LCLS scientific development

LCLS-II, LCLS-II-HE

Mike Dunne

Director, LCLS

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U.S. DEPARTMENT OF ENERGY
Office of Science

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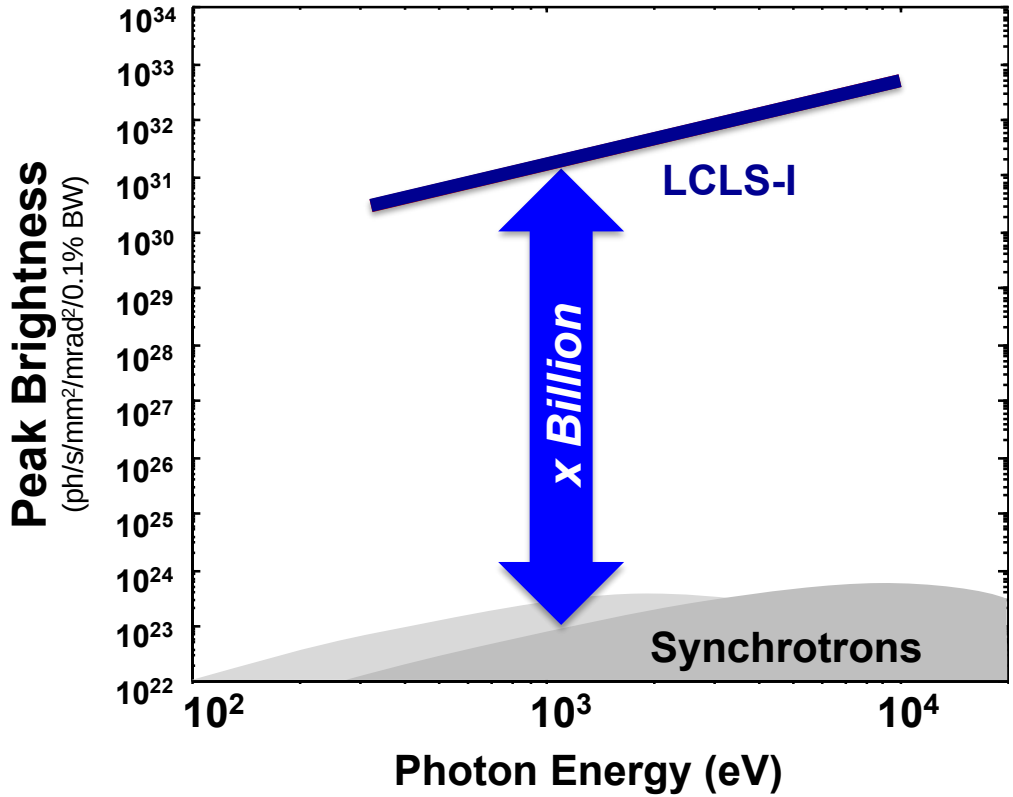
The performance of LCLS was designed to be a true game-changer



Initial expectations:

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

LCLS was a technical and scientific leap into the 'unknown'

The ability to tailor LCLS has far exceeded expectations, with major steps in capability year-on-year

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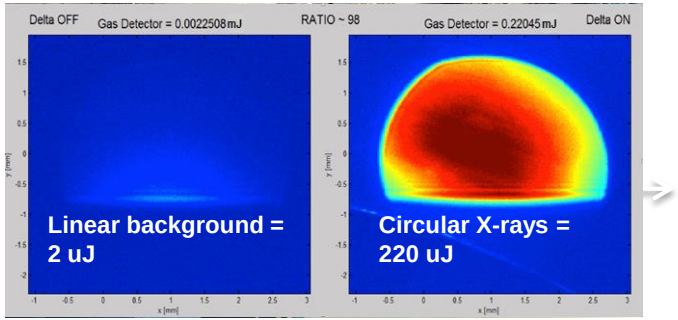
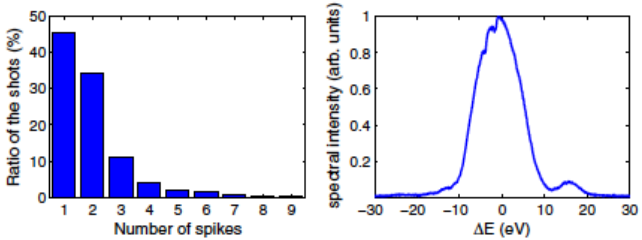
From linear to controlled polarization

