

Future Science Opportunities Enabled by X-ray Free Electron Lasers

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Linac Coherent Light Source, SLAC

Thursday, April 7, 2015



SLAC NATIONAL ACCELERATOR LABORATORY



Fermilab Jefferson Lab



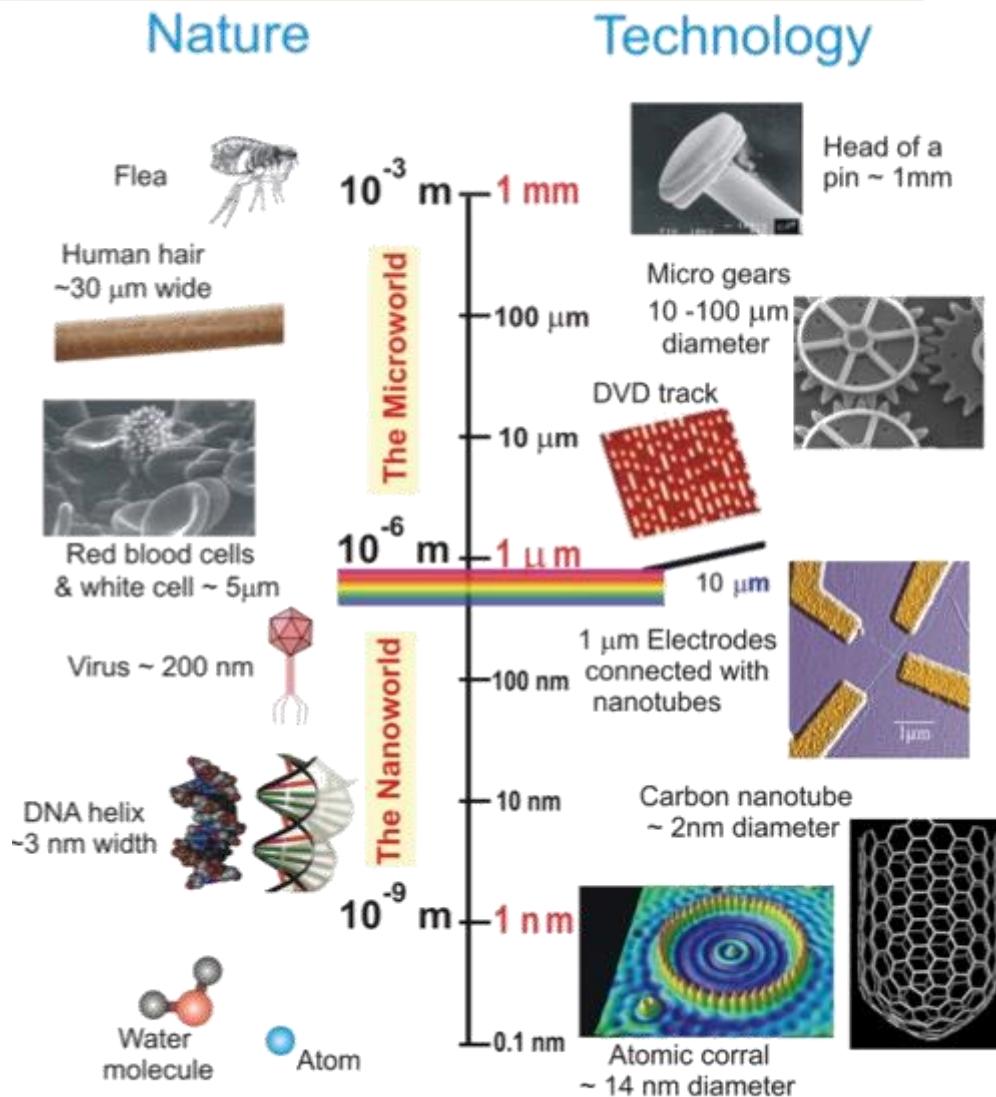
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Outline

- X-ray Science and Methods
- Soft and Hard X-ray Free Electron Lasers
- A Tour of LCLS with some science examples
 - Soft X-ray Instrument for Materials (CXI)
 - Coherent X-ray Imaging (CXI)
- The LCLS-II upgrade
- Further Reading

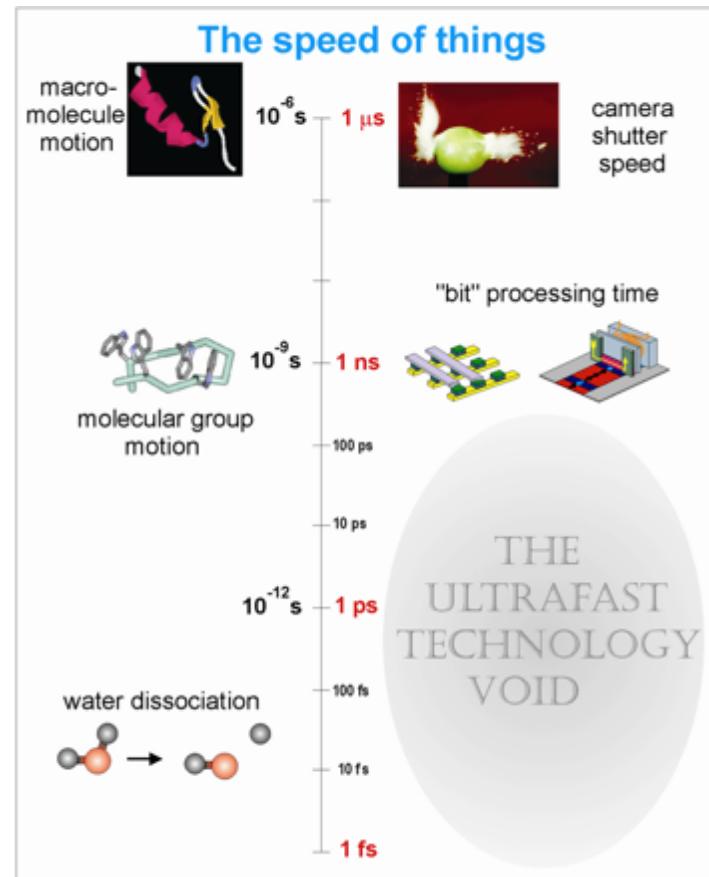
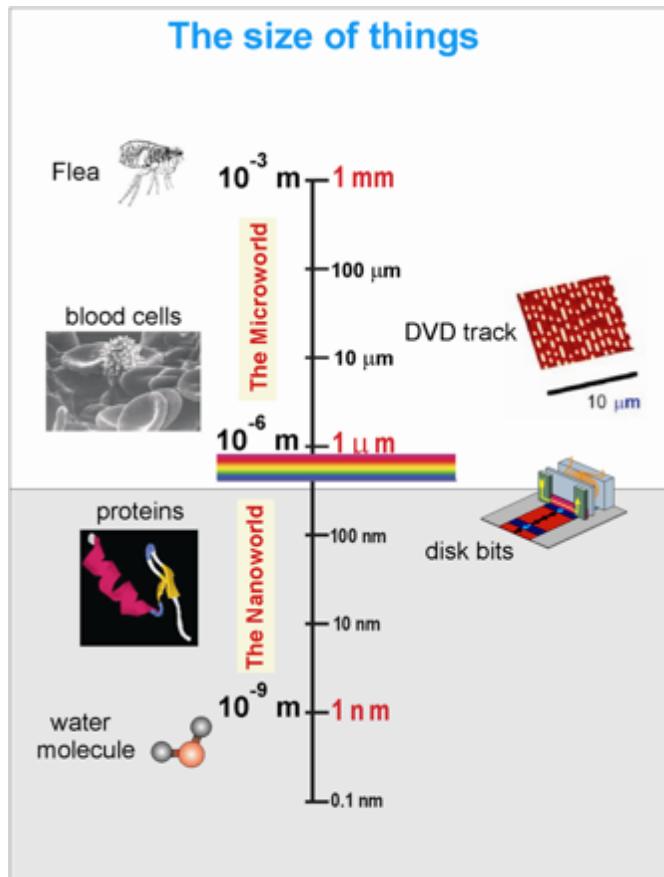
How do we see the nanoworld?

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Relevant Time and Length Scales

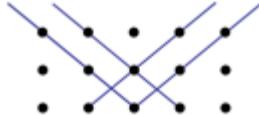
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1 light picosecond = 0.3 mm

Why do we use x-rays?

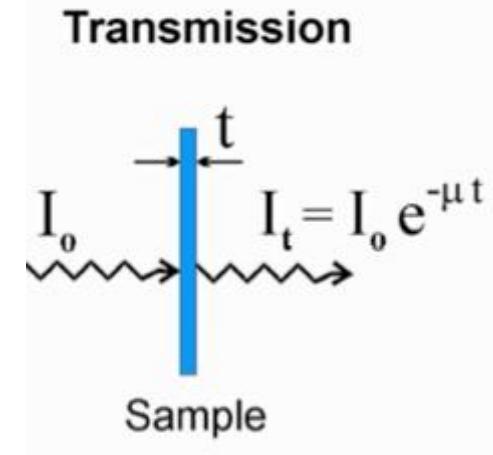
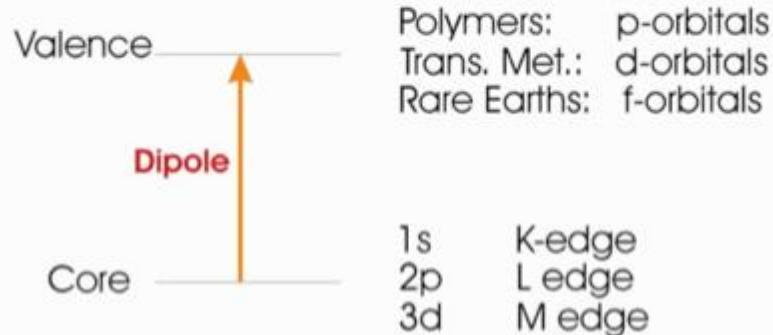
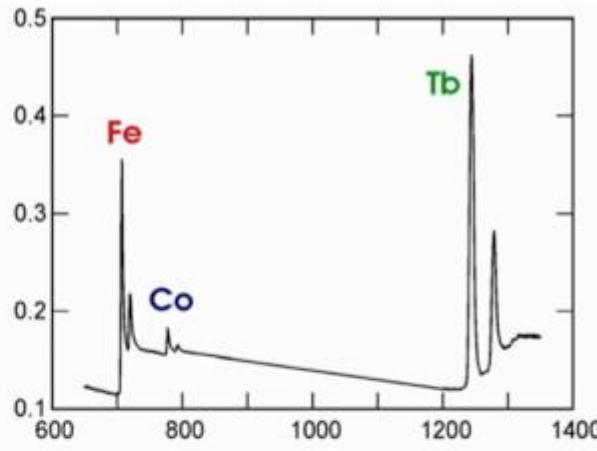
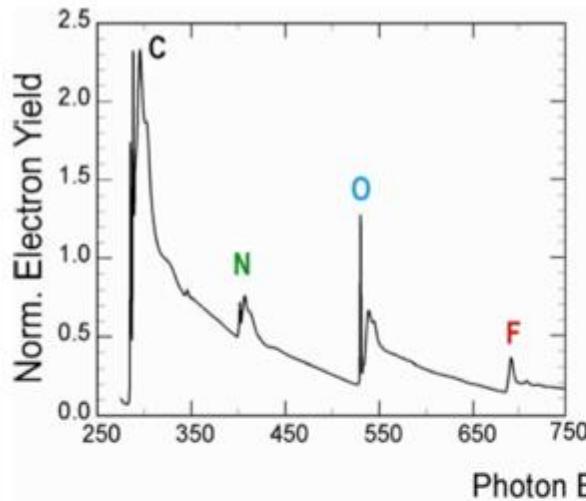
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| Capability | Technique |
|---|---|
| Access to atomic length scales | Scattering  |
| Capture texture exactly and access bulk | Imaging  |
| Element and chemical sensitivity | Spectroscopy  |

X-ray Absorption Spectroscopy

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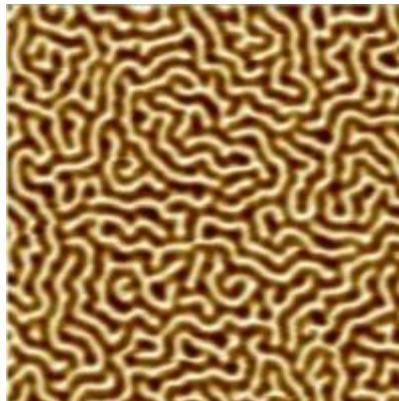
Element Specific Sensitivity and Contrast



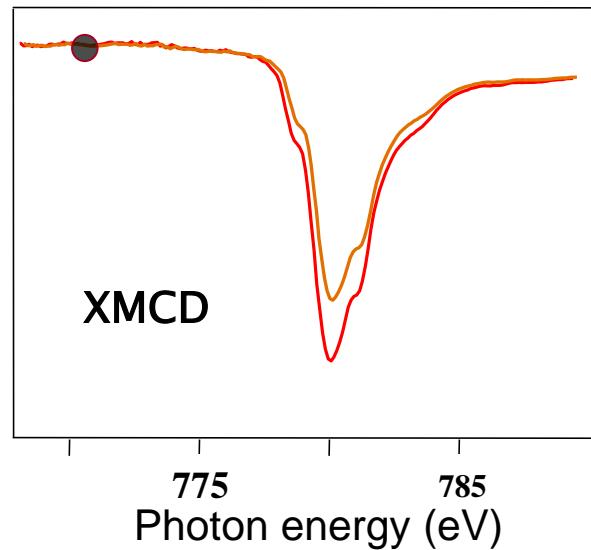
Resonant Coherent Scattering

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magnetic domains
Co/Pd multilayers

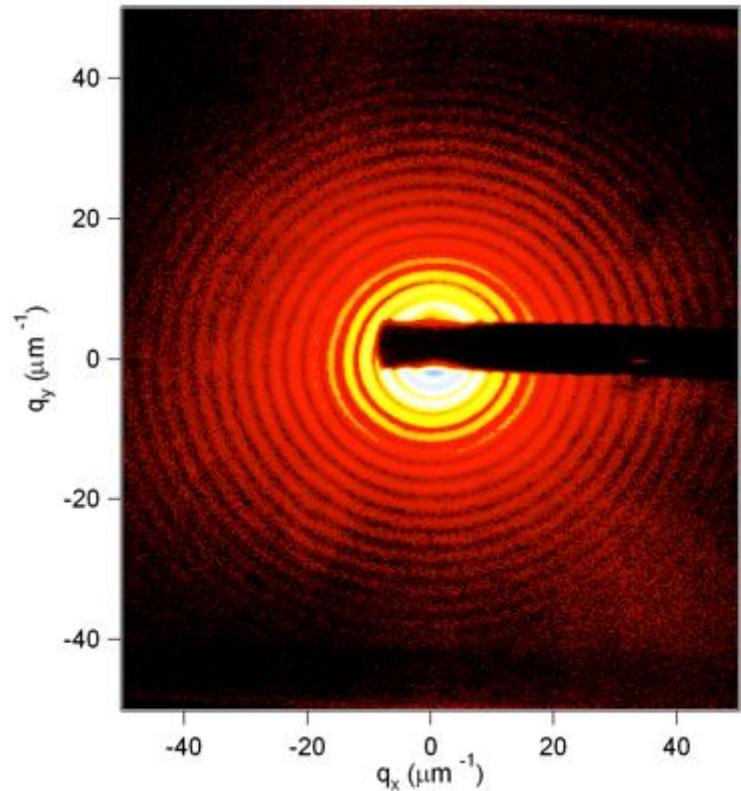
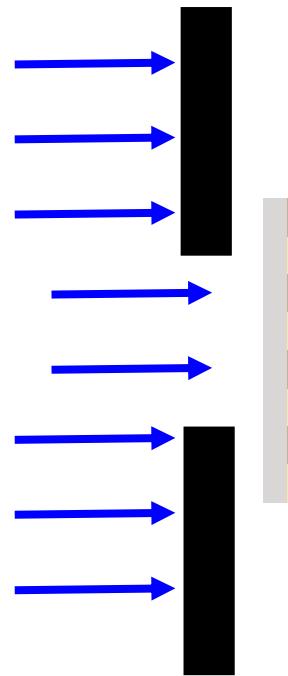


