obvious operational advantages, permitting both SXR and HXR experiments when one of the accelerators is out of operation for whatever reason.

Detailed consideration of this reconfiguration is underway, and will be implemented if deemed sufficiently high priority.

5.2.2 LCLS Beam availability

During the past several LCLS user runs, the FEL beam availability was approximately 95% during user operation, accomplishing our stated goal. We actively manage many technical aspects of accelerator and FEL subsystem performance and maintain a targeted program that is based on quantitative goals for the performance and availability of each subsystem. To achieve high availability during user operation, high risk maintenance and upgrade activities are conducted during non-user times, for example during machine physics and maintenance periods or during start-up periods.

Decisions for maintenance, replacement and system upgrades are guided by statistical parameters, such as Mean Time Before Failure (MTBF) and Mean Time To Repair (MTTR). The main decision making tool is our Work-Planning and Control System (CATER), which tracks all accelerator maintenance activities. Figure 15 illustrates MTBF and MTTR results by subsystems for a recent year-long period.

The continuing goal for future LCLS operation is to maintain high beam availability for the LCLS user program. It is also important to deliver beams with specific performance parameters, such as very short pulses (<10fs), narrow energy bandwidths, or dual bunches separated by time and/or photon energy. This will dictate the evolution of our machine availability program to allow evaluation of system performance under key delivery conditions.
Another aspect of the machine availability program is to deliver our stated goals with less and/or reduced effort. The increase of overall system maintenance efficiency will be an outcome of the Mission Readiness program (see below).

**Figure 15** Mean Time Between Failure (MTBF), Mean Time To Repair (MTTR) for key subsystems

5.2.3 LCLS Cu-Linac Energy Stabilization Program

The level of energy stability and the resulting impact of energy jitter on FEL brightness has been a principal limitation for many LCLS experiments. As such, over the past 2 years, an energy jitter reduction program was established to reliably achieve a beam energy jitter less than ½ of the SASE bandwidth. This has now been demonstrated, by careful attention to stability of the high power RF stations, and in particular the klystron modulator thyratrons, which act as a switch for the high voltage pulse that fires the klystron. We identified a number of RF stations which were the main contributors to the overall machine energy jitter. For example, a single station before the first bunch compressor contributes 50 times more to the machine jitter compared to those downstream. Current jitter...
performance is deemed adequate, and so ongoing work will seek to monitor and maintain at this level (see Figure 16)

**Figure 16** Average X-Ray brightness reduction vs. electron energy jitter

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5.3 **LCLS-I Accelerator “Mission Readiness” Program**

The development of the LCLS-I Accelerator Mission Readiness Program began in fiscal year 2012 by evaluating the state of the various technical systems that support the accelerator’s operation. A number of risks to our mission of reliably delivering a high performance FEL have been identified during this study. The findings have been categorized by technical, safety, operational and financial risks, which served as a basis to rank and prioritize the mitigation tasks. The prioritization process included the operational return of investment of each mitigating activity, where appropriate. An external review was conducted in October 2013 to evaluate and verify the approach of the program. A further review and optimization process was conducted in 2016 by the new Accelerator ALD (Lia Merminga).

LCLS is committed to address the various issues that were identified and a multiyear program was developed in consultation with DOE-BES to carry out the Mission Readiness activities. Work is organized in many subprojects, which are subject to internal reviews both by the senior LCLS management, including representatives of the LCLS-II project. Technical reviews are conducted at various levels including subject matter experts from many SLAC organizations.

Included in our considerations are the boundary conditions that are set by the future LCLS-II FEL systems. This is particularly important for the Mission Readiness Projects that are addressing the various aspects of control system upgrades (e.g. high performance systems such as low-level RF and timing). It is of utmost importance to conduct the system
upgrades with a view of an integrated facility, both LCLS-I and LCLS-II. Another aspect is to evaluate the Mission Readiness benefits to the X-Ray beam line operations. This is the case in particular for the control systems scope, as many systems are common for accelerator and X-Ray beam line operation. Examples are DAQ, timing and safety systems. It is an important goal to develop systems with a high degree of compatibility across the facility to streamline operation, maximize the return of investment and ensure efficient future maintainability.

The main targets of the program are the accelerator control systems, the high power RF systems and a number of accelerator and technical infrastructure systems that are critical to the operation of the LCLS accelerator and FEL. This program is spread out over 5 years. The planning of the overall program takes into account the LCLS-I operating and downtime schedule, the LCLS-II project and commissioning schedule as well as boundary conditions set by other programs at SLAC, such as the FACET operating plans and anticipated FACET-II installation schedules. The Mission Readiness Program is planned to be complete in fiscal year 2020 when the LCLS-II systems will be commissioned and the integrated facility begins to deliver X-Ray beams to users. Table 2 summarizes the baseline scope.