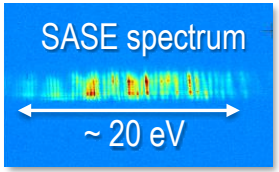


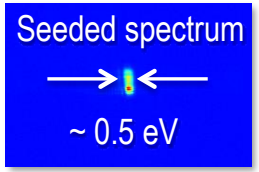
From 200 fs down to 200 as duration



179 ± 58 as @ 9 keV (14.4 eV BW)

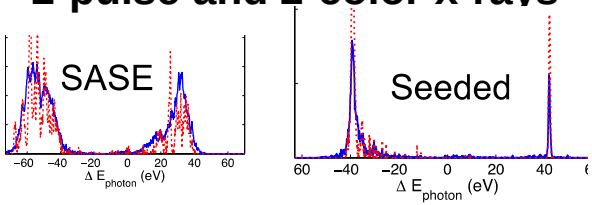
From statistical fluctuations to controlled pulse width and spectrum





40x increase in spectral brightness.

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



From fs to >600 ns separation, and 2, 3, 4 (or more) pulses

The scientific reach of LCLS has been dramatically extended

LCLS has opened new research opportunities to tackle grand challenge problems in multiple disciplines

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Collective dynamics in complex materials

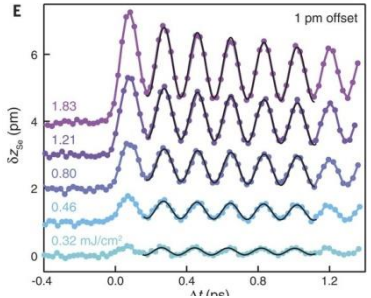
- Direct measurements of electron-phonon coupling (FeSe)
- Field-induced 2D to 3D charge density wave order (YBCO)
- Observation of purely relaxational diffusive dynamics (LBCO)

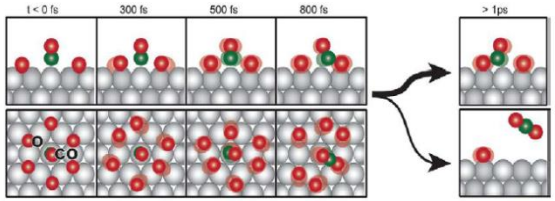
Real-time tracking of chemical bond formation

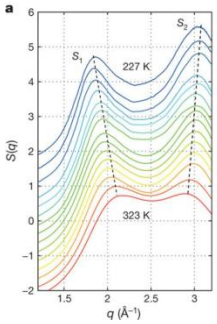
- Transient catalytic states in CO oxidation on metal surface
- Room temperature, damage free PS-II transient states
- Observing ionization and decay pathways (DNA repair)

Molecular dynamics in soft matter and biology

- Water structure below the ice nucleation temperature
- Ultrafast functional motions tracked in CO-myoglobin
- Structures of ligand-triggered riboswitch RNA reaction states

