LCLS scientific leadership strategy

Mike Dunne et al, SLAC

Presentation to BESAC, December 2021

U.S. DEPARTMENT OF ENERGY

Stanford University

SLAC NATIONAL ACCELERATOR LABORATORY

LCLS performance was designed to be a true game-changer ($>10^9$ increase in brightness over prior sources)

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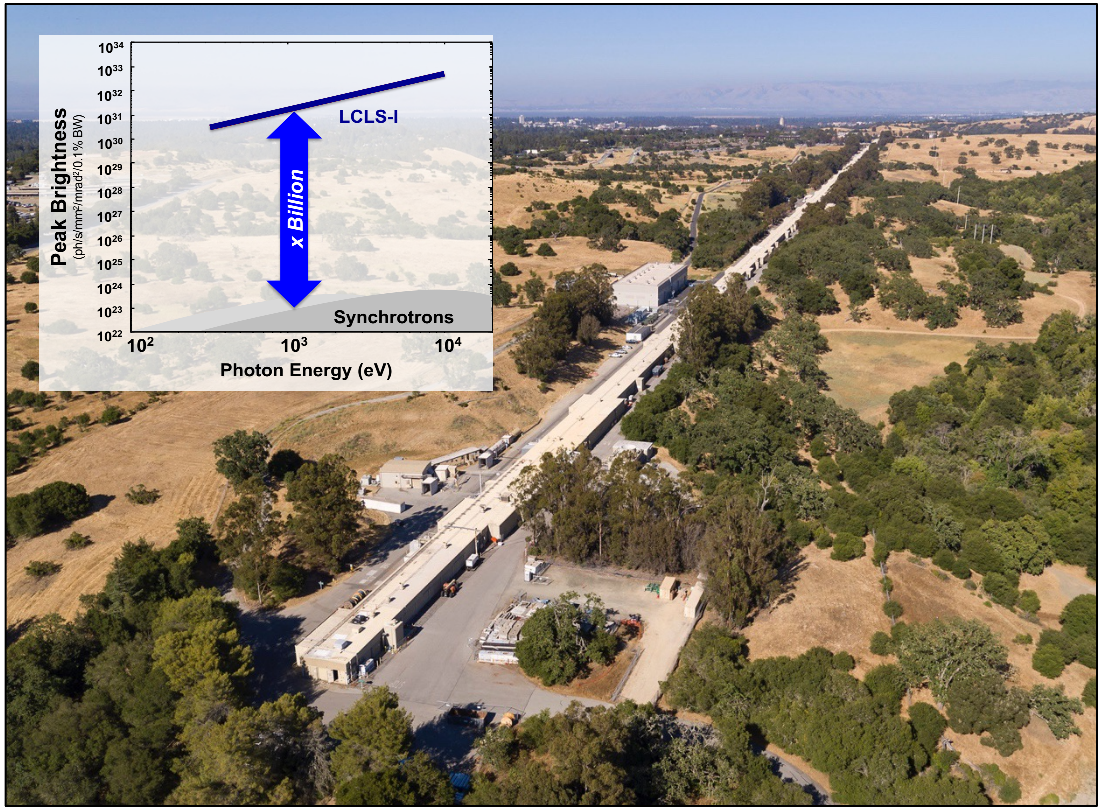
Initial parameters:

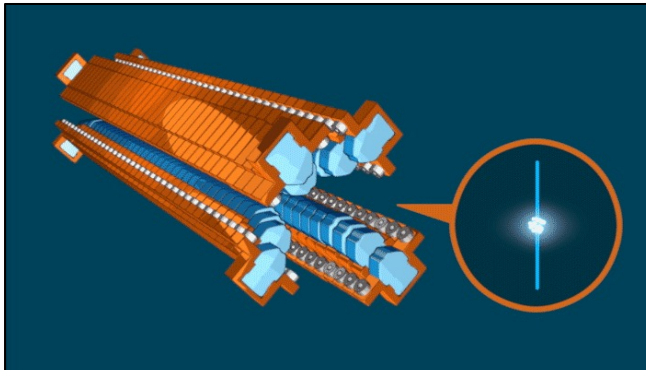
- ~100 fs
- Single X-ray pulse
- 0.8 to 8 keV
- Extreme peak brightness