Table 2 Mission Readiness Program Components

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<th>Controls Projects</th>
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<td>Beam Containment Systems</td>
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<td>EPICS Version 4 and High Level Applications</td>
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<td>Fast Feedback Systems</td>
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<td>Beam Position Monitor Upgrades</td>
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5.4 LCLS-II Strategic Dependency Projects

The LCLS-II strategic projects reflect SLAC's commitment to the success of the LCLS-II project. The goal is to facilitate the installation and commissioning of the superconducting accelerator, new variable gap undulator systems and X-Ray experimental instrumentation. The overall scope is articulated in a memorandum of understanding between the LCLS-II project and SLAC. It covers the contributions of the Accelerator and LCLS directorate as well as the scope of SLAC as an institution.
The list of projects includes:

- **Beam Switch Yard (BSY) Excess Hardware and Removal and Reconfiguration Projects** will reconfigure this area for LCLS-II beamline installation. In addition, we have started to remove unused and obsolete devices and structures that have been used during SLAC’s 50+ year history of high energy physics programs. The goal is to prevent their future activation by high power LCLS-II electron beams, thereby minimizing potential radioactive waste generation.

- Several projects are associated with reconfiguration of the accelerators alignment system. The superconducting accelerator will be installed on pedestals and will use a laser tracker based alignment system. This requires the removal of the historical accelerator support system that is also used to align the current S-band accelerator. A continued use of this system for the remaining sectors (10-30) is currently being evaluated. The associated Alignment Calibration Lab will be moved from its current location (linac tunnel spur at sector-10) to a new location to make room for LCLS-II installation infrastructure.

- To allow installation of LCLS-II equipment in the sectors 0-6 area, an S-band klystron will be moved to other locations throughout the remaining klystron gallery and to the Klystron Test Lab. This includes associated hardware such as modulators, waveguides, vacuum system hardware and control racks.

- A number of conventional infrastructure modifications are necessary to support the LCLS-II installation, commissioning and future operation. Those include the modification of the Magnetic Measurement Facility required to support LCLS-II undulator magnetic measurement, tuning and maintenance, improvements throughout the accelerator tunnel such as upgrades of linac access areas, upgrades of fire alarm and detection systems and the modification of cooling and process water systems for LCLS-II needs.

- Modifications and upgrades of the high voltage infrastructure are needed for all accelerator systems at SLAC and the LCLS-II cryo-plants. Examples are the substations along the linac and the 12 kV electrical distribution systems.

- Equipment removed from accelerator housings will be characterized and inventoried by SLAC’s Radiation Physics group and plans are being developed for near and long term disposal and storage.
6 EXPERIMENT DELIVERY

6.1 Effective and efficient experimental operations

LCLS operations developed in a largely organic manner as the facility transitioned from initial experiments with instruments in the development stage to a more mature facility. Over the past 3 years, considerable attention has been paid to determining how to operate more efficiently, meaning a greater throughput of experiments and users, and a rebalancing of funds from operations towards strategic developments that can build readiness for the increased capacity and enhanced capability of LCLS II experiments.

As LCLS has evolved, it has become apparent that when a pre-experimental setup goes well, experiments can often be completed in significantly less time than was originally planned. This setup and testing of a different instrument configuration is very labor intensive. It was not uncommon for this to occur before almost every week. This was accommodated because LCLS wanted to provide the highest level of experimental flexibility in order to achieve the greatest scientific impact. After five years of running, we found that a recurring suite of particular instrument setups are used in each run, meaning significant duplication of set-up activities. Starting with Run 13 (April 2016), LCLS devoted a fraction of each Run to operate in a mode where each of the instruments is in one of these “standard configurations” for an extended period of time (~25% of the overall Run for this initial phase). This allowed multiple users to exploit this configuration with only one setup and testing period. An extreme example of this would be our recently initiated Protein Crystal Screening program where we run two independent Users through an instrument in a fixed configuration every 12 hours. In order to have enough high profile experiments to take advantage of this, the standard configurations have been defined in each call for proposals (Runs 13 to 16) and factored into the proposal review panel when ranking proposals for beam time. During the non-standard configuration time for a given instrument, the same level of flexibility that we currently accommodate will be accepted in order to address high profile science that requires a specific custom setup. On average to date, we have allocated ~30% of beamtime in this “standard configuration” mode. Feedback from the user community has overall been very positive.

