High energy upgrade: LCLS-II-HE
new insight to structural dynamics at the atomic scale

- Ultrafast coherent X-rays
- ~1 Ångstrom (~12 keV)
- High repetition rate

- 4 GeV \Rightarrow 8 GeV (SCRF linac)
- +20 cryomodules

Greg Hays
Project Director
LCLS-II-HE Dedicated Workshops

2016  Scientific Opportunities for Ultrafast Hard X-rays at High Rep Rate: An Energy Upgrade of LCLS-II

2016  LCLS-II-HE Science Case (CD-0 Approval)

2017  LCLS-II-HE “First Experiments” Meeting: Chemistry & Materials Physics

2017  LCLS-II-HE “First Experiments” Meeting: AMO, Biology, and Quantum Materials

2018  Advanced X-ray Methods & Instrumentation for LCLS-II-HE Science

CD-1 approved by DOE in September 2018
Advanced X-ray Methods & Instrumentation for LCLS-II-HE Science

Workshop Charge

- Identify compelling (transformative) X-ray methods and instrumentation
- Demonstrate that proposed methods exploit (require) the unique capabilities of LCLS-II-HE
- Justify (and prioritize) methods by projected science impact
  - LCLS-II-HE “first experiments” are a starting point (see LCLS-II-HE science case)
  - New “first experiment” ideas are welcome
- Consider both:
  1. Ideas consistent with near-term constraints (e.g. instrumentation that will fit in existing LCLS facilities)
  2. Longer-term ideas with greatest potential science impact
- For both (1) and (2):
  - Define the experimental approach
  - Define the required instrumentation, and key LCLS-II-HE source parameters
  - Feasibility analysis (or plan for one)
Advanced X-ray Methods & Instrumentation for LCLS-II-HE Science

October 16-17, 2018
Plenary: B53 Panofsky Auditorium
Breakouts: Building 48 (Redwood)
SLAC National Accelerator Laboratory - Menlo Park, CA

The LCLS-II project now underway at SLAC represents a major advance in X-ray laser capabilities that will enable compelling new science opportunities as identified by the user community [1]. When it becomes operational in 2020, this next-generation facility will exploit advanced superconducting accelerator technology (CW-JSCF) and tunable undulators to provide ultrafast coherent X-rays in a uniformly-spaced train of pulses with programmable repetition rates of up to 1 MHz and tunable photon energies from 0.25 to 5 keV.

Looking to the future, the proposed energy upgrade of LCLS-II to 8 GeV (LCLS-II-HE) promises to open entirely new areas of science as further identified by the user community [2]. LCLS-II-HE will provide X-ray energies extending beyond 12 keV to 40 keV, 100 times more than LCLS-II (1 keV), with a peak flux of 10^20 photons per pulse.

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Tues. Agenda Overview

8:30 AM  
**Plenary Session**

10:50 AM  
*break – group photo (outside B53)*

12:30 PM  
*lunch (Redwood B48)*

1:30-6:00 PM  
**Science Breakout Sessions**

6:30 PM  
*dinner (B53 SLACáfe)*

after dinner speaker: J.B. Hastings

8:00 PM  
*optional discussion & preparation closeout slides for Wed.*
Science Breakout Sessions

- All are encouraged to present ideas (template provided – see website)
- Breakout summaries at plenary closeout
- Scribes will take notes and collect presented materials (for internal use only)

### Materials Physics:
- heterogeneity, nonequilibrium dynamics

- Diling Zhu
- Aaron Lindenberg
- Mariano Trigo

### AMO Physics, Gas-phase Chemistry, Atto Science

- Mike Minitti
- Peter Walter
- Thomas Wolf

### Quantum Materials:
- correlated/collective phenomena

- Hasan Yavas
- Jun Sik Lee
- Patrick Kirchmann

### Condensed Phase Chemistry

- Roberto Alonso-Mori
- Amy Cordones
- Tim van Driel

### Biological Function & Structural Dynamics

- Mark Hunter
- Cornelius Gati
- Sebastien Boutet
Wed. Agenda Overview

8:30-10:30 AM  **Advanced Instrumentation & Methods**  
*parallel breakouts*

10:20 AM  **Science Breakout Sessions**  
*final discussion & prep for closeout*

11:50 PM  **lunch** (Redwood B48)

12:50 PM  **Plenary Closeout** (Redwood B48)  
*summary presentations from science breakouts*
1. Advanced spectroscopy methods to probe collective excitations, electronic structure, and dynamics (IXS, RIXS, XPCS, HERFD, PES etc.)

2. Advanced scattering methods to probe atomic structural dynamics (Coherent scattering/imaging, XPCS, Bragg CDI, PDF analysis, EXAFS etc.)

3. Advanced methods to map stochastic dynamics, capture “rare” events, characterize non-identical objects, and map potential energy landscapes

4. Nonlinear X-ray & X-ray Pump/Probe Methods (Stimulated X-ray Raman, FT-IXS, extreme states via X-ray pump etc.)
1. What are the most important methods (prioritized list) and essential requirements for each prioritized method that will have the greatest scientific impact
   • Requirements for the proposed methods/instrument/diagnostics
   • Key XFEL and/or beamline capabilities/parameters
   • Requirements should accommodate a reasonably broad range of science applications
   • Identify conflicts, or areas where needs for different science applications begin to diverge i.e. What is an appropriate balance between impact/optimization for one area of science, vs. impact across multiple areas of science?

2. What are the most compelling science applications for each method
   • Should be consistent with above requirements
   • Solicit ideas from the science breakouts
   • Each science breakout will be encouraged to identify at least one representative to attend each of the Advanced Methods breakouts

3. Feasibility, current state of knowledge, next steps
   • Assessment of the feasibility and current state of knowledge for the proposed method/instrument
   • Is this a straight-forward extension of current state of the art?
   • What are the critical open questions, and next steps, to advance the feasibility case
New Experimental Capabilities of LCLS-II-HE

- **Dynamics near the FT Limit**
  - Time-resolved spectroscopy & inelastic scattering
    - RIXS & IXS at high resolution (meV)
  - Excited-state molecular dynamics
  - Time-resolved (diffuse) X-ray scattering (FT-IXS) following impulsive excitation of collective modes

- **Fluctuations & Stochastic Dynamics**
  - Ground-state collective modes via inelastic scattering
  - Photon Correlation Spectroscopy (XPCS, fs and longer):
    - sequential (μs), two-pulse (fs), programmable time structure

- **Heterogeneity**
  - Heterogeneous ensembles at atomic resolution (10^8-10^10 snapshots/day)
  - Time-resolved Pair Distribution Function (PDF)
  - ~100x increase in average X-ray brightness beyond DLSRs at 20 keV
LCLS-II-HE Science Opportunities

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

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

Materials Physics:
Heterogeneity, spontaneous fluctuations, nonequilibrium dynamics, extreme environments

Quantum Materials:
Emergent phenomena & collective excitations

Biological Function & Structural Dynamics
Dynamics in physiological environments