Transmission



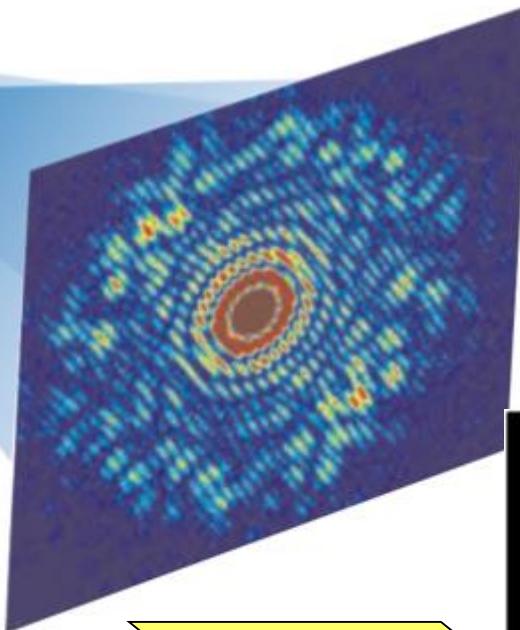
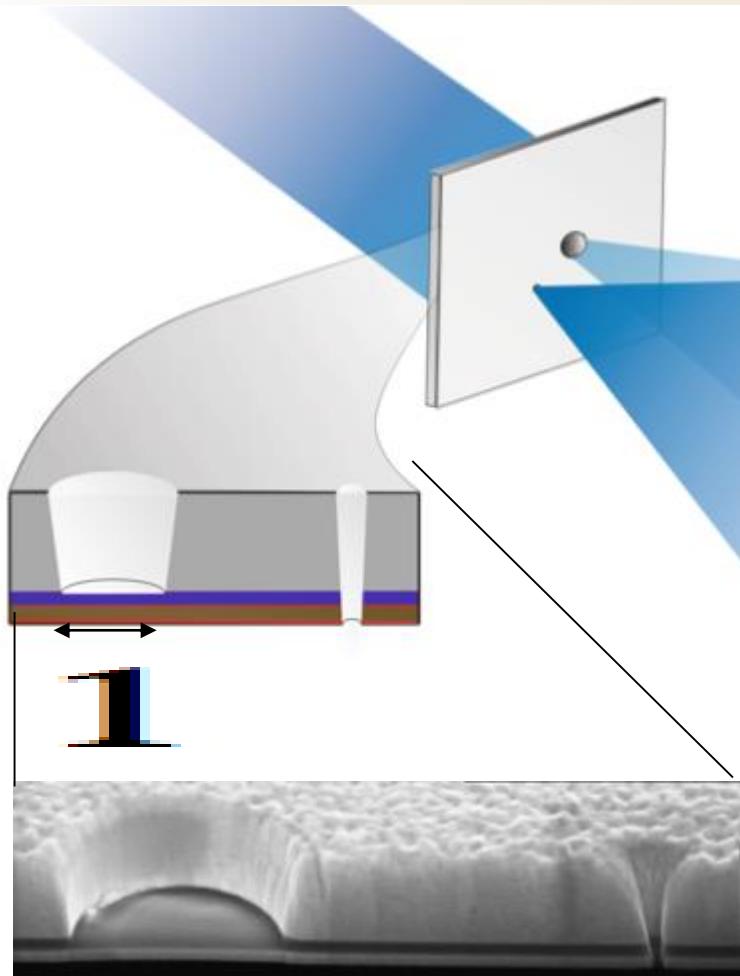
- Perpendicular Magnetization
- X-Ray Magnetic Dichroism

Non-Resonant



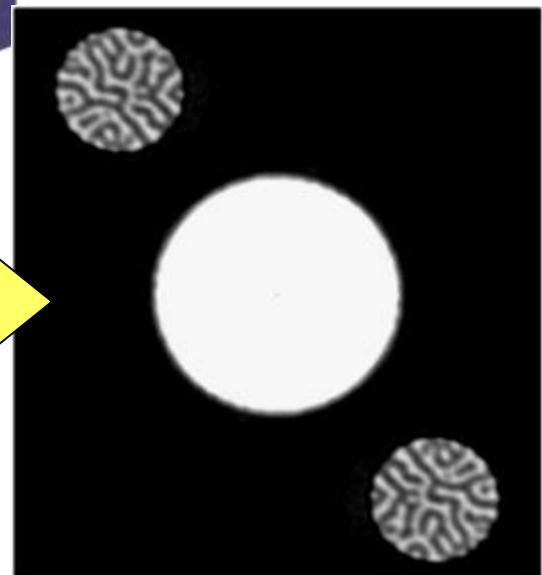
Fourier Transform Holography

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Fourier
Transform

Autocorrelation

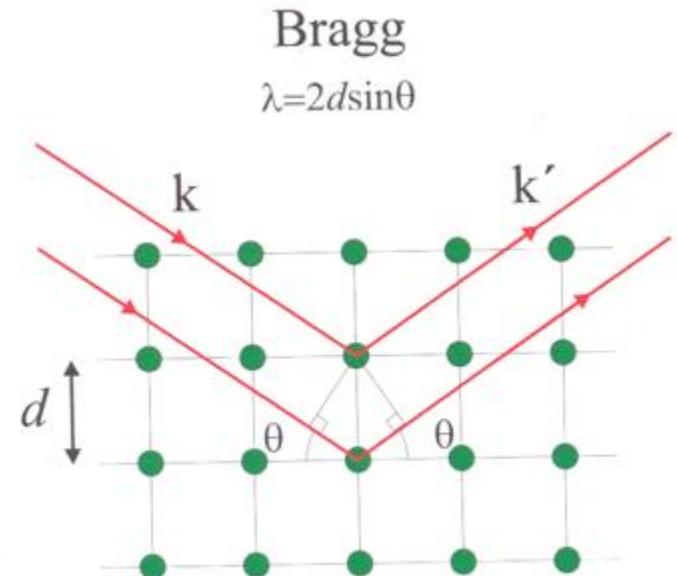
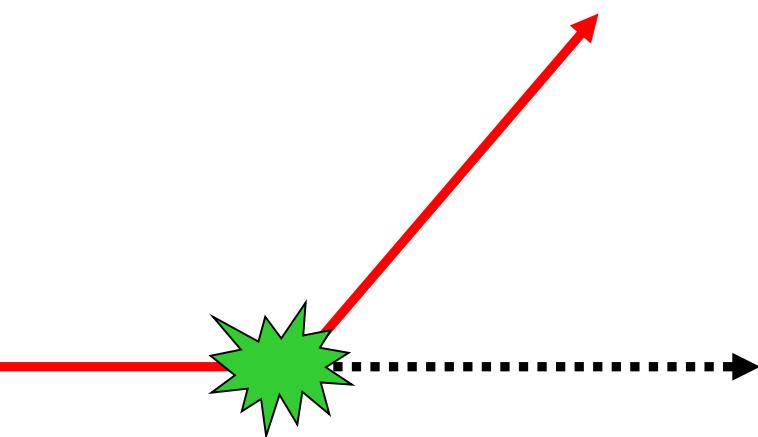


X-ray Scattering & Diffraction

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Wide Angle Scattering Probes
Short Length Scales

Crystallography
Probe Atomic Structure
When Long Range Order is Present



Jens Als-Nielsen, Elements of Modern X-ray Physics, Wiley, (2001)

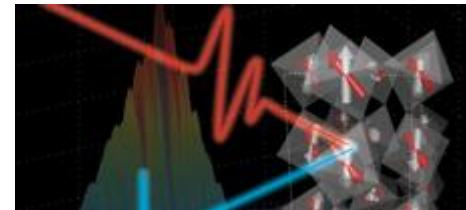
Why do we use X-ray Free Electron Lasers?

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X-rays provide element specificity and atomic resolution...

➤ Ultrashort X-ray Pulses

- Study ultrafast (femtosecond) dynamics
- Out-run damage to samples



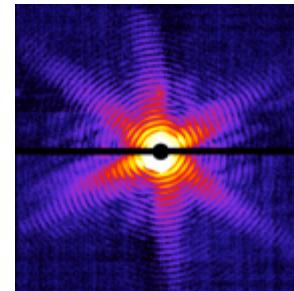
➤ High Energy Per Pulse

- Enables single shot imaging
- Generates unprecedented electric fields



➤ Coherent X-ray Pulses

- Far field scattering methods improved spatial resolution



Hard vs. Soft X-rays



| | Soft X-rays | Hard X-rays |
|--|----------------------|------------------|
| Photon Energy Range | 250eV - 2 keV | 4 keV – 25 keV |
| e-Beam Energy to produce photons* | 3-5 GeV | 8-17GeV |
| FEL gain length** | ~2m | ~5m |
| Transmission through 100 mm Air(1 bar) | 10^{-33} | 89% |
| Transmission through 100 nm of Iron | 34% | 97% |
| Experimental Strength | Electronic Structure | Atomic Structure |

*The photon energy is a function of both the ebeam energy and the undulator period and gap. The values here represent optimized

** Around 20 gain lengths needed to reach saturation

Operating VUV and X-ray FELs Worldwide

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| Location | Name | Linac type | E energy (GeV) | Photon energy (keV) | Rep. rate (Hz) | Start ops. |
|-------------|------------|------------|------------------|---------------------|--------------------------|------------|
| Germany | FLASH | SC | 1.2 | 0.03–0.3 | $(1 - 500) \times 10^3$ | 2005 |
| | FLASH-II | SC | | | | 2015 |
| | XFEL | SC | 17.5 | 3–25 0.2–3 | $(1 - 2800) \times 10^3$ | 2017 |
| Italy | FERMI-FEL1 | NC | 1.5 | 0.01–0.06 | 10–50 | 2012 |
| | FERMI-FEL2 | | | 0.06–0.3 | | 2014 |
| Japan | SACLA | NC | 8 | 4–15 | 30–60 | 2011 |
| Korea | PAL-XFEL | NC | 10 | 1–20 | 60 | 2016 |
| | | | 3 | 0.3–1 | | |
| Switzerland | SwissFEL | NC | 5.8 | 2–12 | 100 | 2017 |
| | | | 3 | 0.2–2 | | |
| USA | LCLS | NC | 16 | 0.25–11 | 120 | 2009 |
| | LCLS-II | NC | 16 | 1–25 | 120 | 2020 |
| | LCLS-II | SC | 4 | 0.2–5 | 10^6 | 2020 |

^aPulsed mode operation at 10 Hz, with each macropulse providing up to 500 bunches.

^bPulsed mode operation at 10 Hz, with each macropulse providing up to 2800 bunches.



VUV: below 0.2 keV

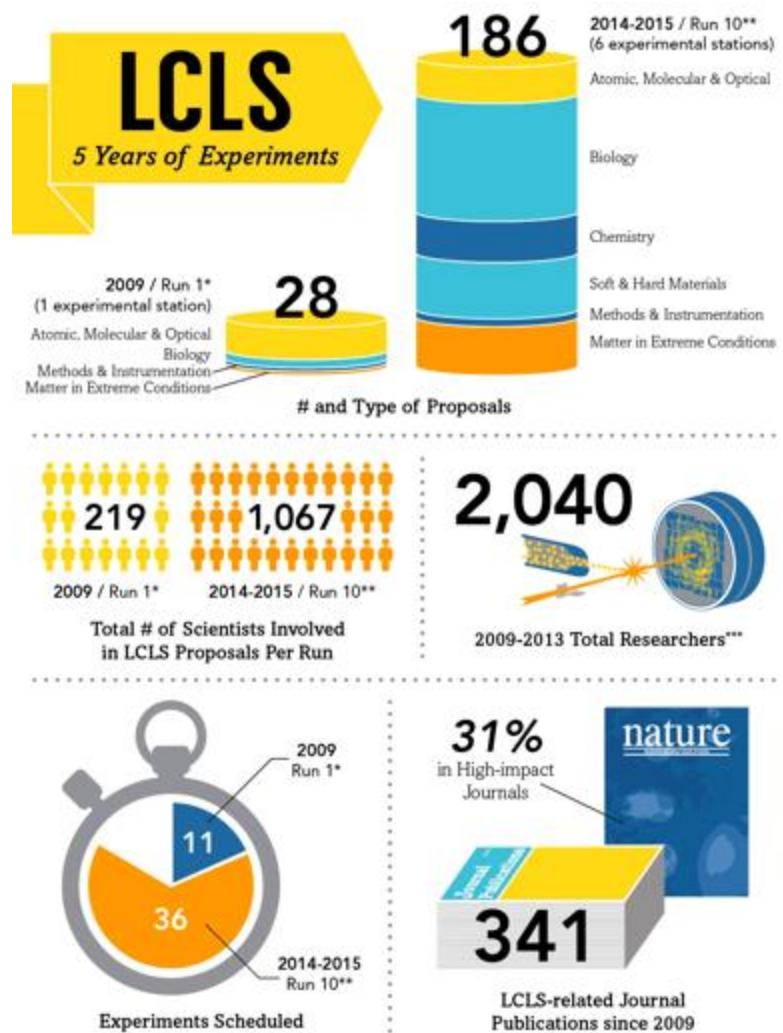
Soft X-ray: 0.2–2.0 keV

Hard X-ray: 4–25 keV

How does LCLS work?

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- Users submit proposals twice a year
- Beamtime proposals are evaluated via peer review
- ~20% of proposals are granted beamtime
- Successful proposals are awarded an average 60 hours of LCLS beamtime
- The average user group is ~15 people



* Run 1, the first operating period at LCLS, was October-December 2009.

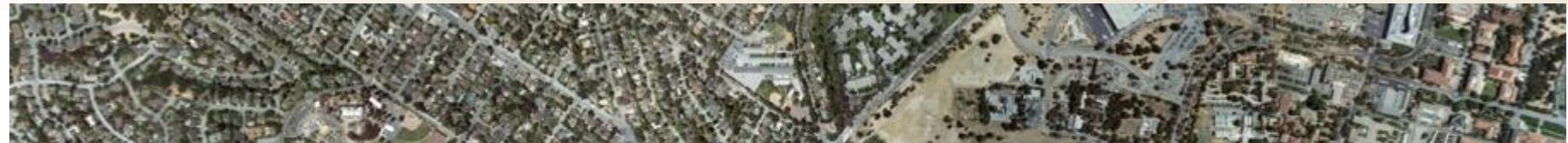
** The Run 10 operating period is scheduled October 2014-March 2015.

*** October 2009-October 2013 total number of scientific researchers engaged in approved research at LCLS.

A tour of the LCLS

LCLS from Above

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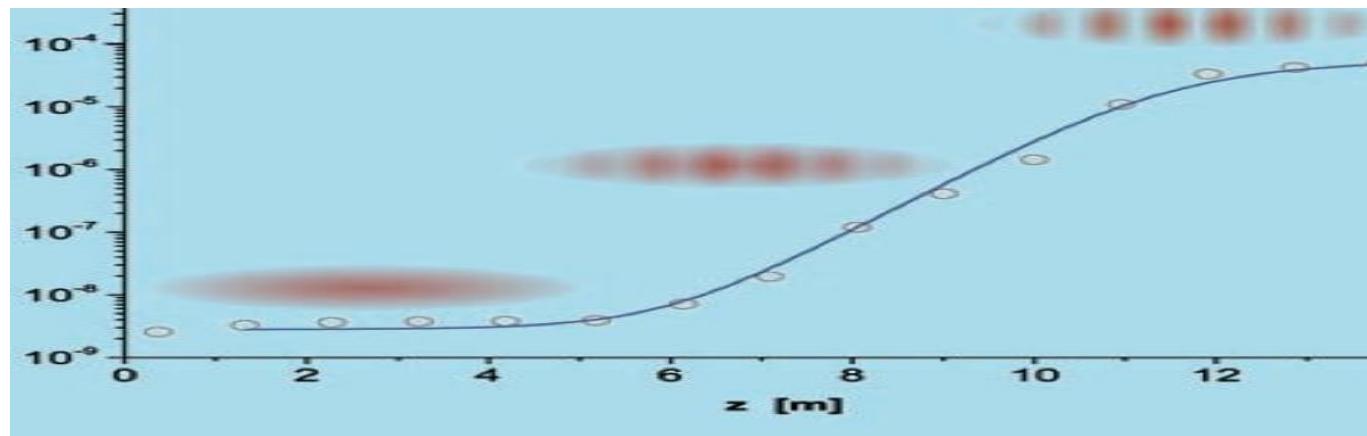
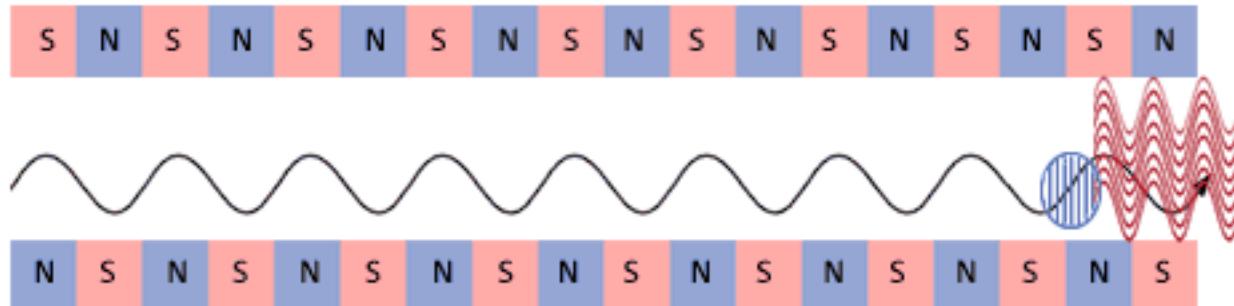