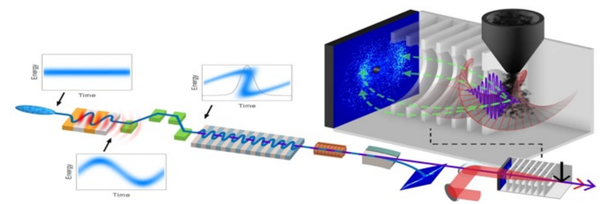
In 2009, LCLS was a technical and scientific 'leap into the unknown'

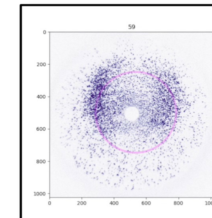
LCLS has demonstrated a remarkable ability to tailor and measure the X-ray beam, enabling precision studies across a wide range of disciplines

From linear to controlled polarization



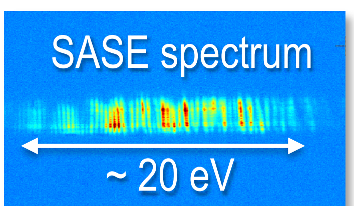
From 200 fs down to 200 as duration

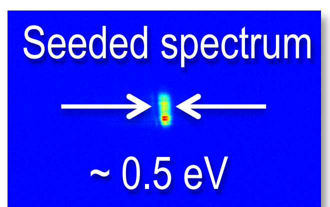




Record to date: 179 ± 58 as @ 9 keV (14.4 eV BW)

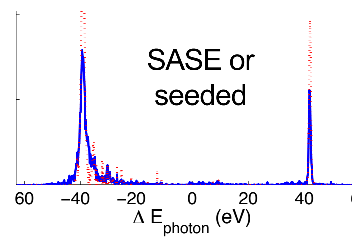
From statistical fluctuations to controlled pulse width and spectrum

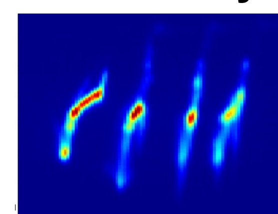




40x increase in spectral brightness.

From single pulse to tunable multi-pulse and 2-color x-rays



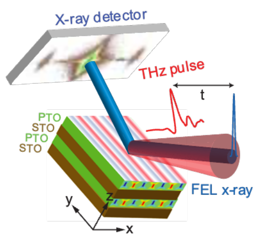


fs to >100 ns separation, and 4 or more pulses

Snapshot of recent scientific highlights from LCLS

Materials Science

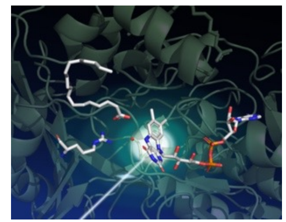
Ultrafast collective dynamics of polar vortices in ferroelectrics



Li et al., Nature (2021)

Chemical Sciences

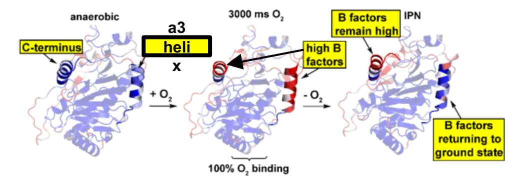
Green chemistry and biofuel: decrypting a key photoenzyme



Sorigué et al., Science (2021)

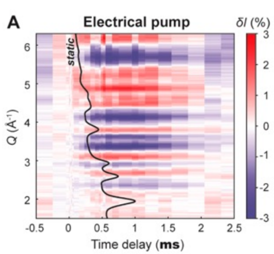
Biological Sciences

Enzyme movie shows how Nature makes penicillins



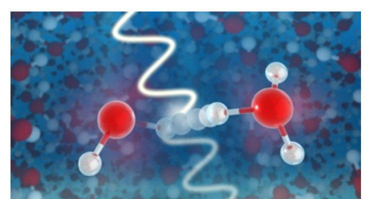
Rabe et al., Science Advances (2021)

Electrically-driven transient phases in an operating device



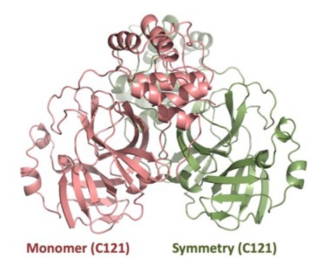
Sood et al., Science (2021) [UED]