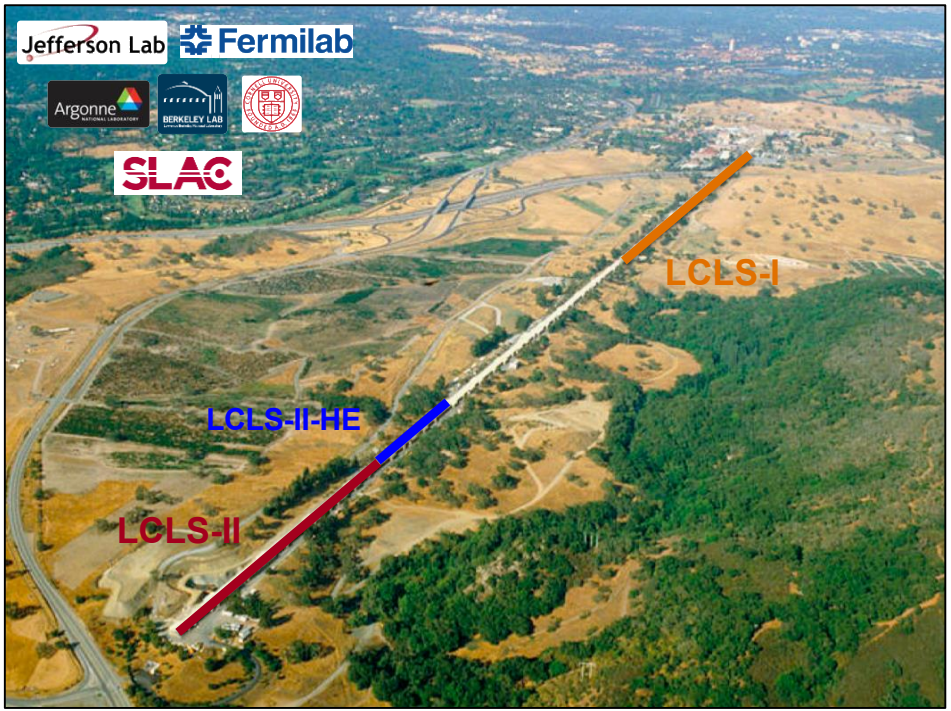


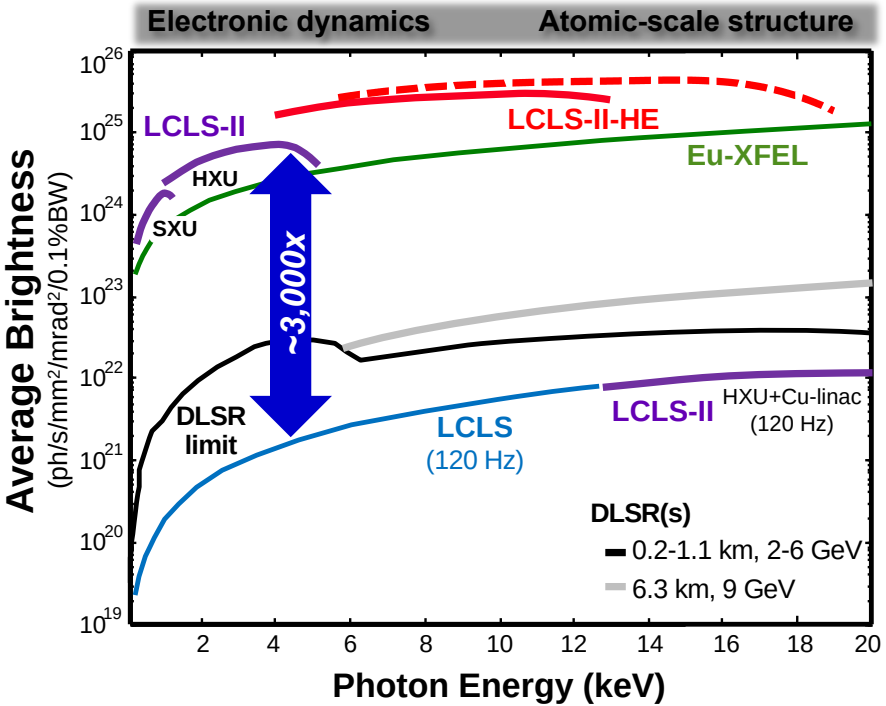




Pioneering results from LCLS have highlighted the key areas where coherence, fs time-resolution, and high power can have a revolutionary impact

LCLS-II and LCLS-II-HE will take us from 120 pulses per second to 1 million pulses per second





LCLS-II Currently 70% complete. Users online in 2021

LCLS-II-HE CD-1 review in June 2018. Targeting mid-decade users

LCLS-II will transform our understanding of dynamics in real-world materials and chemical science systems

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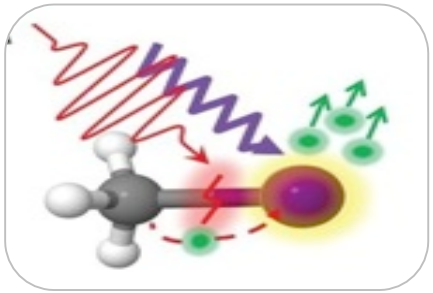
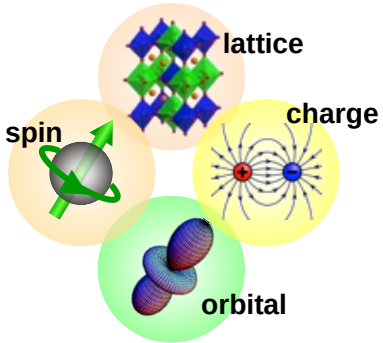
Charge dynamics on fundamental timescales

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



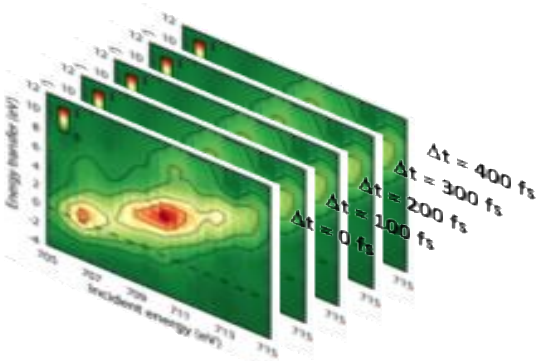
Emergent phenomena in quantum materials

- Connect spontaneous fluctuations, dynamics and heterogeneities on multiple length- and time- scales to bulk material properties
- Study interacting degrees of freedom (e.g. unconventional superconductors)