132 meters of FEL Undulator



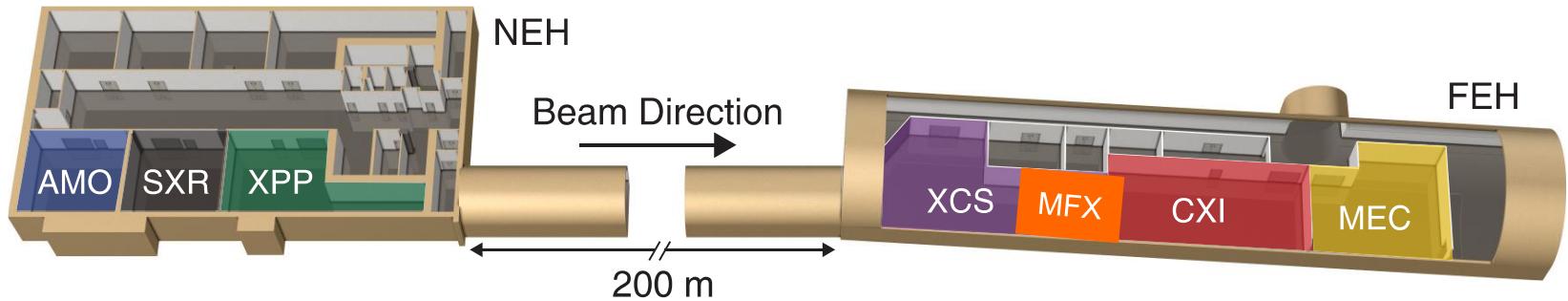
Self Amplified Spontaneous Emission

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LCLS Experimental Instruments

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- AMO: Atomic, Molecular and Optical
- SXR: Soft X-ray Research
- XPP: X-ray Pump Probe
- XCS: X-ray Correlation Spectroscopy
- CXI: Coherent X-ray Imaging
- MEC: Matter in Extreme Conditions

- AMO & SXR: Soft X-ray
- XPP, XCS, MFX, CXI and MEC: Hard X-rays

SXR

Soft X-ray Instrument for Material Science

- Dynamics in strongly correlated electron systems
- Chemical reactivity on both surfaces and in liquids

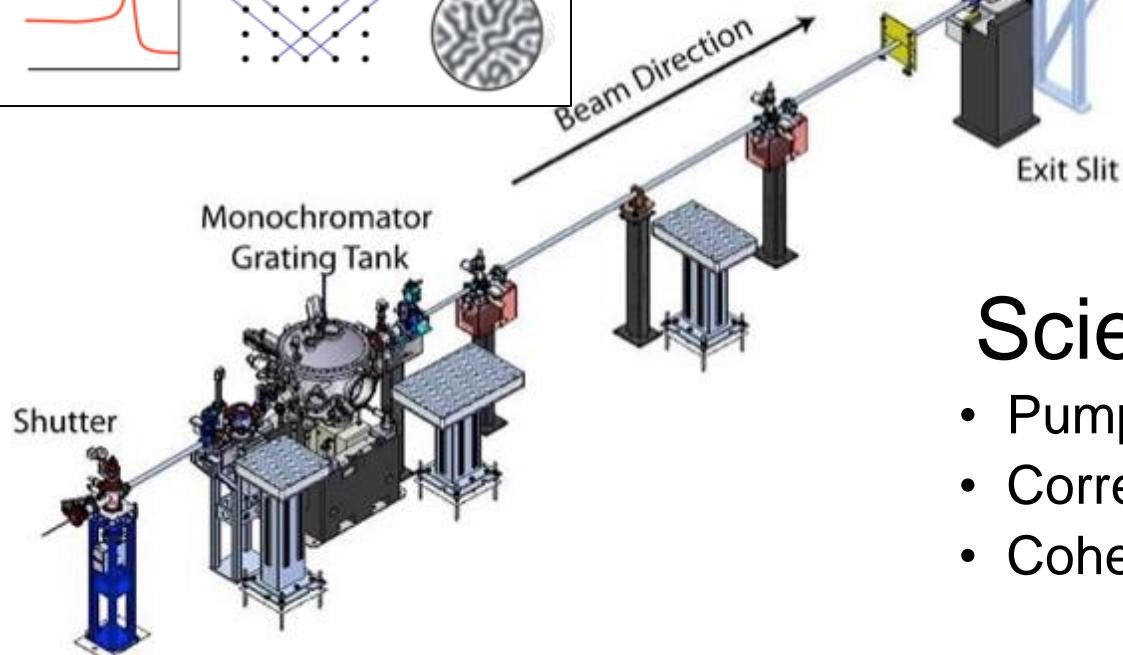
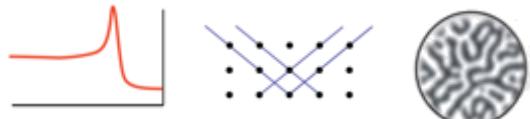
SXR: Soft X-ray Materials Research

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SXR Instrument

First Light: May 2010

Energy : 480eV-2keV



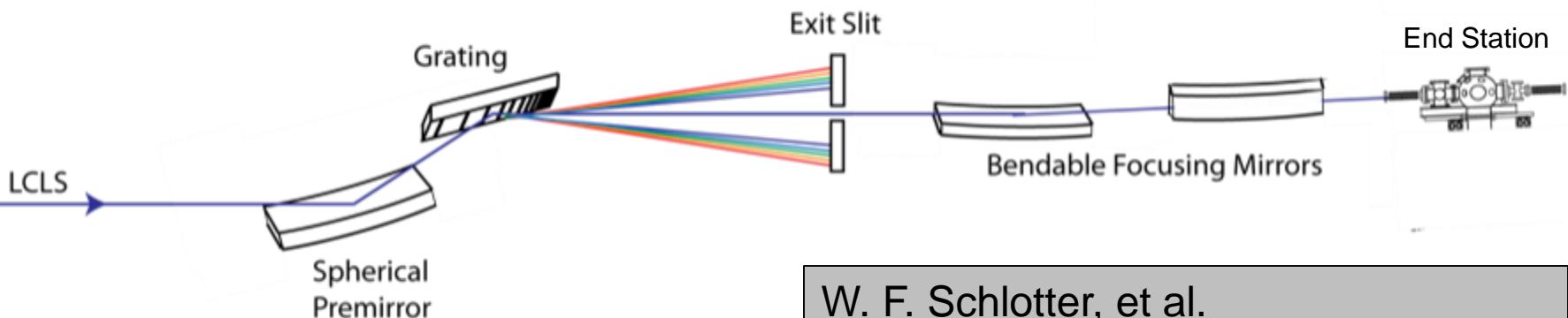
Science Program

- Pump-Probe Ultrafast Chemistry
- Correlated Materials
- Coherent Imaging

The SXR Instrument at LCLS

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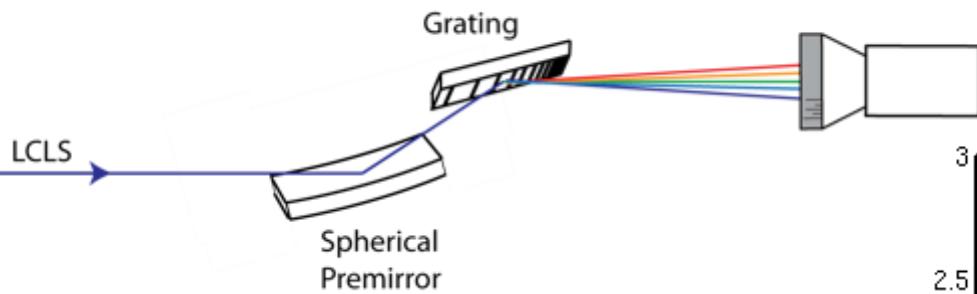
- Soft X-rays (250-2000eV)
- Pulse Energy 10^{12} photons/pulse
- Varied Line Spacing Plane Grating Mono
 - $E/\Delta E \sim 3000$
- KB Focusing
 - $10 \times 10 \mu\text{m}$ is nominal focus spot size.
 - Bendable KB allows for spot sizes up to $\sim 1\text{mm}$
- Optical Pump Laser (Synchronizable with x-rays to $\sim 280\text{ fs}$)



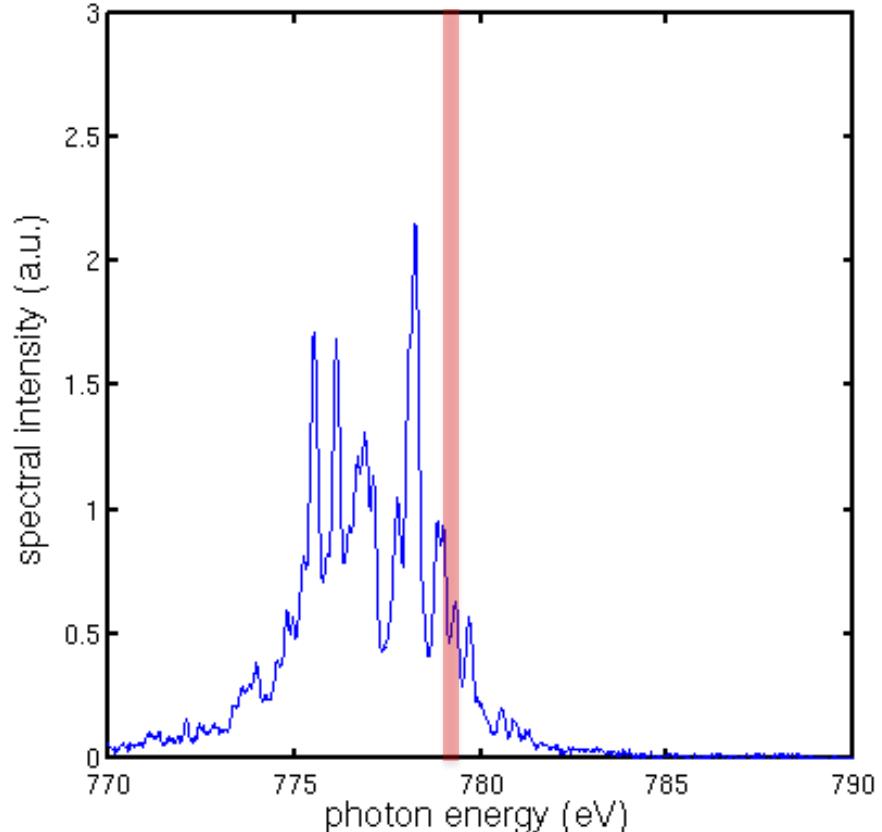
W. F. Schlotter, et al.
Rev. Sci. Instrum. 83, 043107 (2012)

Spectrometer + Monochromator

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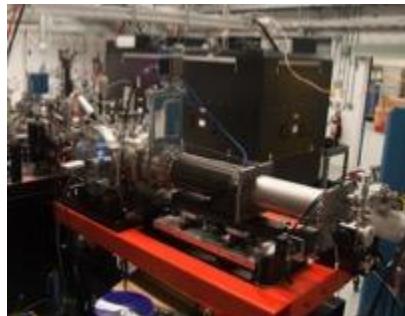
Spectrometer allows for an entire spectrum to be acquired from a single FEL pulse



P. Heimann, et al.
Rev. Sci. Instrum. 82, 093104 (2011)

Commissioned SXR End Stations

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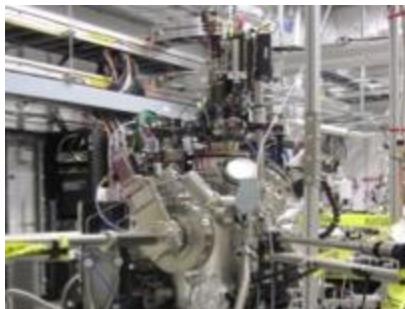
Resonant Coherent Imaging Station

Coherent scattering from fixed target and structured samples



Surface Science End Station

Ultrafast surface chemistry



Soft X-ray Scattering

Resonant and non-resonant diffraction



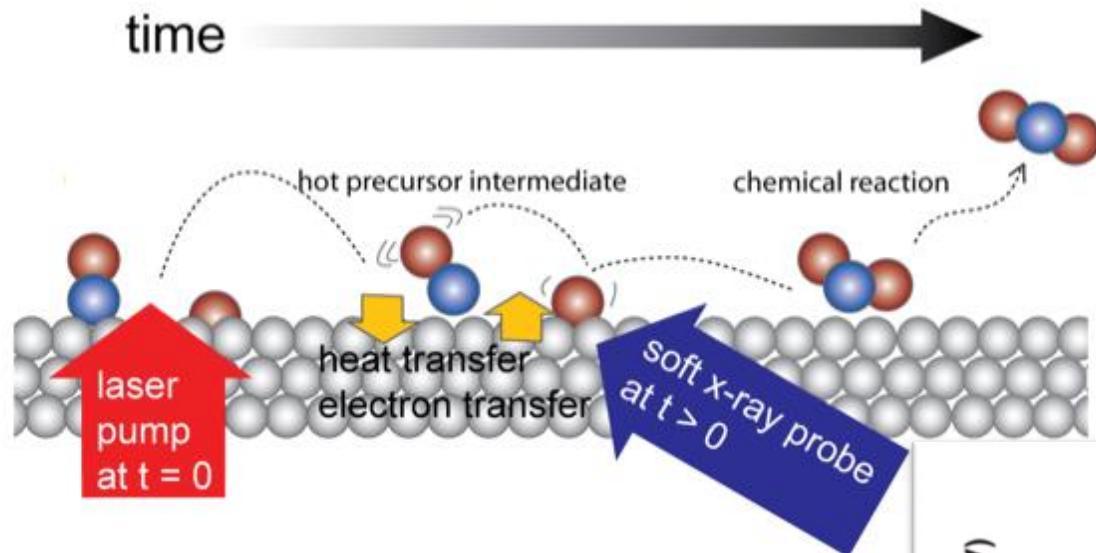
Liquid Jet End Station

Photochemistry in solution

Watching surface bonds break in real-time at LCLS:

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Transient weakly bound state observed in desorption process

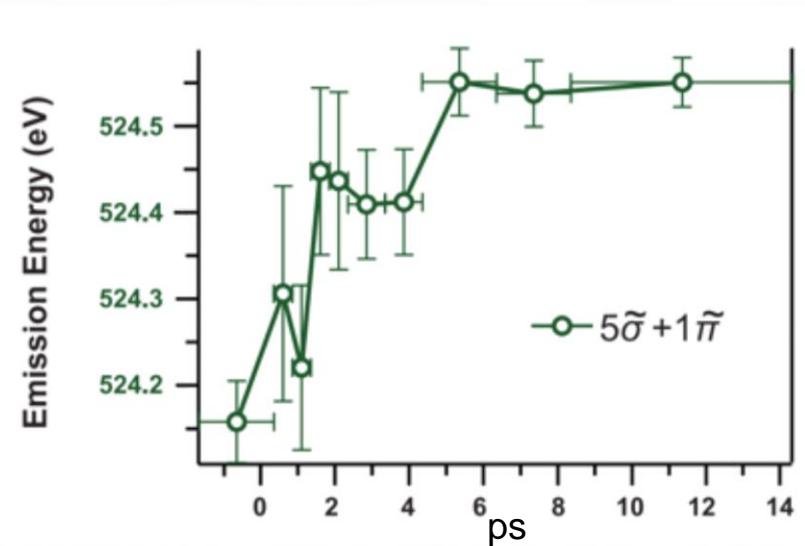


Bond formation of carbon monoxide on a ruthenium substrate

Electronic structure changes consistent with a weakening of the CO interaction with the substrate but without notable desorption.