Observing the birth and evolution of free radicals in water



Loh et al., Science (2020),
Lin et al., Science (2021)

SARS-CoV-2 mPro structure at near-physiological temperature



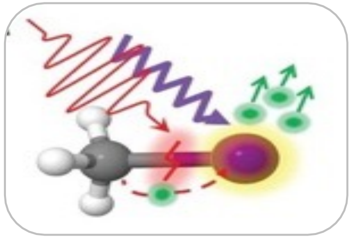
Durdagi et al., Structure (2021)

Results from LCLS have highlighted the key areas where coherence, fs time-resolution, and high rep-rate can have a revolutionary impact

SLAC

Seeing how physics drives chemistry

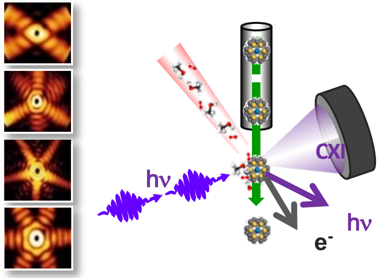
- Reveal coupled electronic and nuclear motion in molecules
- Capture the initiating events of charge transfer chemistry with sub-fs resolution



Ultrafast

The origins of catalytic acceleration

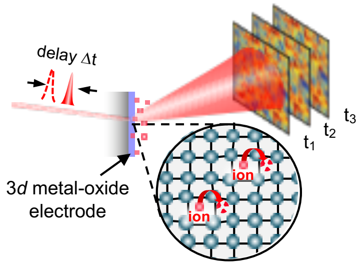
- Directly correlate catalytic reactivity with atomic structure in real-time
- Identify design principles for far-from-equilibrium chemical transformations



High repetition rate

Understanding material function and failure

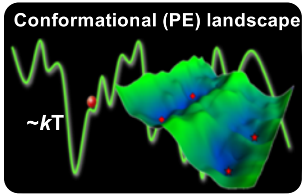
- Characterize dynamic systems without long-range order
- Directed design of energy conversion and storage materials



Coherence

Watching biology in action

- Study large scale conformational changes via solution scattering
- Physiological conditions
- Dynamics ties structure to function



Extreme brightness

The impact of XFELs will define X-ray science in the 21st Century

XFEL capabilities are now available around the world

EuXFEL, Germany

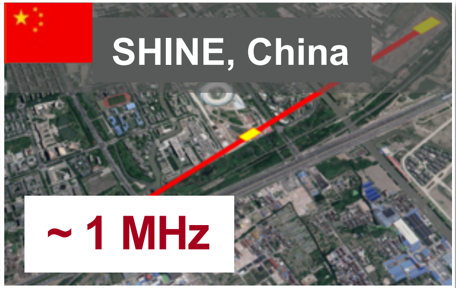
(10 Hz / 4.5 MHz)