This change in the way we schedule and support experiments means that when an instrument is in a standard configuration, fewer resources are needed which means those resources would be available to spend time supporting strategic development projects or to support experiments at one of the instruments that is not in a standard configuration. In order to better support this mode of operations, we have fewer staff assigned to the scientific support departments and more resources assigned to general support across various instruments. This hybrid mode of support allows better response as support needs surge, while maintaining the departmental focus on planning and strategic development, which is critical to keep the instruments operating at the edge of the state of the art.

How we schedule experiments also impacts our efficiency in another manner: In normal operations we run one shift from 9 am to 9 pm and another from 9 pm to 9 am. When we can exploit one of the available multiplexing schemes, we can simultaneously run two experiments during one of those shifts. Historically, it has been difficult to build a schedule that allowed multiplexing on more than approximately 30% of the days, which improved
our throughput by 15%. These standard configurations have also allowed longer blocks of multiplexed operations, with 25% seen in Run 14 for example. Going beyond this was strongly limited by our instrument configurations and scheduling logistics so we will continue to invest in instrument upgrades that facilitate more beam multiplexing (such XCS and MFX).

The results of these significant efforts to increase the number of experiments performed per year, and to increase the number of users at the facility, are shown in Figure 17. These increases have been achieved while reducing the cost of experimental delivery over the past year by ~18% overall (or ~45% per experiment), allowing a greater fraction of DOE funding to be used to develop the technical capability in preparation for LCLS-II.

**Figure 17** The number of experiments and users at LCLS has increased significantly.

![Graph showing the increase in the number of experiments and users at LCLS](image)

We are also investing in instrument changes that will improve efficiency beyond multiplexing. One major problem we had that limited our ability to schedule experiments in the most efficient manner was the fact that when XPP was running in “pink beam” mode (non-monochromatic), it blocked the beam from being transported to the Far Experimental Hall. Since the majority of XPP experiments needed “pink” beam, we were forced to schedule these experiments opposite experiments in either AMO or SXR. To mitigate this issue, we are installing a hard X-Ray periscope that will allow “pink” beam to be taken to XCS by inserting a mirror, in much the same way as we send beam to MEC. Since XCS does not have a pump-probe laser and most of the XPP experiments required an optical laser, we are also building a laser room and adding this capability to XCS. These upgrades will allow the majority of “pink” beam experiments that would have been scheduled in XPP to be moved to XCS. This means XPP can stay in “mono” mode most of the time, which allows multiplexing to the far hall by using the non-monochromatic beam that transmits through the diamond crystals in the monochrometer.
6.2 Scalable and sustainable roles for LCLS staff

A major element for our Preparation for LCLS-II (and –HE) is to transform the “day in the life” of LCLS staff into more sustainable roles with higher scientific and creative impact, and more attractive career development opportunities.

This requires us to develop systems that can maximize the options for automated, robust operation, along with intuitive software, documentation and equipment protection systems. This will enable users to take greater control of their experiments, and to “make it easy to get to the hard stuff”, providing greater time for innovative and creative science.

We seek to minimize repetitive work and staff call-outs by assessing predictable failure modes and finding engineered / system solutions. Areas that currently require regular intervention by uniquely-skilled staff will be at the center of attention (lasers, injectors, DAQ, beam alignment, etc.)

We seek to phase-out technology that does not scale, and identify where R&D is needed to transform areas where there are substantial gaps.

The near term focus is in 3 areas:

(1) **Run 15 / 16 Planning and Delivery**

- Further development of a detailed User Questionnaire to improve planning
- Definition of a baseline scope for each experiment, formally agreed with the PI
- Rigorous implementation of detailed delivery plan based on this baseline scope, to improve user & facility readiness and expectations of timely delivery
- Creation of an ‘Operations Delivery Team’ comprising key scientific, technical and logistics staff
- **PURPOSE is to embed operational improvements, ready to scale to LCLS-II**

(2) **LCLS-II Instruments (L2S-I)**

- Definition of a suite of “First Experiments” to guide facility-wide prioritization
- Creation of a set of SLAC-led teams for early science on LCLS-II, with broad user engagement
- Definition of detailed, time-phased plans for the required instruments and associated systems, and delivery to this plan
- Design of the new facility systems based on stable, low-maintenance platforms
- **PURPOSE is to ensure early success & create a scalable mode of working**

(3) **Hard X-Ray Instruments**

- Translation of experience during 2017/18 to inform L2S-I (e.g. operation of the new HOMS mirrors and the new ‘Split and Delay’ unit)
- Capture ideas from the L2S-I process and identify implementation path for the enduring Hard X-Ray instrument suite
- Ensure readiness for LCLS-II-HE via suitable community engagement, design work, and integrated facility planning.
- **PURPOSE is to ensure LCLS-wide scalability and impact.**
7 LEVERAGING STANFORD AND SLAC – AN INTEGRATED APPROACH TO ULTRAFAST X-RAY SCIENCE

The rest of the world is now responding to the success of LCLS with well-developed projects to replicate or advance the capabilities we offer. Recognizing this, SLAC and DOE are pursuing a vigorous and well-coordinated series of developments to keep the U.S. facility in a preeminent state, as described above.