M. Dell'Angela, et al., Science **339** 6125 (2013)
M. Beye, et al., Phys. Rev. Lett. **110** 186101 (2013)

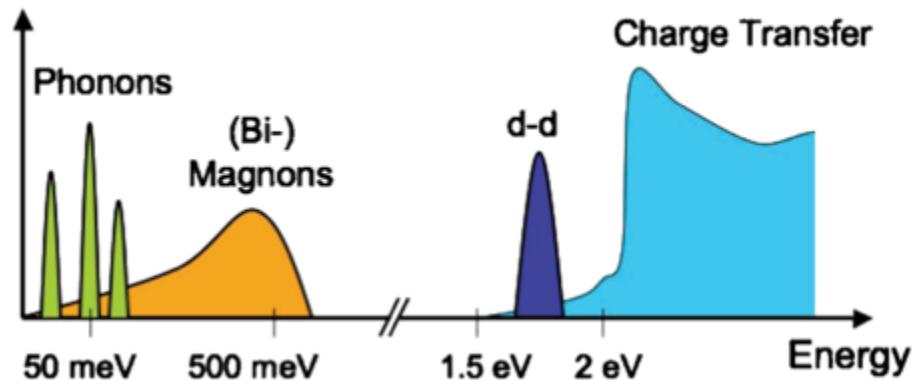
Bill Schlotter wschlott@slac.stanford.edu CLIC April 7, 2016



What can be done with X-ray Emission

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- Resonant Inelastic X-ray Scattering (RIXS)
 - Maps occupied density of states
- To study
 - Chemical reactivity on surfaces and in solution
 - Electronic excitations in correlated electron systems



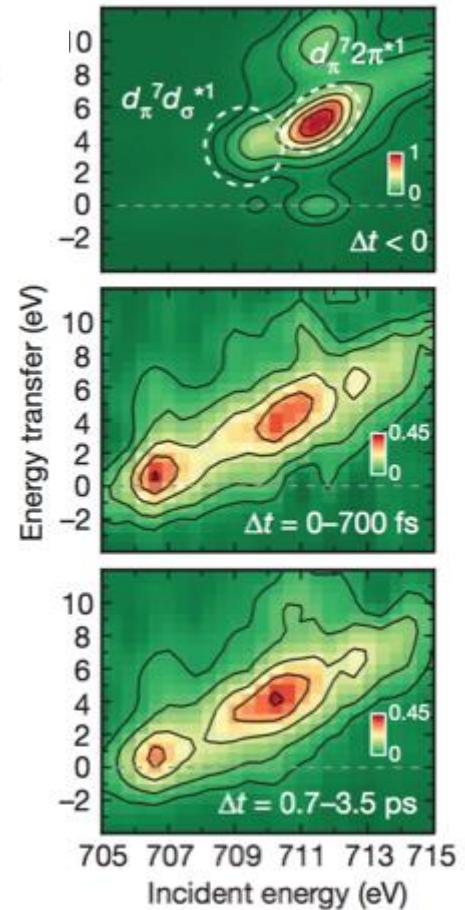
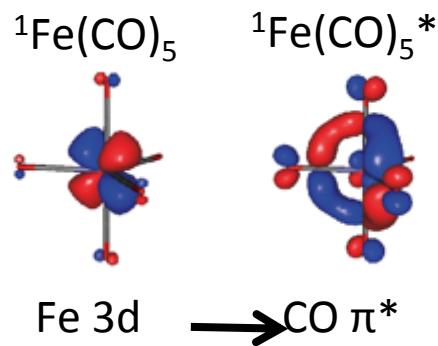
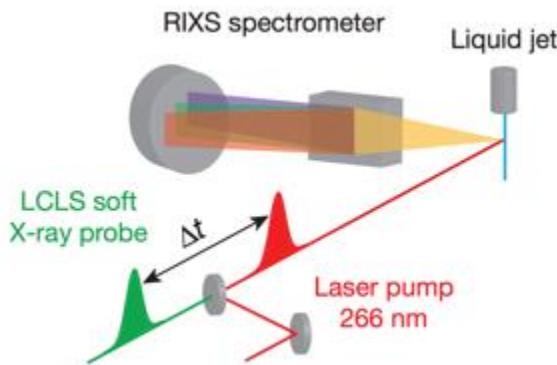
L. Ament, et al. Rev. Mod. Phys.
Vol. 83 (2) April June 2011

Example: X-ray Raman Studies of Molecular Dynamics

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- Soft X-ray RIXS maps molecular orbitals & their evolution
- Element-specific: transition-metals & ligands
- Local chemical structure & bonding
- Current limitations:
 - Sensitivity - observe only large molecular changes, in model complexes, at high concentrations
 - Limited time information - average X-ray flux (rep rate)

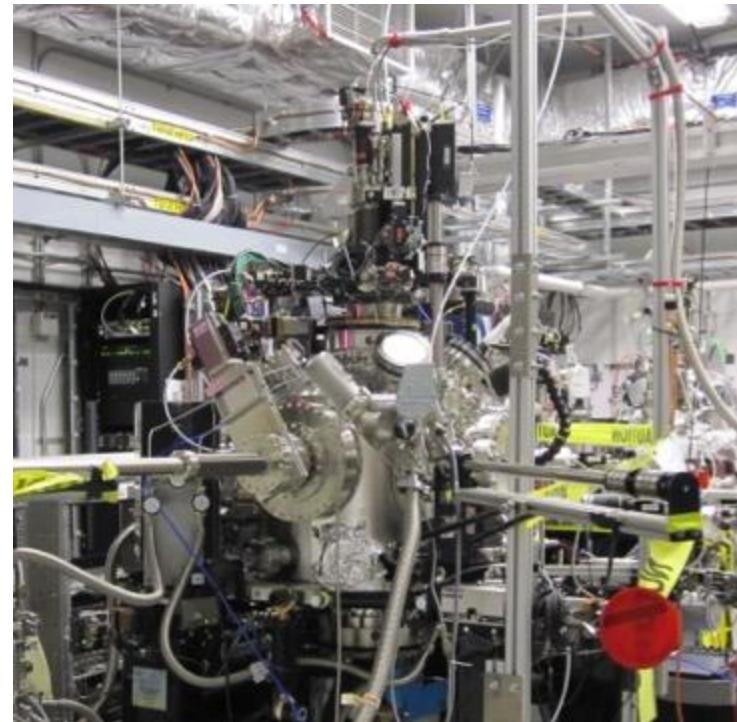
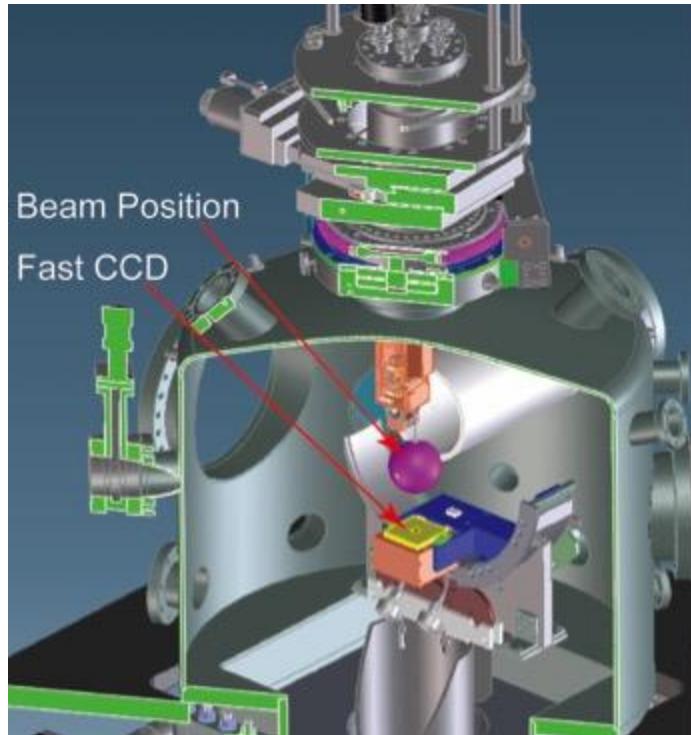
Ultrafast X-ray Raman Spectroscopy (resonant inelastic X-ray scattering – RIXS)



Resonant Soft X-ray Scattering

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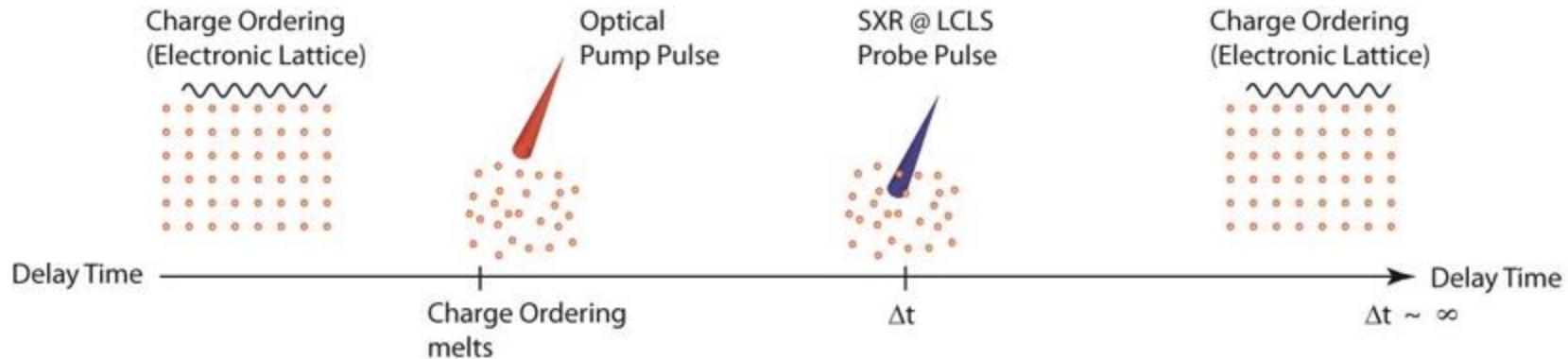
- **RSXS** Resonant Soft X-ray Scattering
- Resonant Soft X-ray Diffraction
- Strongly correlated systems



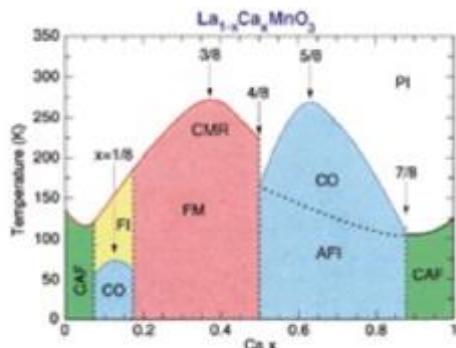
Fast CCD
In-vacuum diffractometer
Cryo sample environment

Probing Long Range Order with Soft X-rays

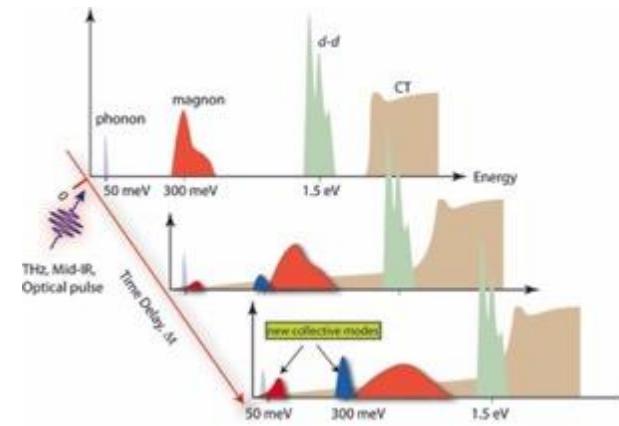
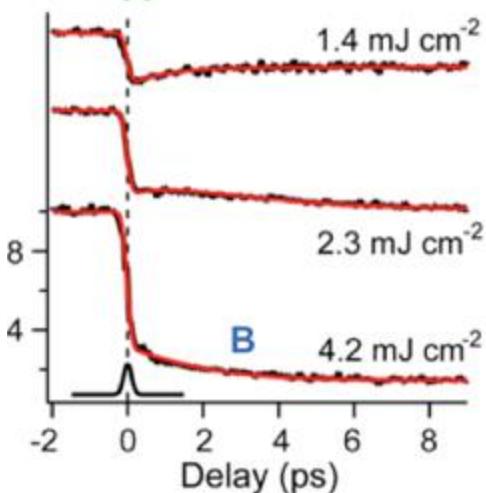
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Correlate:
charge-order insulating and
ferromagnetic metallic phases



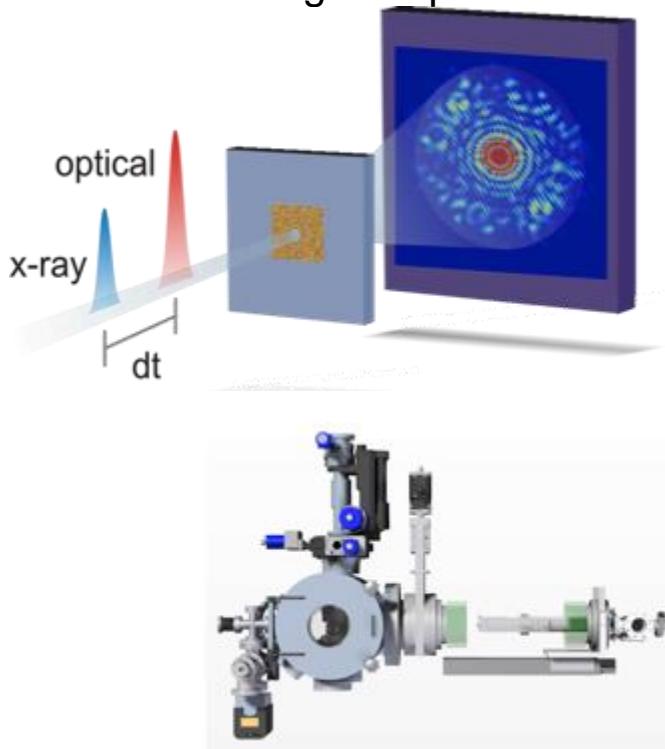
Laser induced phase transition in magnetite



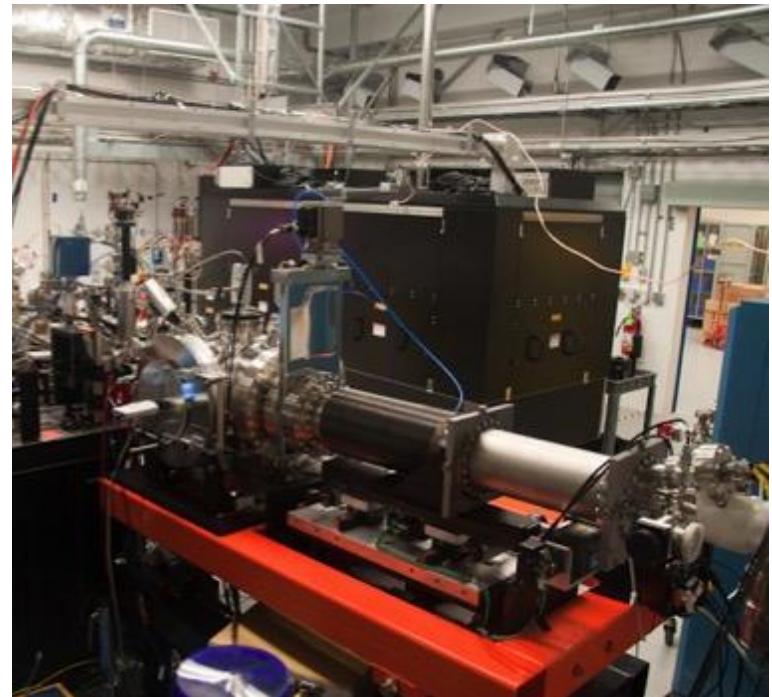
Resonant Coherent Imaging

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- **RCI** Resonant Coherent Imaging
- Coherent Scattering from fixed target and structured samples
- Ultrafast magnetic phenomena