SACLA, Japan

SwissFEL, Switzerland

PAL-FEL, Korea

Under construction

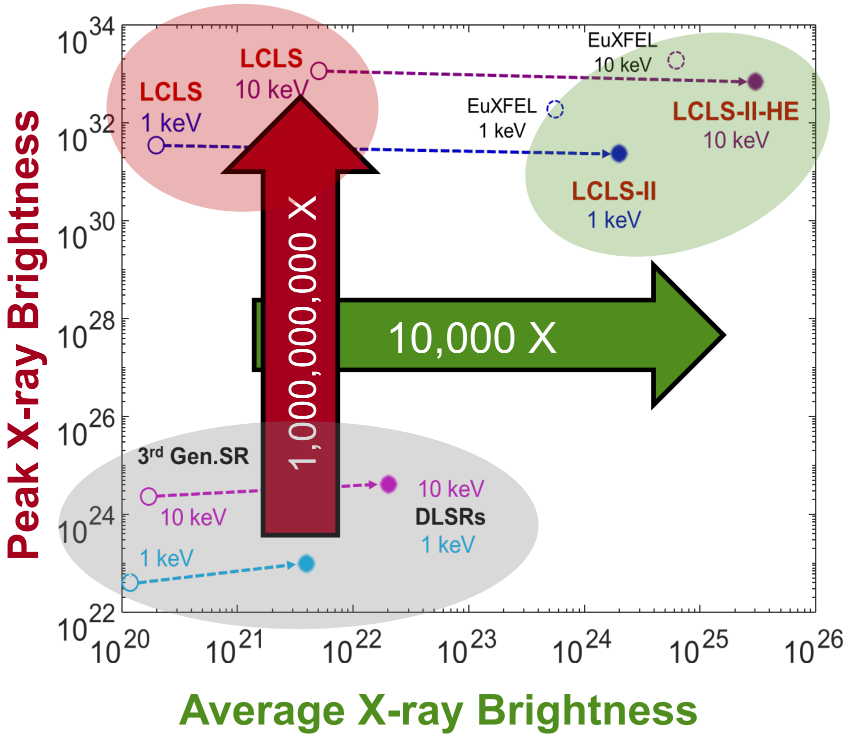


~2025

These facilities are demonstrating impressive performance & driving community growth

LCLS facility development via DOE-BES construction projects will provide an internationally leading capability throughout the next decade

SLAC



Phase 1: 2020

- **2 LCLS-II variable gap undulators**
- 0.25 to 25 keV (fundamental) at 120 Hz
- XLEAP pulse(s) at 200-400 attoseconds
- 4 pulses at 0.35 ns to >500 ns separation

Phase 2: 2022

- **LCLS-II 4 GeV superconducting accelerator**
- 0.25 to 5 keV at 1 MHz (CW, programmable)
- >5 new endstations

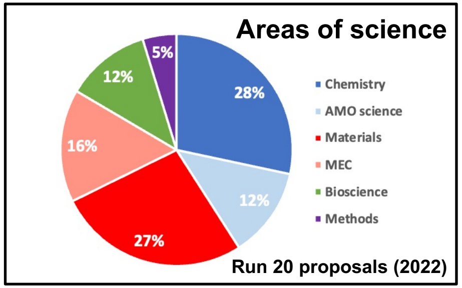
Phase 3: ~ 2027

- **LCLS-II-HE 8 GeV superconducting accelerator**
- 0.25 to >15 keV at 1 MHz
- 5 new or upgraded instruments
- Reconfiguration to increase experimental capacity

The leap from 120 Hz to 1 MHz will transform the breadth and scale of the impact of LCLS

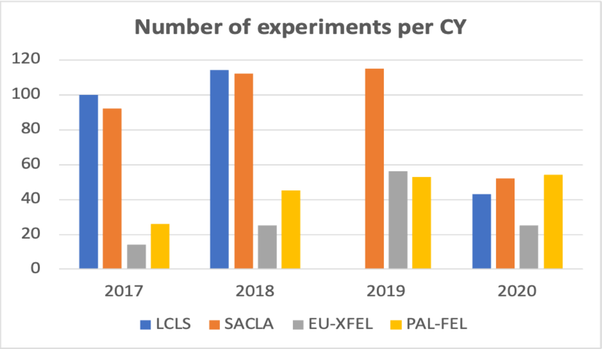
International comparison on facility productivity

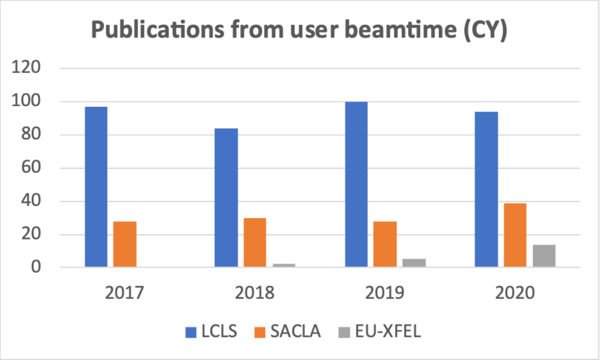
Broad community



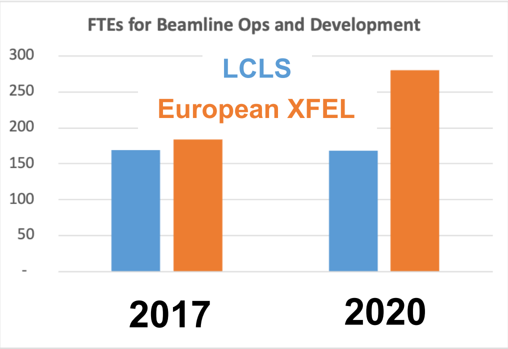
1268 registrations for the annual users meeting 2021