More broadly, a widespread series of developments are underway to prepare for early science on LCLS-II (and subsequently LCLS-II-HE), with a view to maintaining leadership in the field of ultrafast X-Ray science. Our plans integrate theory, simulation and experiments; pursue focused R&D in critical technologies; integrate new approaches to data analysis both onsite and offsite; ensure alignment between the local SLAC science programs and the evolving LCLS facility; and engage the wider user community in an organized series of events leading up to first experiments to exploit the new facility capabilities.

Specific areas of activity and planning include the following:

i. LCLS-II scientific priorities

   o An integrated facility development program for LCLS-II has been established to take the community's identification of priority scientific goals and translate these into a phased delivery of instrument upgrades, new detector systems, data analysis capability, pump/probe laser performance, and commissioning of the new accelerator and undulators. This program is timed to deliver initial capability for early light (2020) and over the subsequent 3-year period.

   o Instrument Advisory Panels (with members drawn from the LCLS user community) have been formed for each of the areas under development for LCLS-II. These IAPs help to steer the design choices and time-phasing of capability throughout the development phase, and will be key to ensuring early exploitation after initial commissioning.

   o LCLS has initiated a series of “digital Town Hall” meetings with the broader user community, aimed at conveying recent developments and upcoming issues to increase the awareness and involvement of users in the rapidly evolving facility.

ii. R&D to maintain leading edge capability

   o FEL performance: Intensive work is underway to assess novel modes of operation for LCLS-II, consistent with the successful approach adopted for LCLS-I. Current focus is on attaining sub-femtosecond pulse durations (with coordinated SLAC and BES grants) via the XLEAP program; assessing design options for an LCLS-II dechirper capable of enabling fresh bunch lasing; design of cross-over optics to transport the existing Cu-linac through the new LCLS-II soft X-Ray undulator to achieve the highest focused intensities; and designs for very high time resolution synchronization between LCLS-II and optical pump lasers. The latter will require additional investment if it is to be made available for early LCLS-II science.
o **Advanced Optics:** Good progress is being made in the development of advanced X-Ray optics systems capable of handling the high average power beams from LCLS-II, and measuring residual errors in the propagating wavefront. This is in concert with other BES national laboratories (BNL, ANL, LBNL), with targeted funding from BES. This work is progressing alongside SLAC investment into diamond nano-optics capable of measuring and tailoring the phase profile of the LCLS-II beam, to provide balanced development across the soft and hard X-Ray spectrum.

o **Computing and Data Analysis:** Particular attention is being paid to the development of new data analysis capabilities that are able to scale to the data rates and volumes predicted from LCLS-II. We have launched a widespread consultation with the LCLS user community, via the Users Executive Committee, to assess options for a data reduction pipeline (DRP) that would be consistent with expected capacity limits. The newly formed SLAC Computer Science Division, led by the chair of the Stanford CS Department, is providing direct input to this process. In parallel, SLAC has initiated work on a new ASCR grant for exascale computing ("ExaFEL") in concert with groups from LBNL (MBIB, ESNet, NERSC and CAMERA), LANL and Stanford. This seeks to reduce the data analysis timescale by orders of magnitude for large-area pixel array images, consistent with the needs of LCLS-II and LCLS-II-HE.

o **Development Laboratories:** Priority is being given to laboratory capabilities in the new **Photon Science Laboratory Building (PSLB)**\(^{16}\) and associated lab space at SLAC that can augment our ability to exploit LCLS-II. In particular, a new high power 100 kHz OPCPA laser under development at SLAC will be coupled to high-harmonic (EUV/XUV) experimental capabilities within PULSE and SIMES to allow co-development of HHG-based attosecond and EUV chemical and material science together with the attosecond LCLS-2 timing and synchronization developments.

A new ‘Nano-X” laboratory is being constructed to manufacture diffractive optics to measure and manipulate the LCLS-II beam; calibration laboratories are planned for the new suite of X-Ray detectors and reflective X-Ray optics for LCLS-II; and development space for new laser capabilities is targeting an extended wavelength reach for pump/probe studies, and phase-space manipulation of the LCLS-II electron beam.