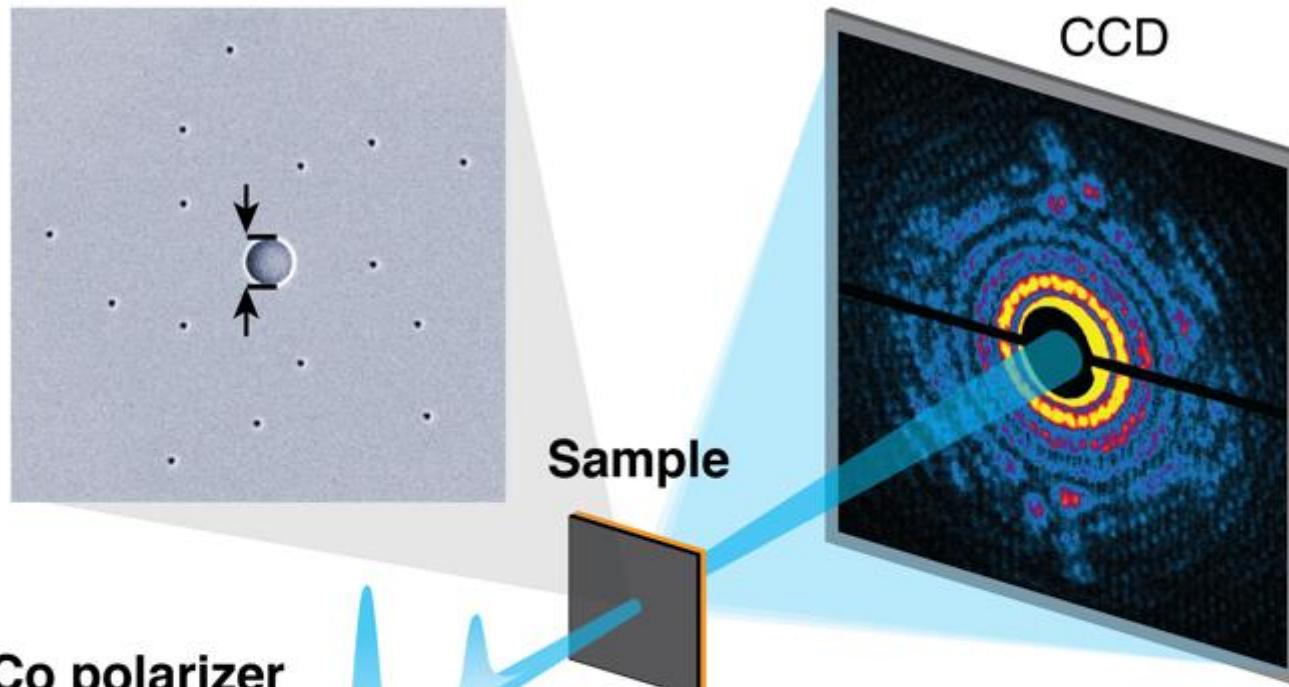


- In-vacuum sample manipulation
- 2k x 2k CCD
- In-situ magnetic field

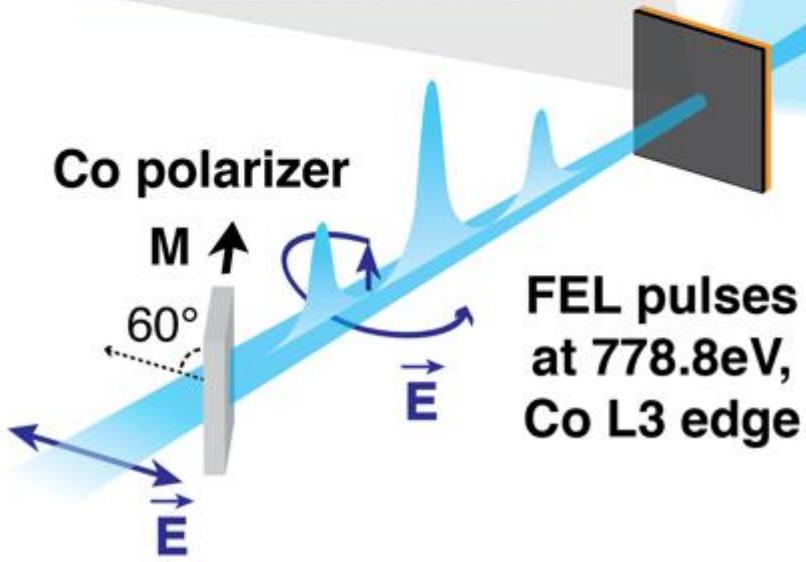


Femtosecond single-shot imaging of ferromagnetic nanostructures

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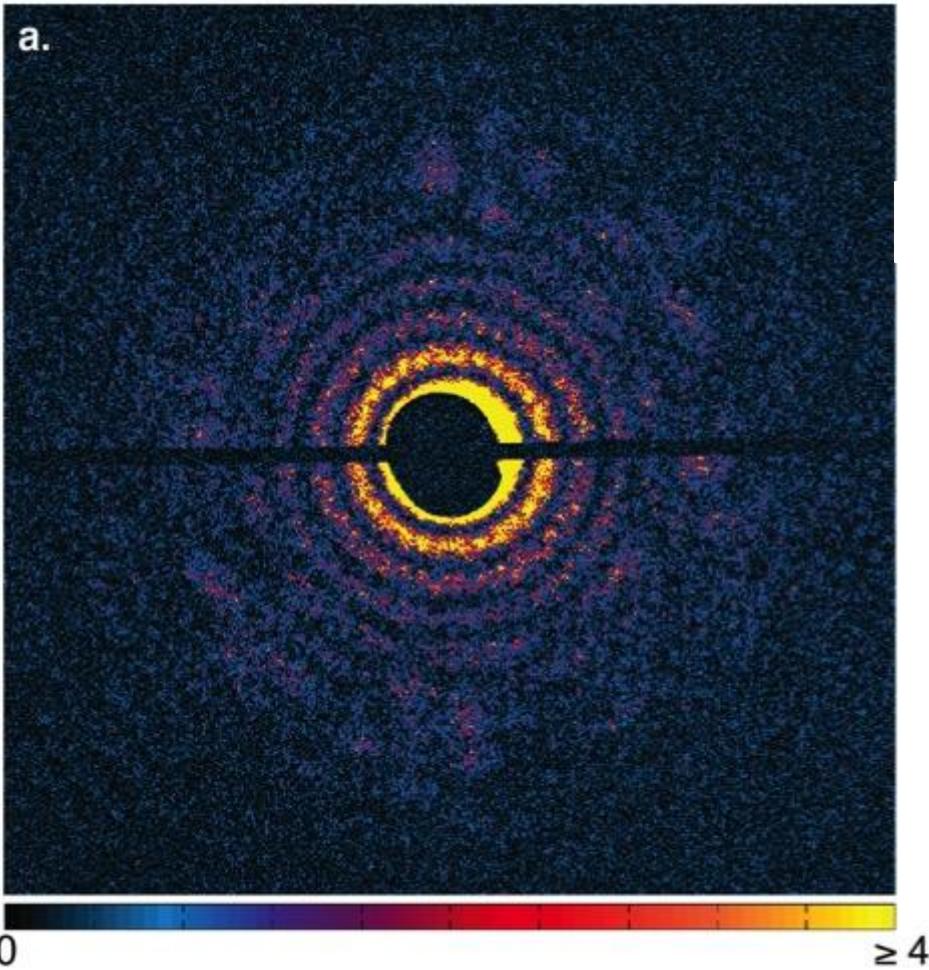
T. Wang, et al,
PRL 108,
267403 (2012)



Monochromator: Co L3 edge (778.8eV) with 0.5eV bandwidth
Photons after the polarizer: 1×10^9 photons/pulse
Focus at sample: $10 \times 30 \mu\text{m}^2$
Shot-shot intensity jitter: Fluences from 1 to 30 mJ/cm^2
Nominal pulse durations: 80fs and 360fs

80 fs single-shot Hologram with spatial multiplexing

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1.5×10^5 detected photons in hologram

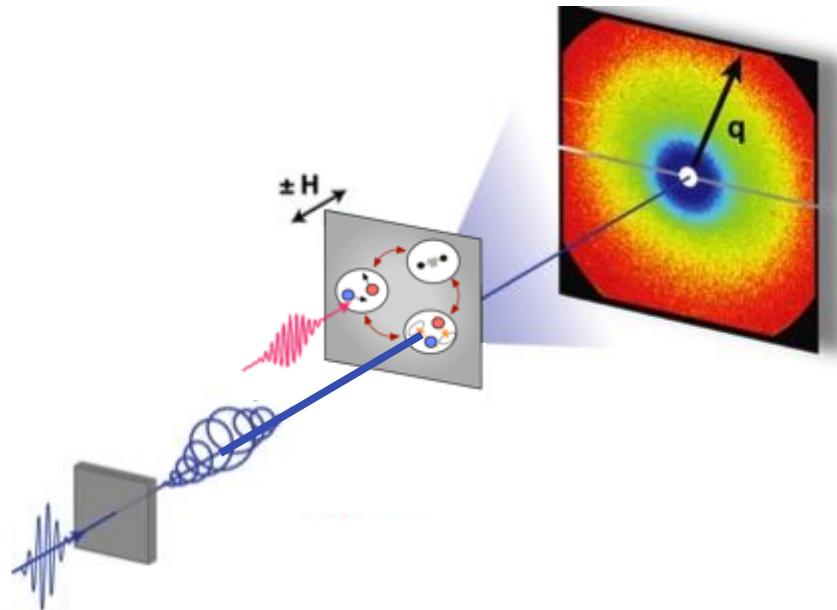
Bill Schlotter wschlott@slac.stanford.edu CLIC April 7, 2016

T. Wang, et al, *PRL* 108,
267403 (2012)

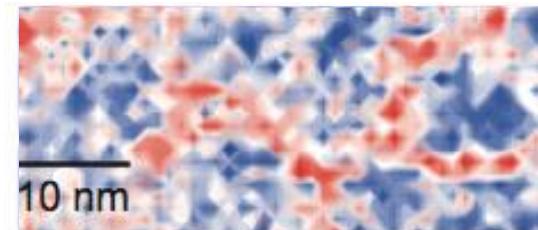
Optical control of nanoscale spin order in $\text{Fe}_{66}\text{Co}_{10}\text{Gd}_{24}$

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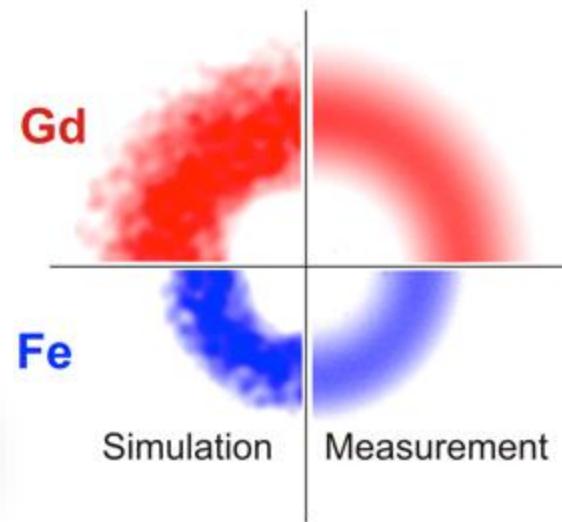
Diffraction



Real Space



Scattering Pattern



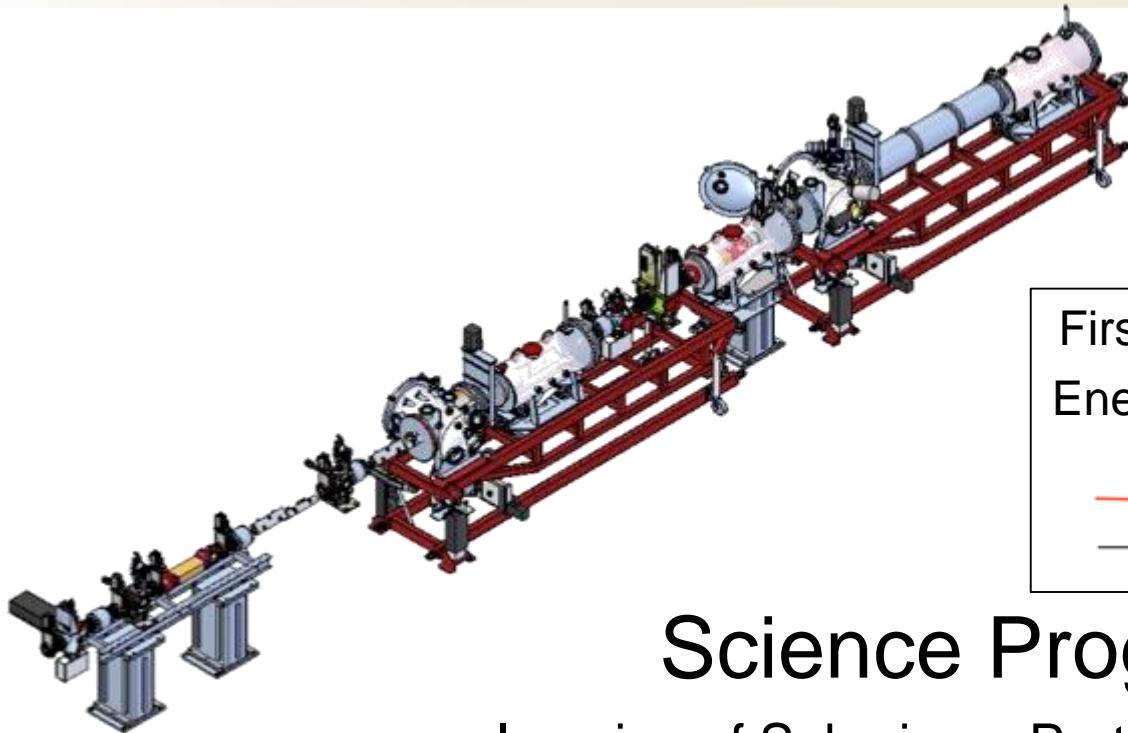
C. Graves, et al., Nature Materials, 12 293 (2013)

CXI

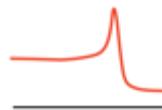
Coherent X-ray Imaging

CXI: Coherent X-ray Imaging

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First Light: December 2010
Energy : 4 keV-10 keV

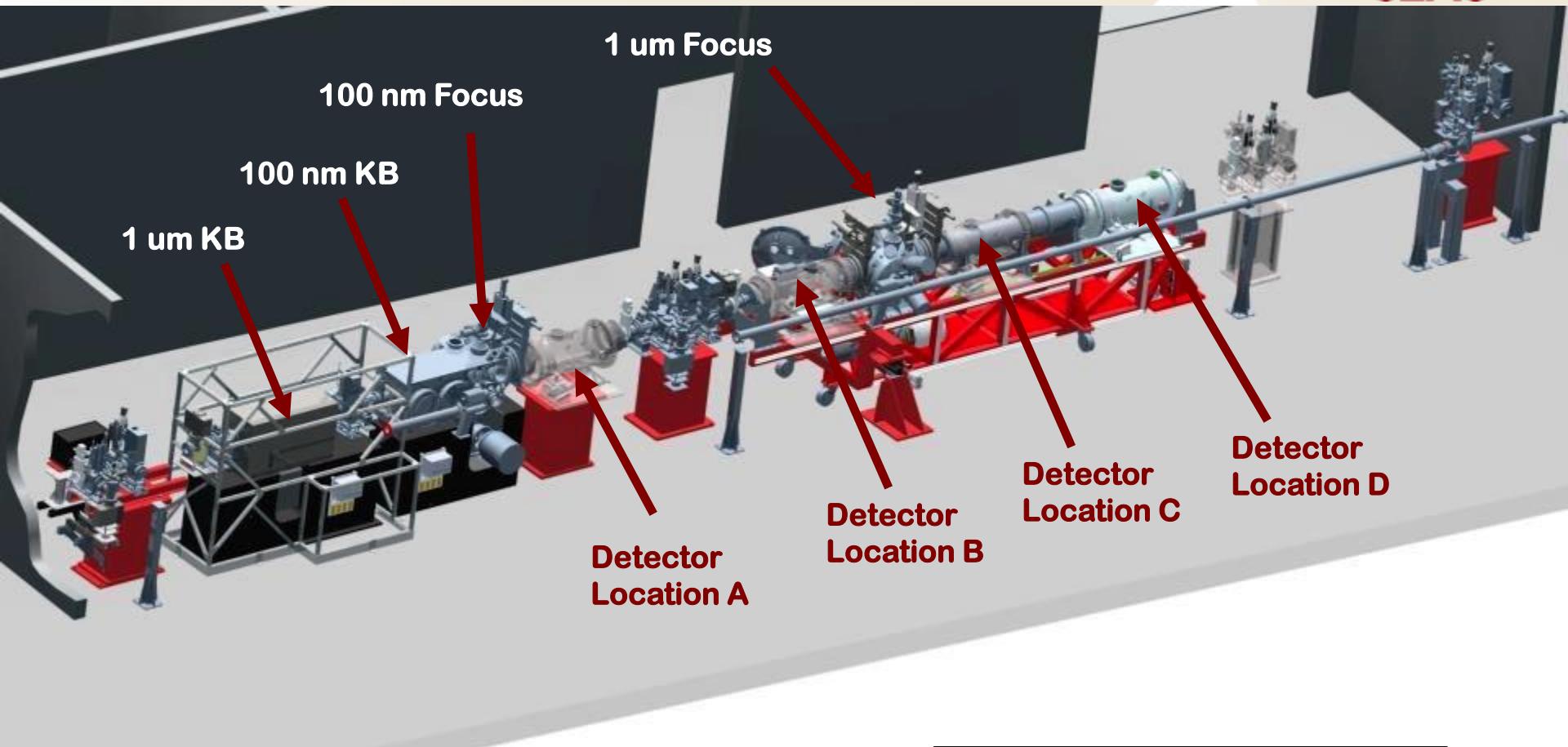


Science Program

- Imaging of Submicron Particles
 - Atomic Structure Determination: Protein Nanocrystals
 - Biological Nanoparticles Beyond the Damage Limit
 - Amorphous Nanoparticles