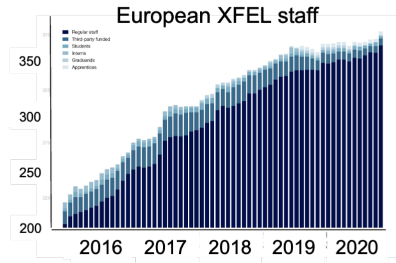
Highly productive





Rebalancing underway





Materials budget ($k)	2017	2020
LCLS	18,721	22,938
European XFEL	17,500	37,500

LCLS productivity compares very favorably, but a rebalancing is underway

International competition could increasingly challenge U.S. leadership

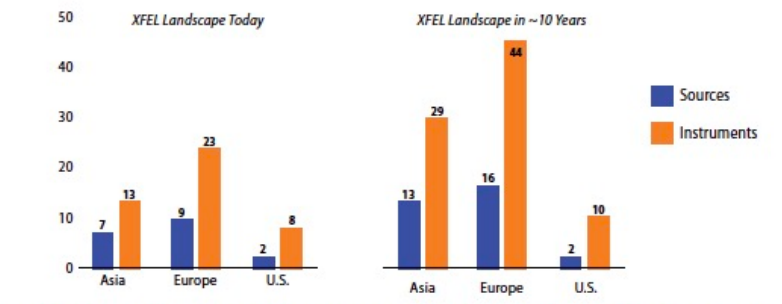


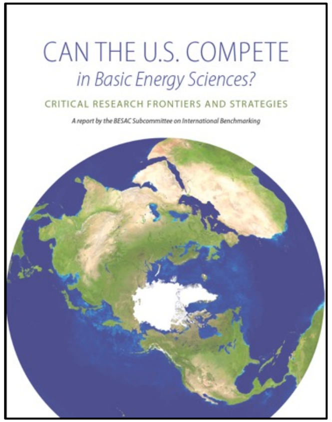
FIGURE 3. Comparing numbers of independent XFEL sources (i.e., undulator beamlines) and instruments (i.e., physically separate, independent experimental stations) in the U.S., Asia, and Europe today vs. 10 years from now, based on announced projects

SHINE (Shanghai)

- Higher energy operation (75 vs 55 cryomodules)
- Superconducting undulators
- SXR FEL, SSRF synchrotron, SULF lasers
- Shanghai Tech

Eu-XFEL / DESY upgrades

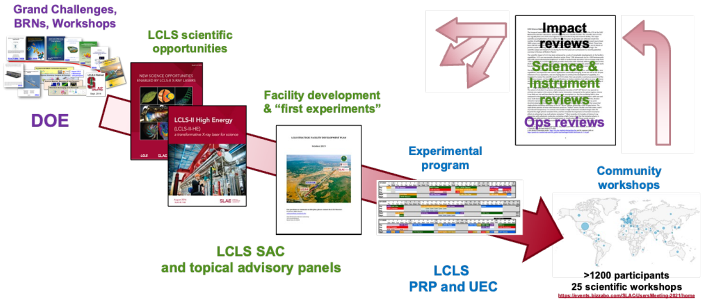
- Second instrument fan for XFEL
- MHz CW operation for XFEL
- FLASH-2 CW operation, PETRA-IV
- U Hamburg + science institutes



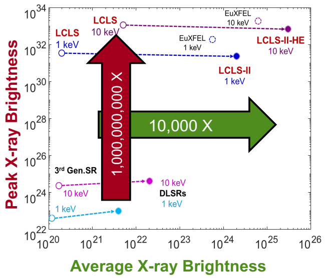
XFELs in Europe and China are building rich research ecosystems and facilities that will support dedicated, specialized instruments

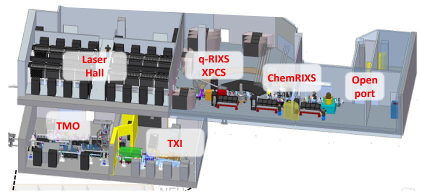
Our strategy is to provide a differentiating capability that leverages the integrated nature of SLAC/Stanford and DOE programs