Molecular dynamics with exquisite resolution

- Measure element-specific, local chemical structure and bonding
- Study efficient, robust, selective photo-catalysts



The leap from 120 Hz to up to 1 MHz will be transformative

LCLS-II-HE will enable structural dynamics at the atomic scale – a key aspect of the BESAC Transformative Opportunities

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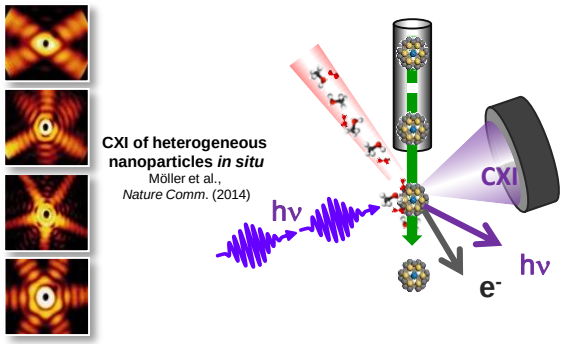
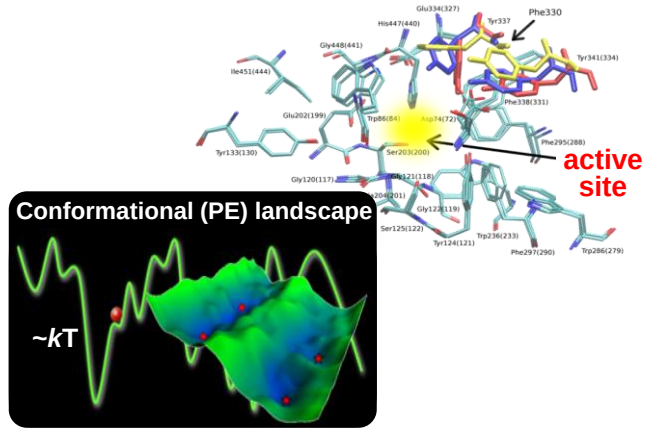
Heterogeneity & complexity in ground & excited states

- Correlate catalytic reactivity and structure
- Real-time evolution with chemical specificity and atomic resolution



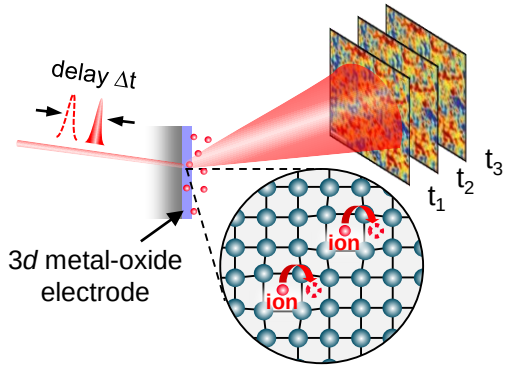
Dynamics of biomolecules & molecular machines

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



Ground State Fluctuations & spontaneous evolution

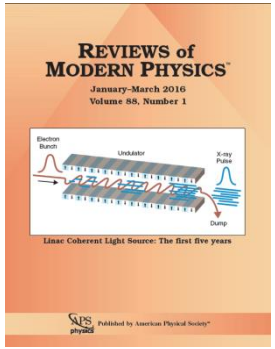
- Characterize statistically dynamic systems without long-range order
- Inform directed design of energy conversion and storage materials



LCLS-II-HE provides the ability to study non-equilibrium phenomena and move beyond idealized materials and systems

The X-ray laser revolution is set to drive a new era of Grand Challenge discovery science

From early scientific impact,



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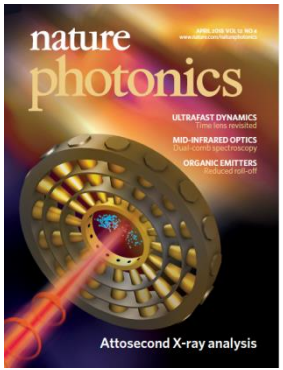
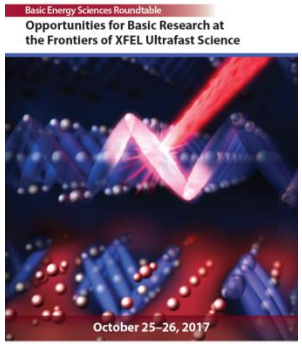
… to unprecedented measurements,



… to accessing critical new regimes,



… to full exploitation and exploration of new frontiers