CXI Instrumentation Description

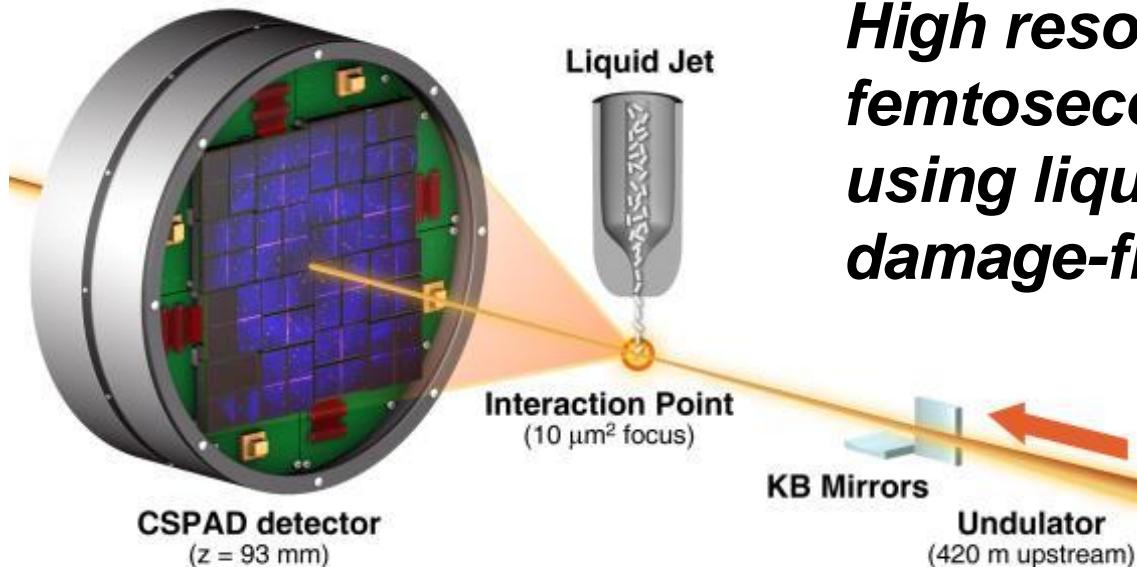
SLAC



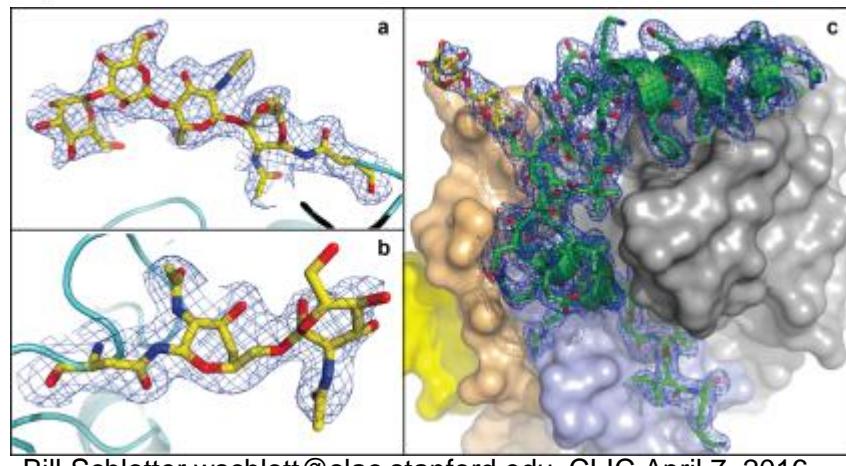
First Light: December 2010
Energy : 4 keV-10 keV

Nano-crystallography at LCLS

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High resolution serial femtosecond crystallography using liquid jets can produce damage-free structures



In-vivo grown crystal of a glyco-protein

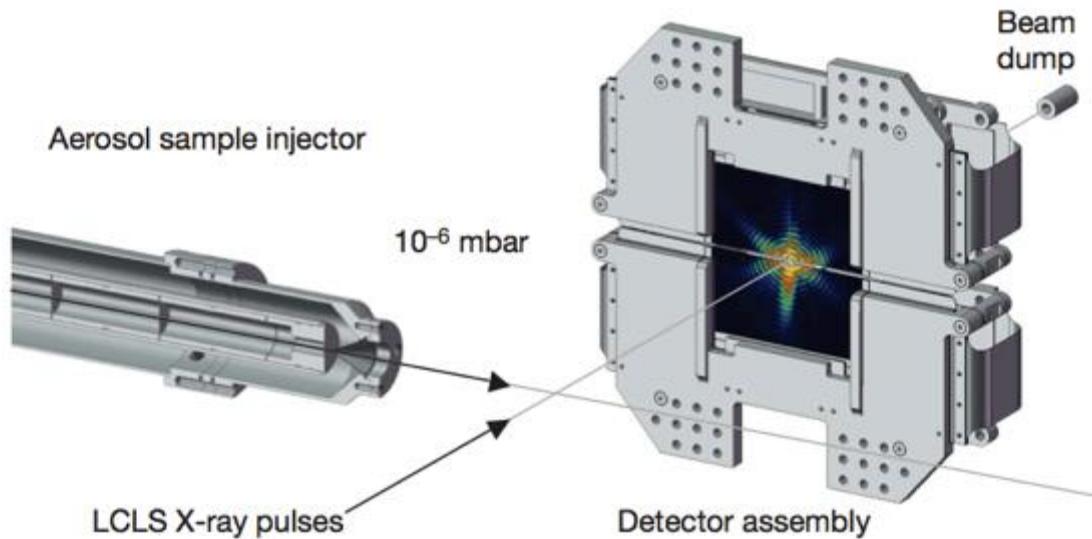
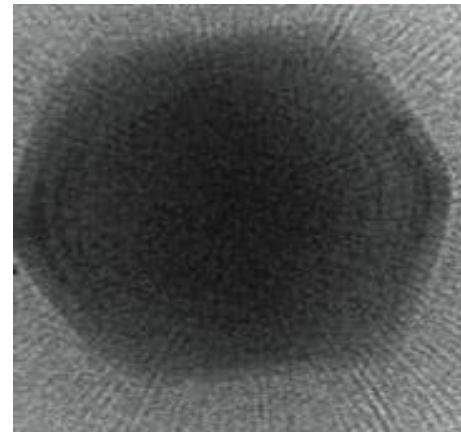
Redecke et al, Science **339**, 6116 (2012)

Boutet et al. Science, **337** (6092) 362 (2012)

Imaging of the Mimi Virus

SLAC

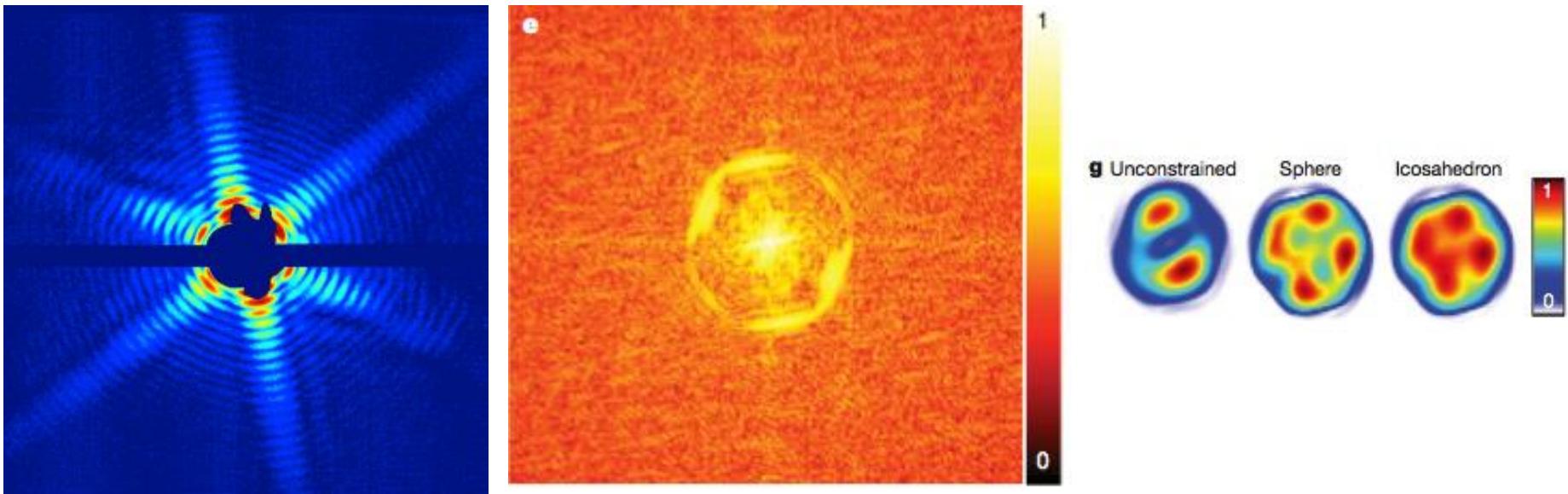
- Mimi Virus is the largest known virus (0.5 um)
- It is too big for cryo-electron microscopy
- It does not crystalize because of dense outer fibrils



M. Seibert, et al, *Nature*
470, p78 (2011)

Mimi Virus

SLAC



Energy: 1.8 keV

Photons per pulse: 1.2×10^{12}
photons/pulse

Focus at sample: 10 μm

Nominal pulse durations: 70 fs

Demonstrates that short XFEL pulses can outrun sample damage

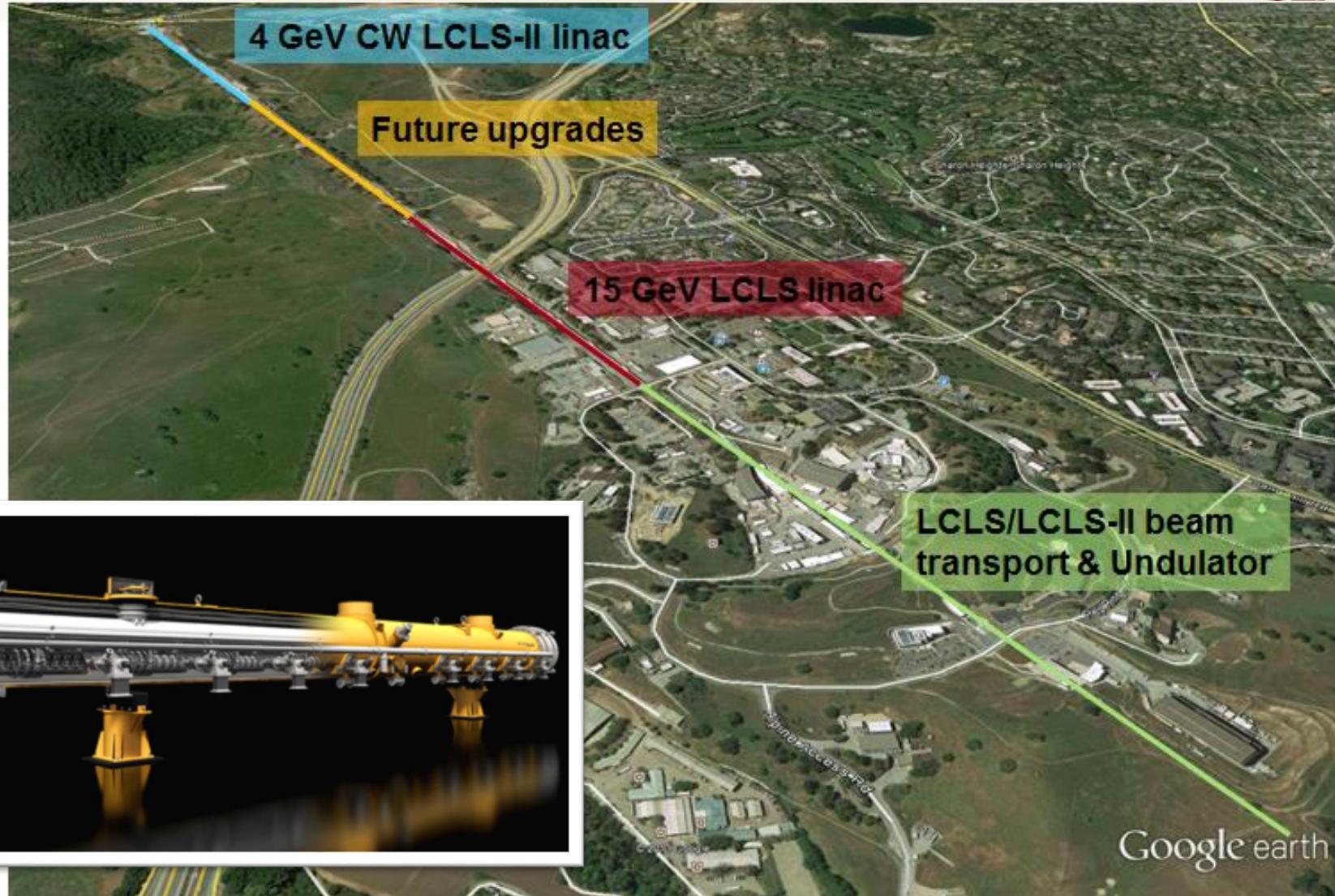
M. Seibert, et al, *Nature*
470, p78 (2011)

LCLS-II

LCLS-II Upgrade

Use 1st km of SLAC linac tunnel for Super Conducting linac

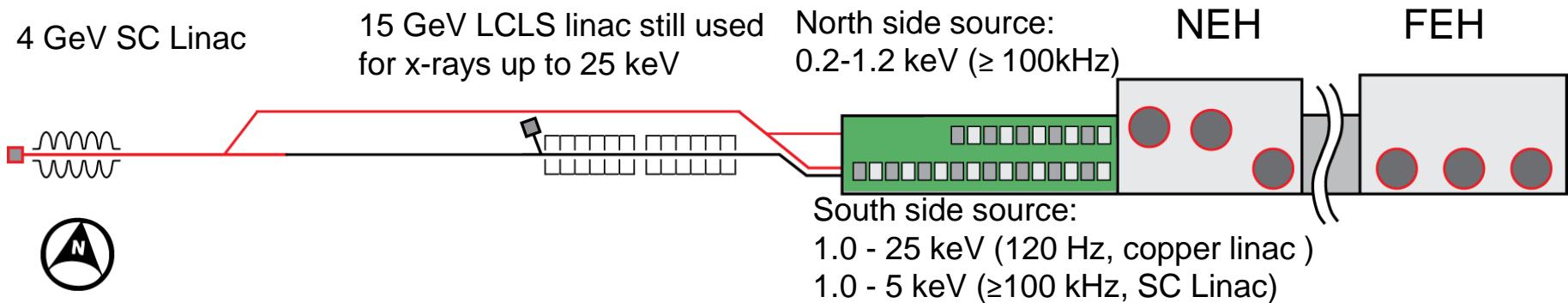
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LCLS-II Project Scope

SLAC

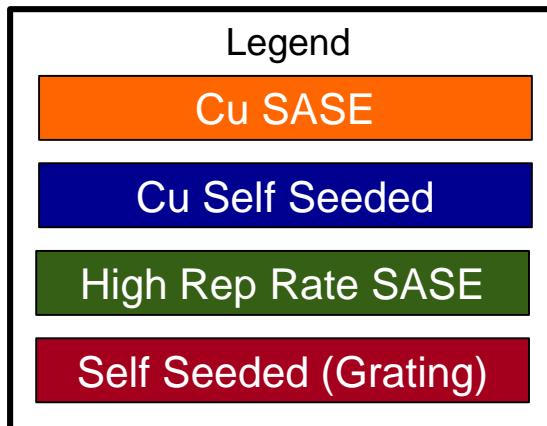
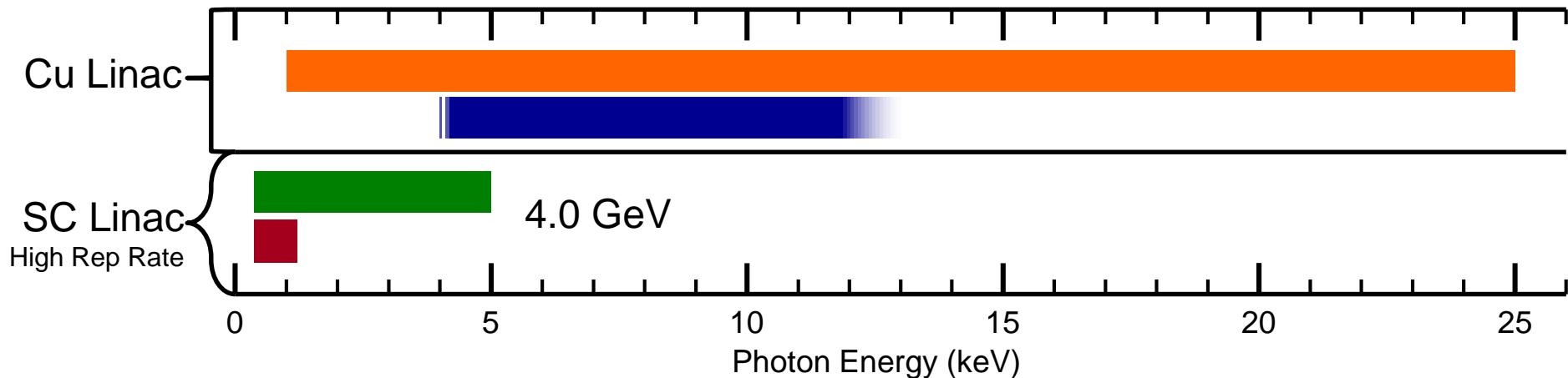
| | |
|---|--|
| Accelerator | Superconducting linac: 4 GeV |
| Undulators in existing LCLS-I Tunnel | New variable gap (north) New variable gap (south), replaces existing fixed-gap und. |
| Instruments | Re-purpose existing instruments (instrument and detector upgrades needed to fully exploit) |



| | LCLS-I | New for LCLS-II |
|---|---|--|
| Accelerator technology | SLAC copper linac  | New superconducting linac  |
| X-ray pulses per second | Up to 120 | Up to 1 million |
| Time to produce 10 billion X-ray pulses | 4 years | 2 hours |