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



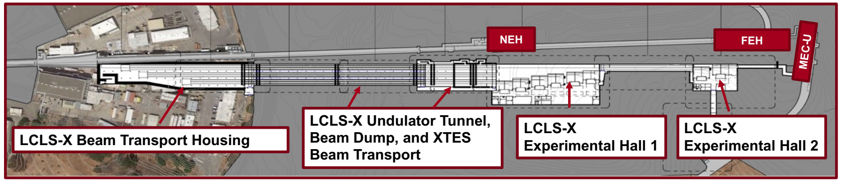
2. Drive step-changes in source and facility performance





3. Foster a vibrant research ecosystem, taking advantage of our unified structure

4. Full build-out and exploitation of the LCLS platform

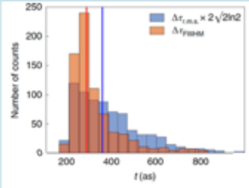


Positions LCLS to sustain a world-leading position over this decade and beyond

LCLS Scientific Campaigns have been created to allow community-wide teams to tackle strategic "grand challenge" questions

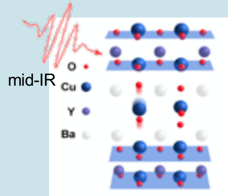
SLAC

Attosecond science



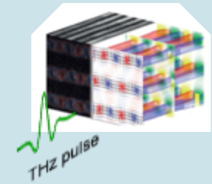
- Control and observation of coherent electronic motion on natural attosecond timescales
- J. Cryan (PULSE) leading 39 PI's from 16 institutions

Collective dynamics



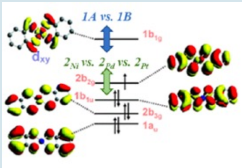
- Nonlinear coupling of collective modes in quantum materials
- Control of electronic order by coherent phonon excitation
- M. Trigo (SIMES) leading 21 PI's from 13 institutions

Topological Materials



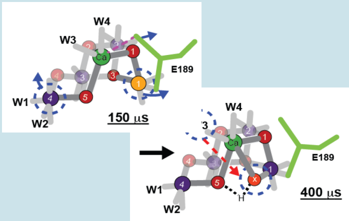
- Dynamics of complex topological structures by design
- Collective modes, transformation pathways, and fluctuations
- Gopalan et al (PSU),14 PI's from 5 institutions including SLAC

Controlled reactivity



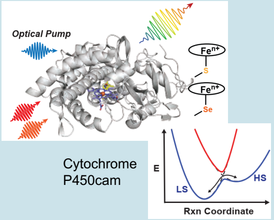
- Design Principles for Covalent Control of Electronic Excited State Reactivity in Transition Metal Complexes
- K. Gaffney et al (SLAC), 14 PI's from 5 institutions

Photosynthesis PS II



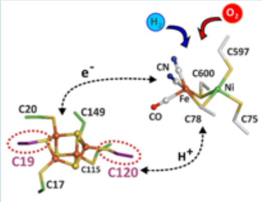
- Understand light-driven multi-electron catalysis of the water oxidation in PS-II
- Junko Yano et al.
  (20 investigators from 8 institutions)

Quantum Enzyme Catalysis



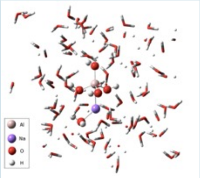
- Understand electronic properties and quantum effects in enzyme function
- Ryan Hadt et al.
  (17 investigators from 10 institutions)

Enzyme Catalysis for Energy



- Understand structural dynamics of metallo-enzymes for the energy economy
- Jan Kern et al.
  (25 investigators from 15 institutions)

Radiolysis in remediation

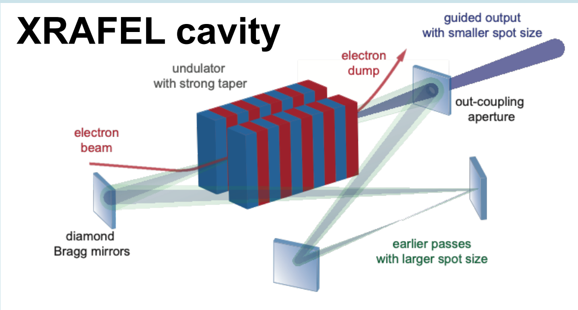


- Understanding radiation-induced chemistry in the condensed phase
- IDREAM environmental remediation
- L. Young (ANL) and C. Pearce (PNNL), 27 from 6 institutions