Also in the area of materials science, PSLB will provide new space for THz laser development, linking to the Martinez theory group and Computer Science groups working on real-time data processing for LCLS-II.

### iii. Growth and alignment of the user community, and the local SLAC/Stanford programs

o SLAC is organizing a series of focused workshops with Stanford faculty, with the first on the science of ‘imaging at the extremes of spatial and temporal resolution’.

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\(^{16}\) Now known as the Arrillaga Science Center (ASC)
This will help strengthen the alignment between local research programs and the capabilities of LCLS-II and LCLS-II-HE. Building on this, SLAC seeks to take advantage of the strategic prioritization process currently underway at Stanford, which is likely to offer substantial new opportunities for developments in this area.

- More broadly across the user community, SLAC is driving an analysis of “First Experiments” for both LCLS-II and LCLS-II-HE, consistent with the successful approach adopted for LCLS a decade ago. This involves a series of workshops, study groups, prioritization activities, theory/modeling development, and test experiments using LCLS. This informs the path to early exploitation of the first instruments on LCLS-II, and will refine the detailed down-selection of techniques that will exploit the high energy regime.

- The teams at SSRL and LCLS are continuing to identify opportunities for scientific alignment, including the offering of joint beamtime to users. Key areas of co-development include: resonant soft-X-Ray scattering (e.g., testing of TES detectors on BL13-3); tender X-Ray emission spectroscopy (BL15-2 and TXI) and extension to nonlinear X-Ray probing of combustion processes, and possible alternatives to RIXS; multimodal structural molecular biology (BL12-1,2 and MFX); material dynamics of quasi-2D materials (including work using the UED facility); accelerator and X-Ray optics design; theory development for RIXS and other advanced spectroscopies.

iv. Longer-term growth

- We foresee many options for future development of LCLS at SLAC, including making full use of the LCLS-II accelerator as a robust platform for sustained growth that ultimately can drive up to 8 or 10 undulators simultaneously. Ongoing consultation is underway to inform these options, with studies focusing on technology options (such as the ‘X-Ray FEL oscillator’), as well as use-inspired directions (such as the recent solar energy workshop), in addition to the regular meetings with the existing user community. The rapid and widespread development of XFEL facilities around the world necessitates a sustained commitment to scientific improvements in order to retain leadership.
8 NEXT STEPS

The purpose of this document is to lay out a suite of facility development priorities for the next 5+ years of LCLS operation, in the context of the LCLS-II Project and the envisioned LCLS-II-HE extension, based on the assessments of science opportunities conducted over the past three years or so.

It is intended that this document (and subsequent updates) be used as the basis of a broad, ongoing consultation across the community, to help prioritize the suite of developments according to available funding and resource limitations, and to drive partnerships for delivery of capabilities that extend beyond the internal LCLS portfolio.

We are adopting the following assumptions to guide our selection of investment priorities:

- LCLS-II dependency projects (site & facility readiness) maintained as high priority.
- Enabling high impact science in for early LCLS-II operations (following commissioning) will be a primary driver for prioritization of project activities and their detailed scope and phasing.
- Instrument priorities will incorporate the following:
  - Modification of the Near Experimental Hall (NEH) to accommodate the revised suite of instruments, as described above.
  - Instrument development will adopt the following order of delivery:
    - (i) NEH1.1 DREAM then LAMP endstations;
    - (ii) NEH 2.2 moderate-resolution SXR monochromatic beamline;
    - (iii) Adaptation of XPP to make early use of the new Hard-X-Ray undulator;
    - (iv) NEH1.2 Tender X-Ray instrument;
    - (v) NEH 2.1 High resolution monochromatic RIXS beamline;
    - (vi) Adaptation of the other hard-X-Ray instruments (CXI, XCS, MFX, MEC), pending LCLS-II-HE.
  - Detector, Laser, Controls and Data Systems consistent with LCLS-II science priorities and efficient and effective user delivery.
- Increase user throughput and efficiency (modifications of XCS to accept pink beam and optical lasers; continued deployment of a set of “standard configurations”; etc).
- The budget for long-term R&D (accelerator and photon systems) will be kept approximately at its current level to preserve long-term capability development.
- All other (intermediate-scale) development projects will be treated as the principal area of flexibility, subject to community requirements and LCLS ability to deliver in a timely manner. These will be prioritized in an integrated manner for the facility for each year and the 5/10-year period.
- Any upgrade to PW-scale peak-power and/or high pulse energy (>100 J) optical laser systems for MEC will be treated as a separate activity, dependent on its own funding stream.

Feedback should be provided directly to the **LCLS Director**.