LCLS-II Operating Energy Range

SLAC

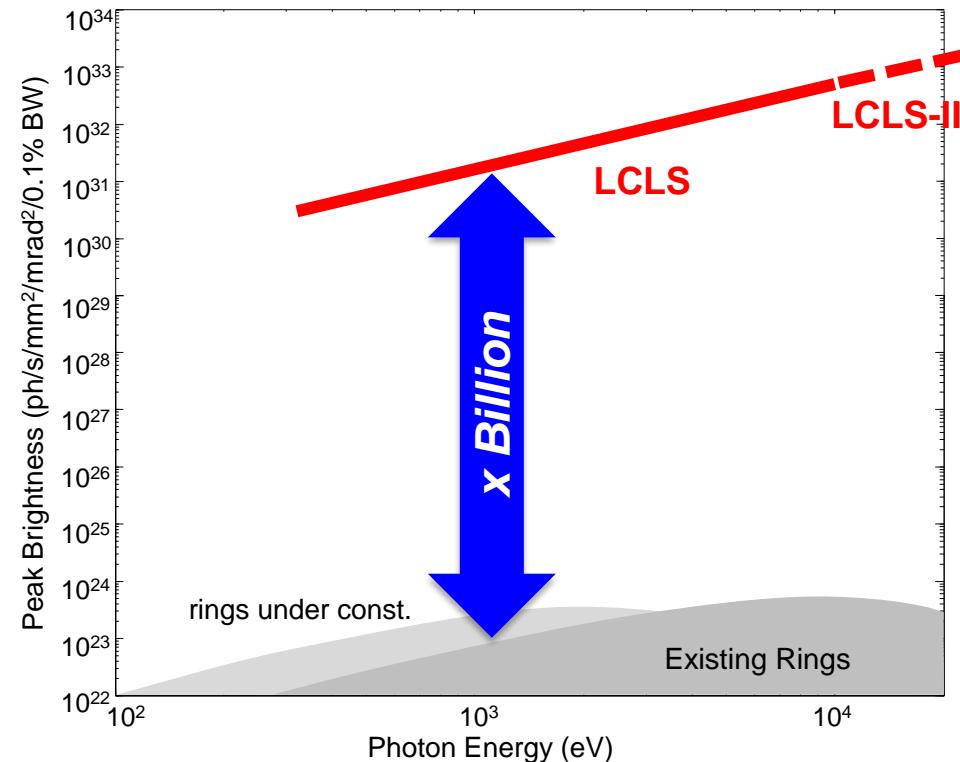


- Hard X-Ray Source:
 - 1-5 keV w/ 4 GeV SC linac
 - Up to 25 keV with LCLS Cu Linac
- Soft X-Ray Source:
 - 250 eV-1.2 keV w/ 4 GeV linac
 - 200 eV requires <4 GeV

LCLS-II: A Revolution in X-ray Science

SLAC

Peak Power



- LCLS-II:
- Repetition rate
 - Stability
 - Coherence (seeding)
 - Photon energy reach

High Repetition Rate Revolution

SLAC

- LCLS-II upgrade will deliver
 - High repetition rate → 10^4 fold increase in data collection
 - High stability → high throughput measurements
 - Second source capable of multiplexing → doubles access
- New Scientific Opportunities at LCLS-II
 - Photo and heterogeneous catalysis
 - Follow molecular transformations & bond formation
 - Revealing interacting degrees of freedom in correlated electron systems

LCLS-II Science Opportunities Document

SLAC

https://portal.slac.stanford.edu/sites/lcls_public/Documents/LCLS-IIScienceOpportunities_final.pdf

SLAC-R-1053

NEW SCIENCE OPPORTUNITIES ENABLED BY LCLS-II X-RAY LASERS

June 1, 2015

LCLS SLAC NATIONAL ACCELERATOR LABORATORY ENERGY Office of Science

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LCLS

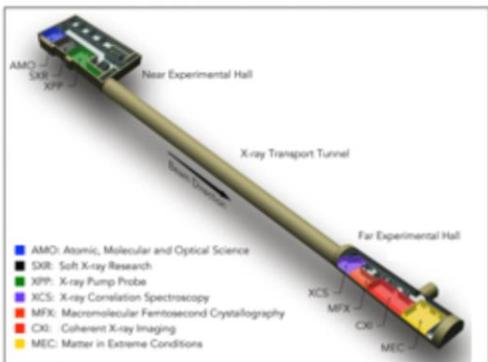
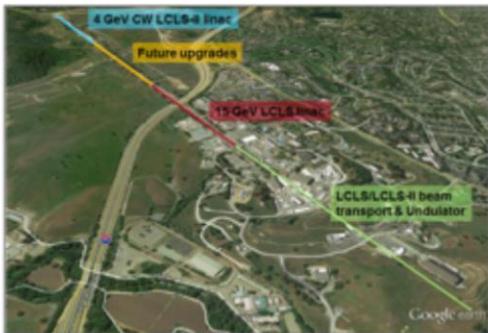
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LCLS Strategic Facility Document (July 2015)

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LCLS STRATEGIC FACILITY DEVELOPMENT PLAN
July 2015



- LCLS Facility generated a strategic development plan to outline an approach to enable LCLS-II scientific objectives
- The plan was released in July 2015 as a draft to solicit feedback.

Review of Modern Physics: LCLS

SLAC

REVIEWS OF MODERN PHYSICS, VOLUME 88, JANUARY–MARCH 2016

Linac Coherent Light Source: The first five years

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(published 9 March 2016)

A new scientific frontier opened in 2009 with the start of operations of the world's first x-ray free-electron laser (FEL), the Linac Coherent Light Source (LCLS), at SLAC National Accelerator Laboratory. LCLS provides femtosecond pulses of x rays (270 eV to 11.2 keV) with very high peak brightness to access new domains of ultrafast x-ray science. This article presents the fundamental FEL physics and outlines the LCLS source characteristics along with the experimental challenges, strategies, and instrumentation that accompany this novel type of x-ray source. The main part of the article reviews the scientific achievements since the inception of LCLS in the five primary areas it serves: atomic, molecular, and optical physics; condensed matter physics; matter in extreme conditions; chemistry and soft matter; and biology.

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- Recently published review article
- Provides an excellent overview of the accelerator, instrumentation and scientific developments of the first five years

Rev. Mod. Phys., Vol. 88, No. 1, January–March 2016

Conclusions



- X-ray Free Electron Lasers are well suited to study nano- and atomic scale dynamics on ultrafast timescales
- Soft x-rays provide access to study specific elements while hard x-rays view atomic structure
- FEL Facilities serve a wide variety of scientific communities.
- The number of operating x-ray FEL facilities will double in the next three years

The Linac Coherent Light Source (LCLS), SLAC National Accelerator Laboratory, is supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Contract No. DE-AC02-76SF00515.

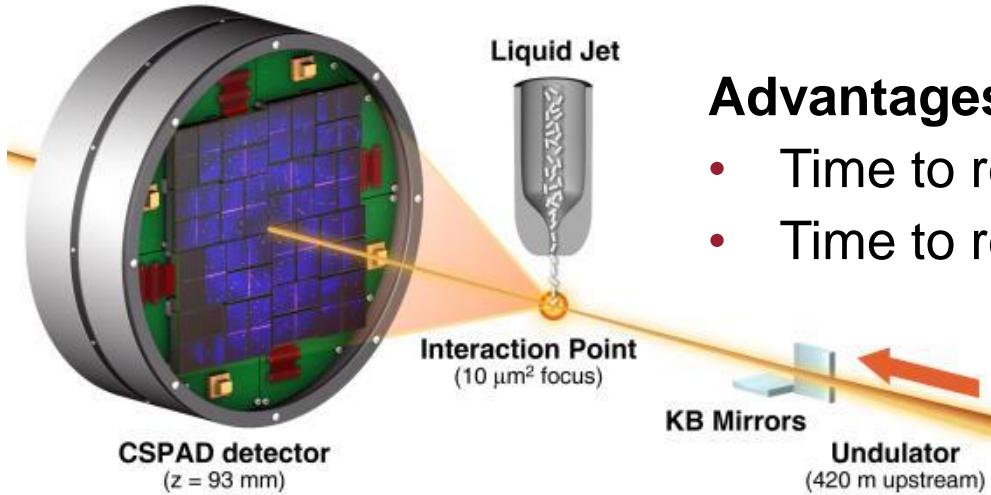
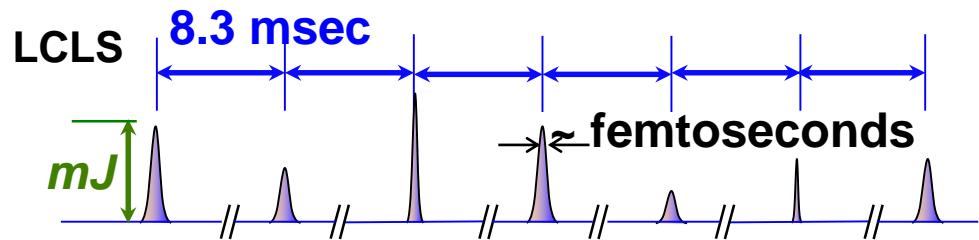
END
Backup Slides

How we detect x-rays at LCLS?

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Single shot mode

- All experimental parameter that may change are recorded for each pulse
- Data must be sorted by the *independent variable* after the experiment
- Each x-ray pulse is different



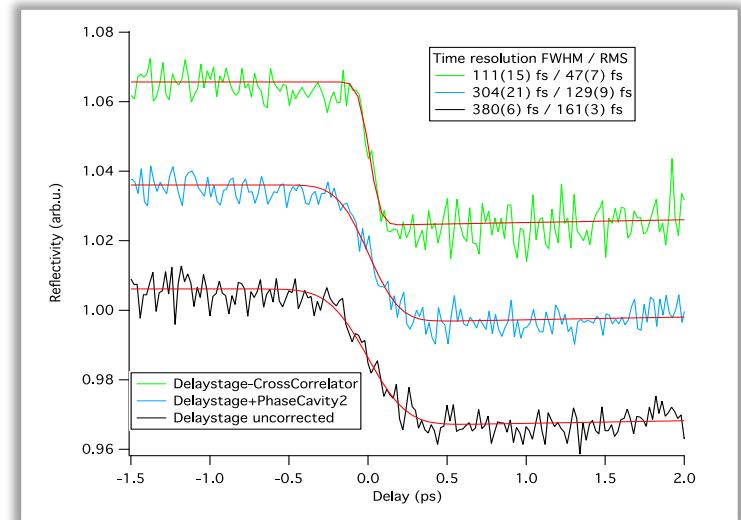
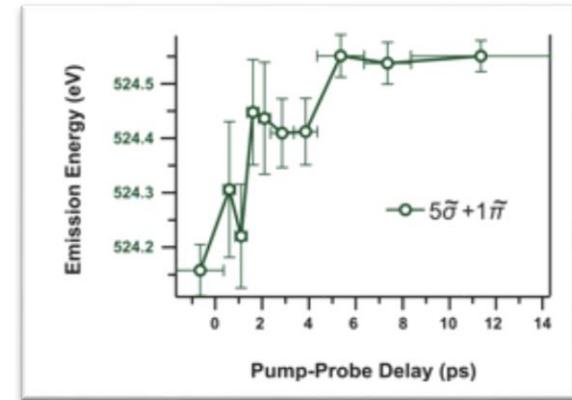
Advantages of single shot mode

- Time to read out detectors
- Time to renew destroyed samples

Limitations to single shot data collection at 120Hz

SLAC

- Limited data collection volume
 - Low repetition rate (120 Hz)
 - Only 60 hours to collect data
- Source stability
 - Energy
 - Arrival time
 - Duration
 - Wavelength & Bandwidth
- Limited Access
 - Only one x-ray source
 - One size fits all experiments

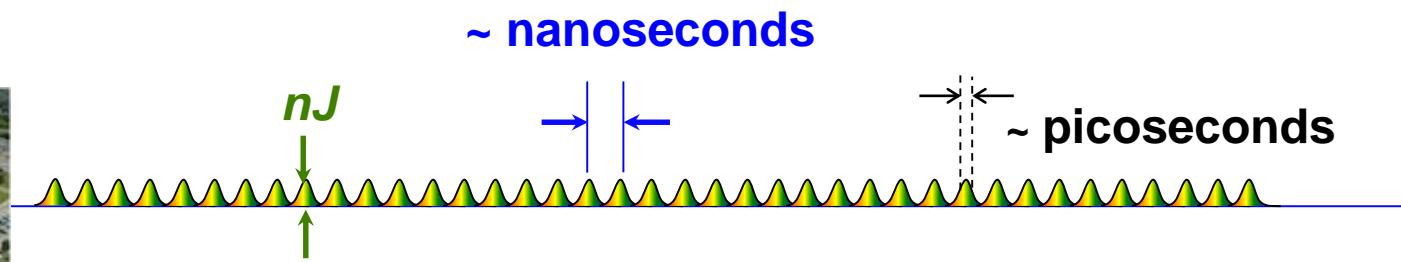


Accumulation Data Collection

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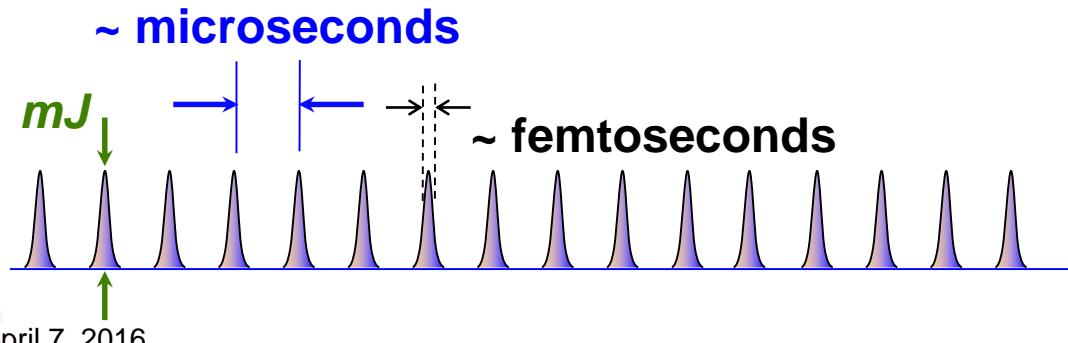
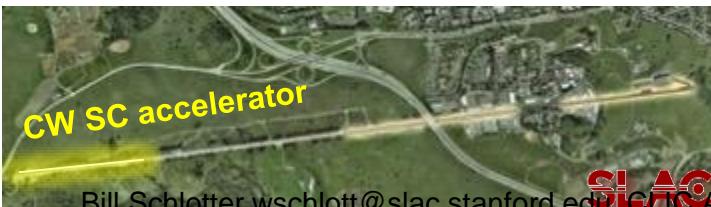
- To the extent each x-ray pulse is the same, we can accumulate the detected photons over many pulses
- But this is exactly how experiments are done at storage ring sources

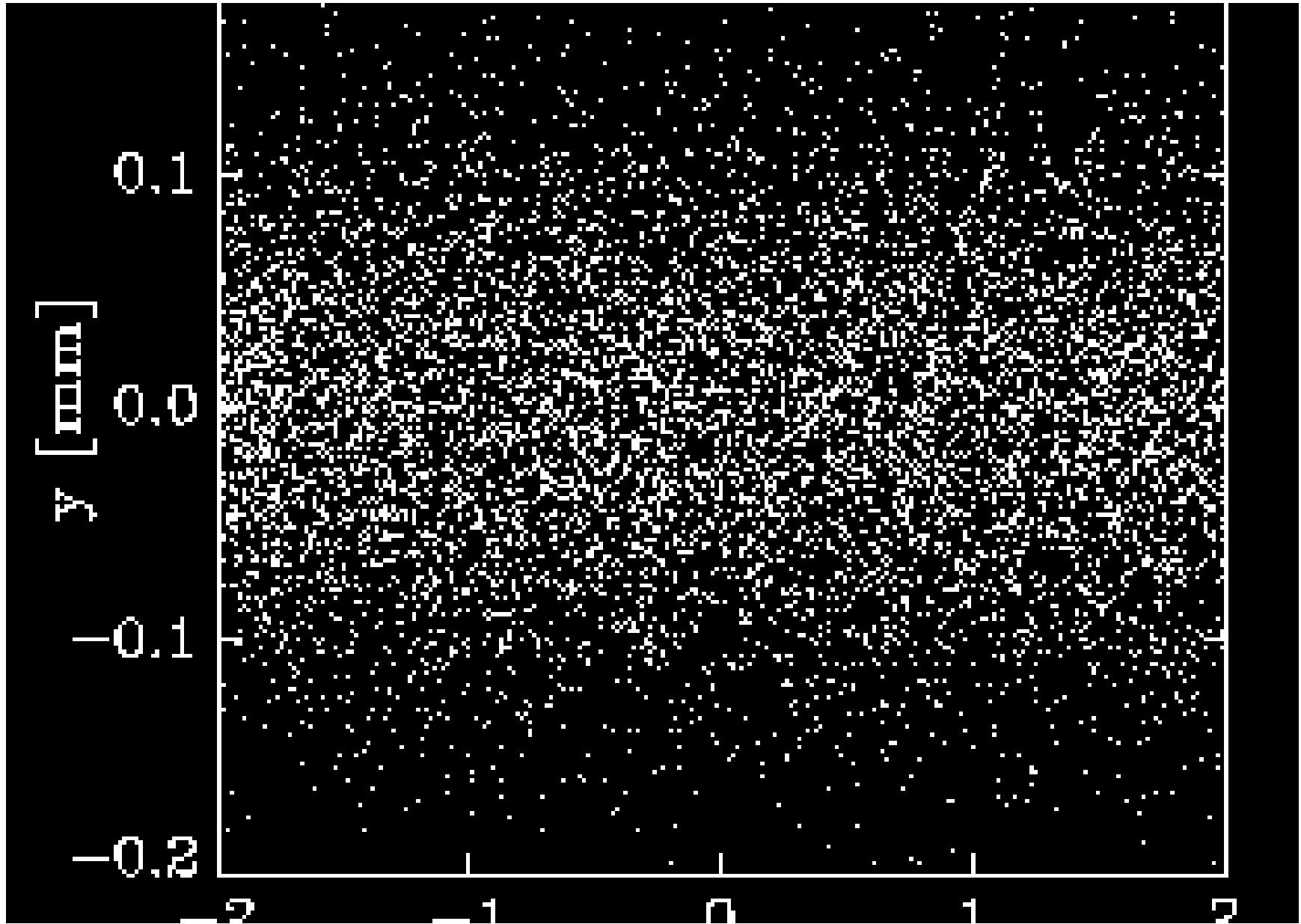
storage ring X-ray source (NSLS-II)



- Combining the mJ, fs pulses of an FEL with the stability of a storage will revolutionize x-ray experiments.