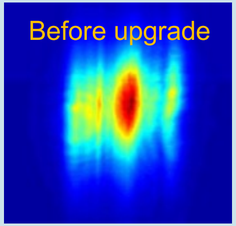
We plan for ~8-10 concurrent Campaigns, each representing a major cross-community effort of theory, synthesis, experiments, and analysis – with beamtime allocation over 3+ years

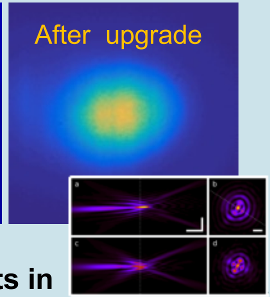
The scientific goals drive strategic R&D to transform the facility’s capabilities, and inspire entirely new approaches to X-ray science

Innovative X-ray sources



Transforming beam quality

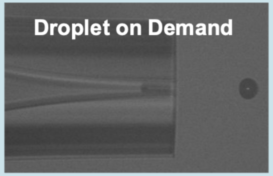




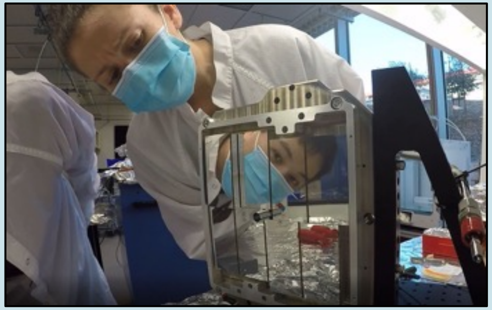
Major improvements in throughput, uniformity & measurement

Ultra-stable X-ray optics

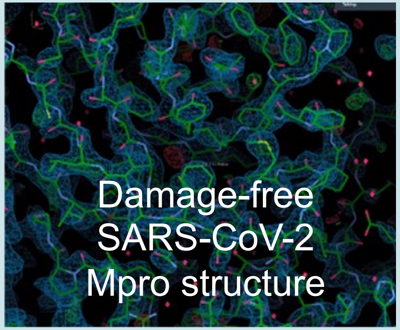
New sample environments



kHz to MHz X-ray detectors



Real-time data analytics

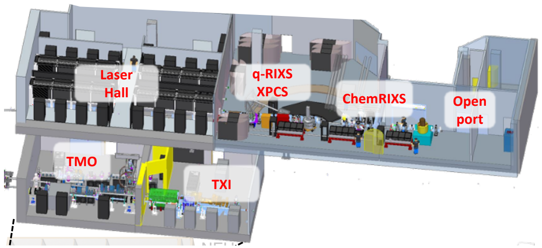


This is an integrated technology development program to drive full exploitation of the major upgrades

The instrument development plan is informed by extensive community engagement to serve a broad science program

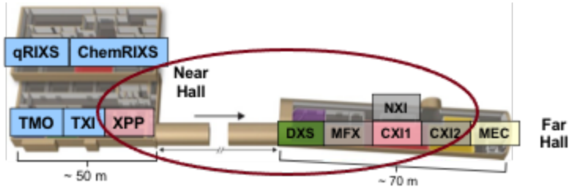
SLAC

LCLS-II instruments



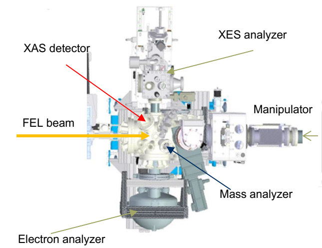
- AMO science
- Condensed phase chemistry and catalysis
- Quantum materials
- Nonlinear X-ray science

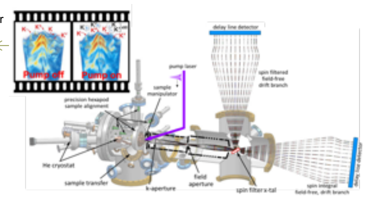
LCLS-II-HE instruments



- Complex materials
- Biological dynamics
- Heterogeneous catalysis
- Gas phase chemistry
- Quantum materials

Community-led instruments





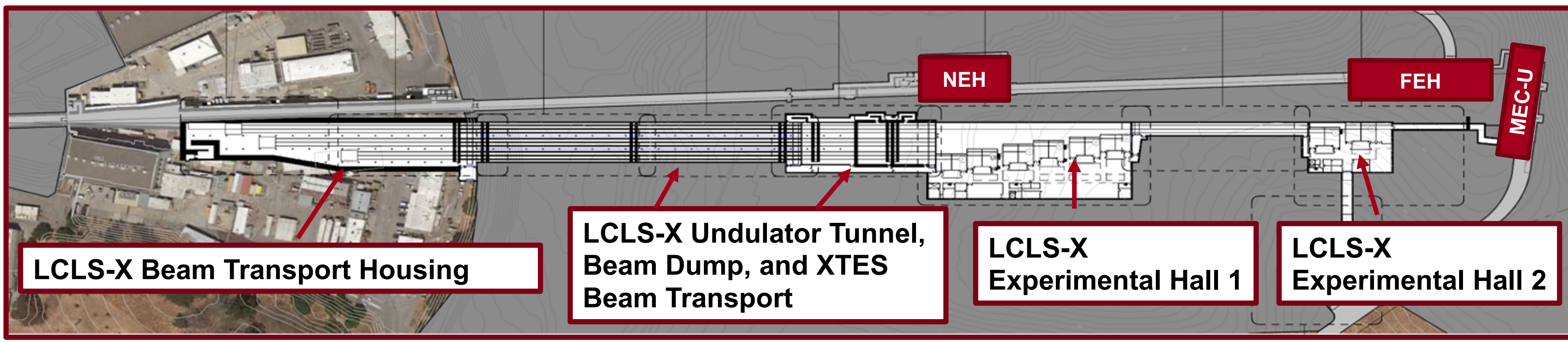
- Surface science (Heinz et al)
- Momentum microscope (Shen et al)

Designed to provide the range and versatility needed to keep our user community at the forefront

Long term competitiveness: Realizing the full potential of the LCLS platform

Analysis of the priority scientific requirements drives the need for a suite of dedicated, specialized instruments:

- The existing LCLS-II-HE accelerator will be sufficiently powerful to feed 10 undulators
- Expand LCLS from 2 beamlines to ~10, and thus number of instruments to >30
- Enable the highest performance beamlines (superconducting undulators, RAFEL, …)
- Phase the delivery to allow staged growth, responsive to emerging priority directions

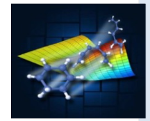


This plan fully leverages the large-scale investments at SLAC over the period 2005-2027

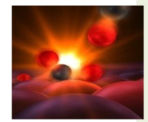
Summary: XFELs will define the frontiers of 21st Century X-ray science

SLAC

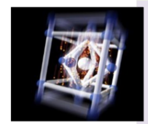
- LCLS performance has shown where coherence, ultrafast pulses, and extreme brightness are most impactful.
- LCLS-II and LCLS-II-HE will provide a transformational capability.
- Co-location of capabilities and scientific programs at SLAC and Stanford provides critically-enabling opportunities.
- Long-term leadership and exploitation of XFELs requires dedicated beamtime and specialized instruments. Advancement of the LCLS-X concept is timely given the international competition.



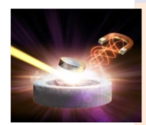
Chemical dynamics:
Reaction dynamics, charge transfer, molecular photocatalysts, natural & artificial photosynthesis



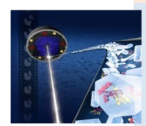
Catalysis:
Homogeneous and heterogeneous catalysis, interfacial & geo/environmental chemistry



Materials Physics:
Heterogeneity, nonequilibrium dynamics & spontaneous fluctuations



Quantum Materials:
Emergent phenomena & collective excitations



Biological Function & Structural Dynamics
Dynamics in physiological environments

DOE-BES has created a platform for sustained international leadership in X-ray science

LCLS | Linac Coherent Light Source