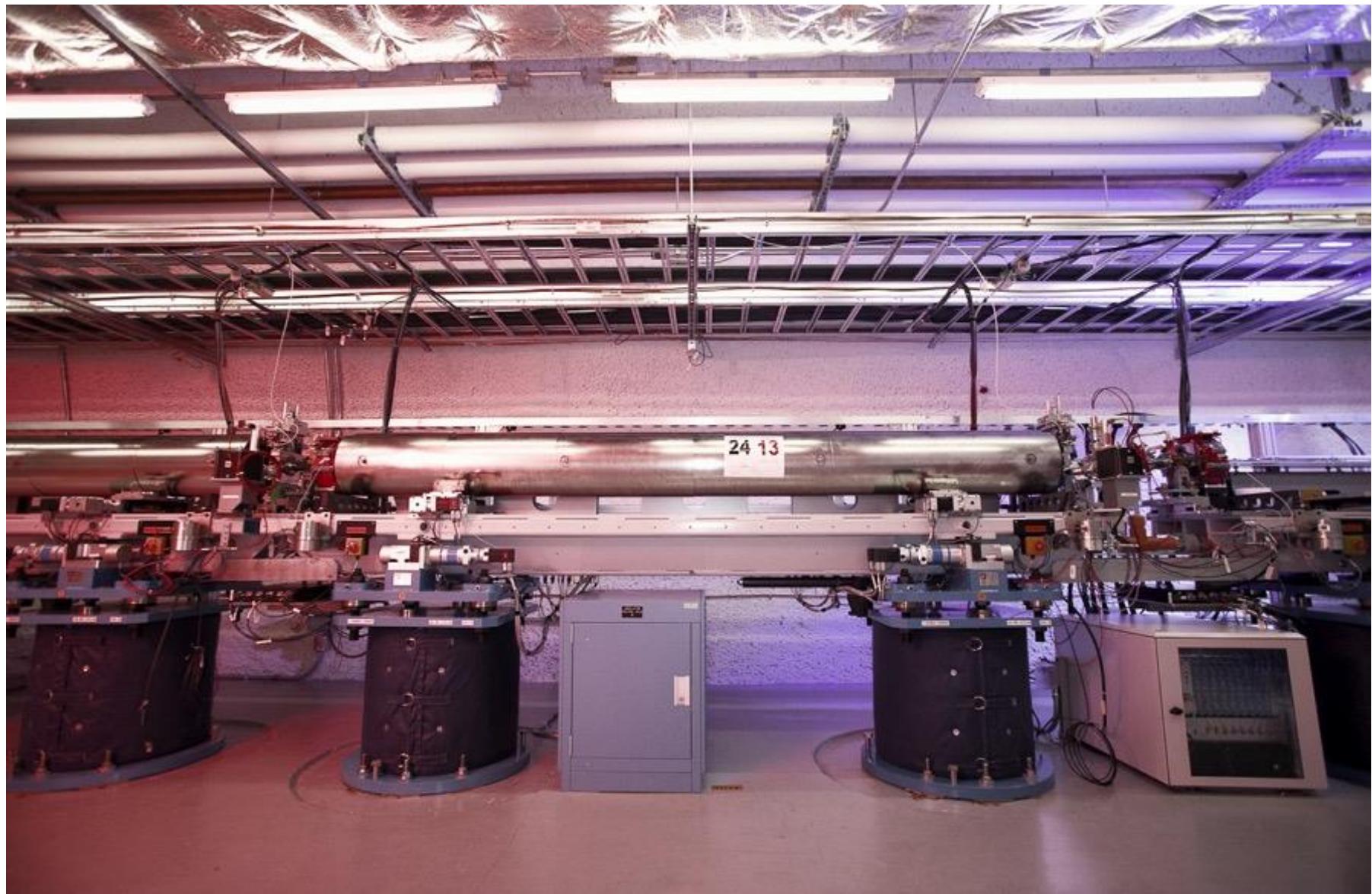
2019 LCLS-II



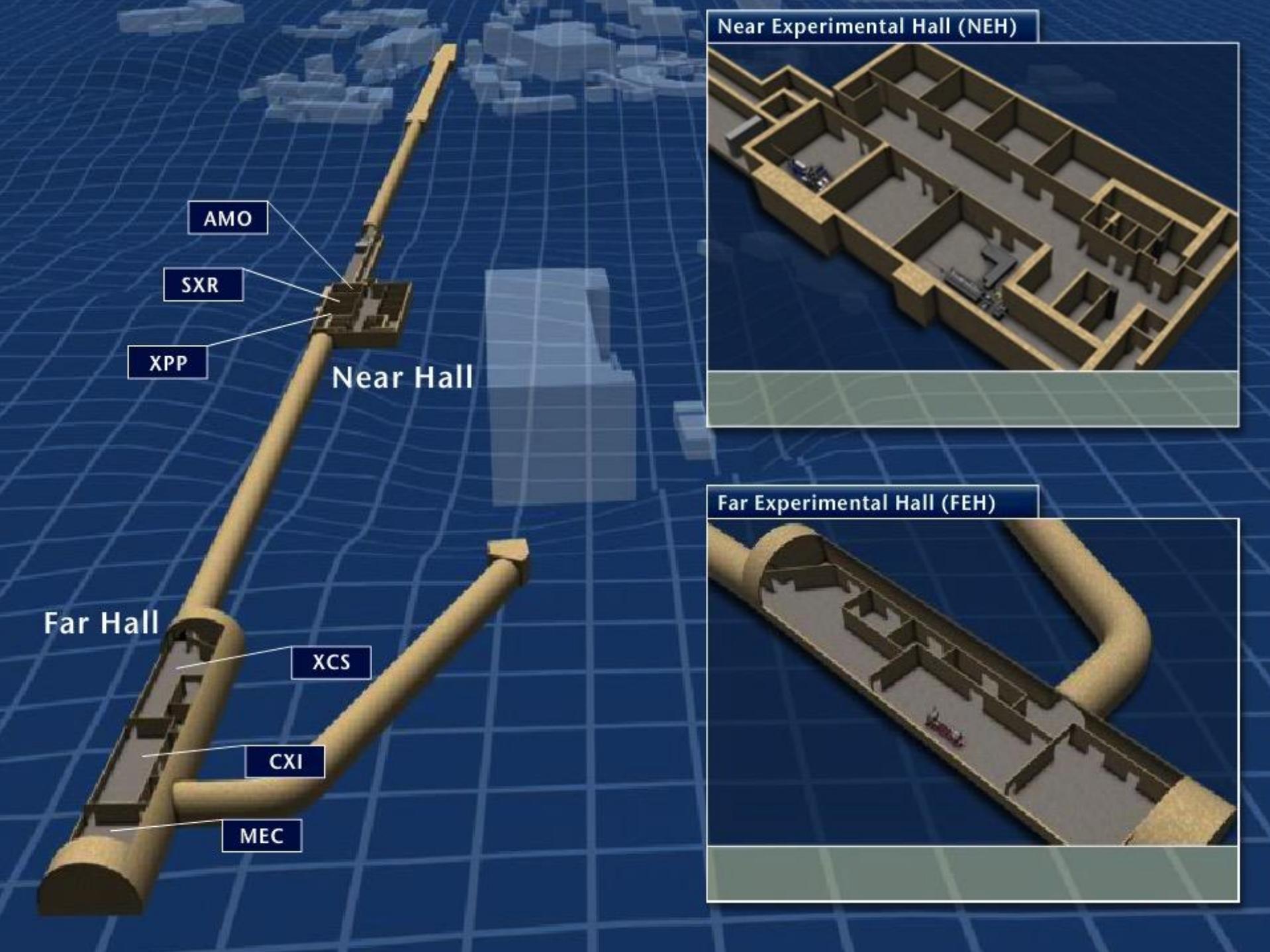


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CLIC April 7, 2016

S. Reiche UCLA



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CLIC April 7, 2016



LCLS Instrument Backup AMO,XPP,MEC

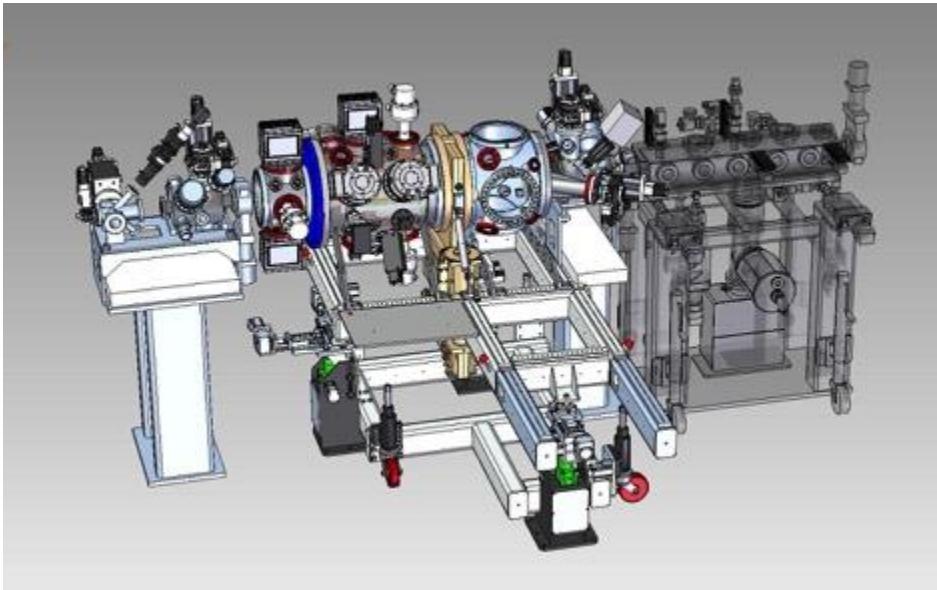
AMO

Atomic, Molecular & Optical Physics

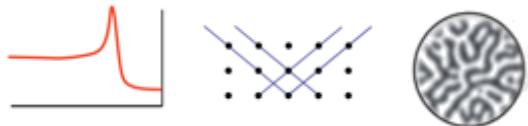
- Intense x-ray interactions with atoms and molecules
 - Non-linear x-ray interactions
- Ultrafast chemical dynamics of molecular gases
- Soft X-ray imaging
- Structure and evolution of clusters

AMO: Atomic, Molecular and Optical Physics

SLAC



First Light: August 2009
Energy : 480eV-2keV



Scientific Scope

- Intense x-ray interactions with atoms and molecules
 - Non-linear x-ray interactions
- Ultrafast chemical dynamics of molecular gases
- Soft X-ray imaging
- Structure and evolution of clusters

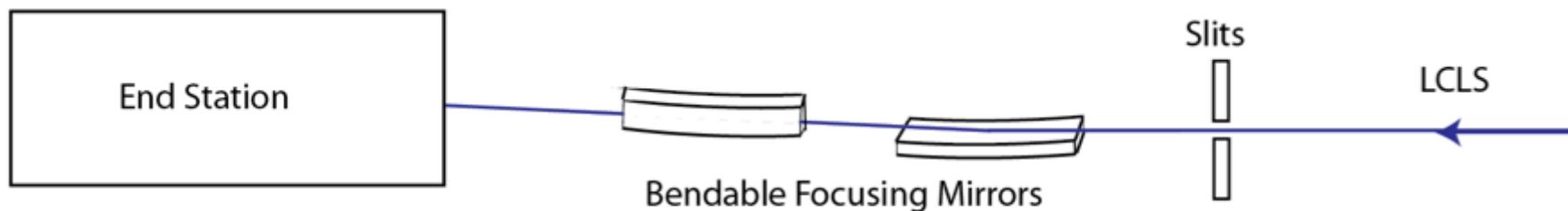
Machine and Instrumentation Development

- X-ray pulse characterization
- X-ray / optical timing
- Accelerator-based x-ray/x-ray pump/probe

The AMO Instrument

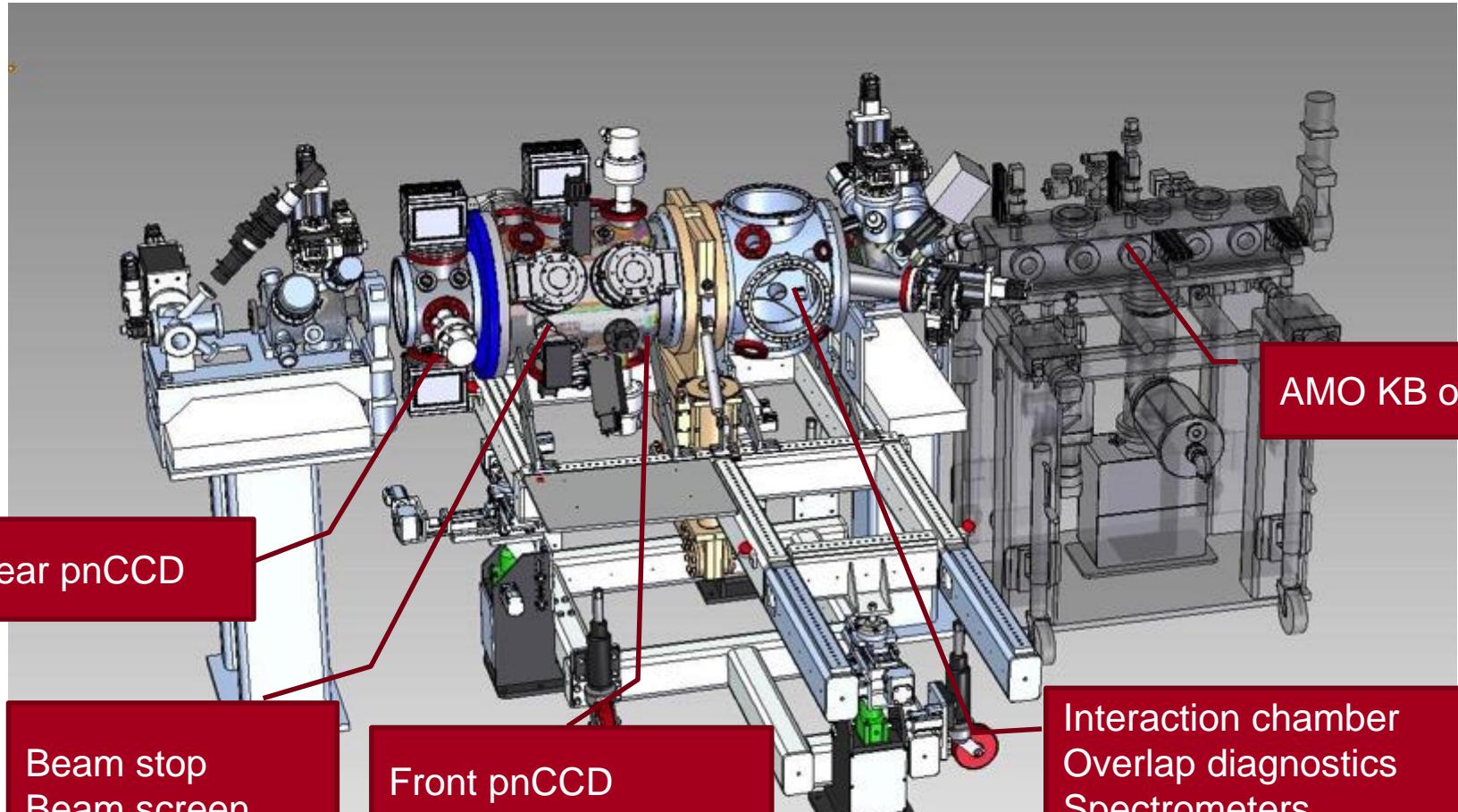
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- Soft X-rays (275-2000eV)
- Pulse Energy 10^{12} photons/pulse
- KB Focusing
 - $1.5 \times 1.5\mu\text{m}$ is minimum focus spot size.
- Optical Pump Laser (Synchronizable with x-rays to < 50 fs)



AMO Instrument: LAMP

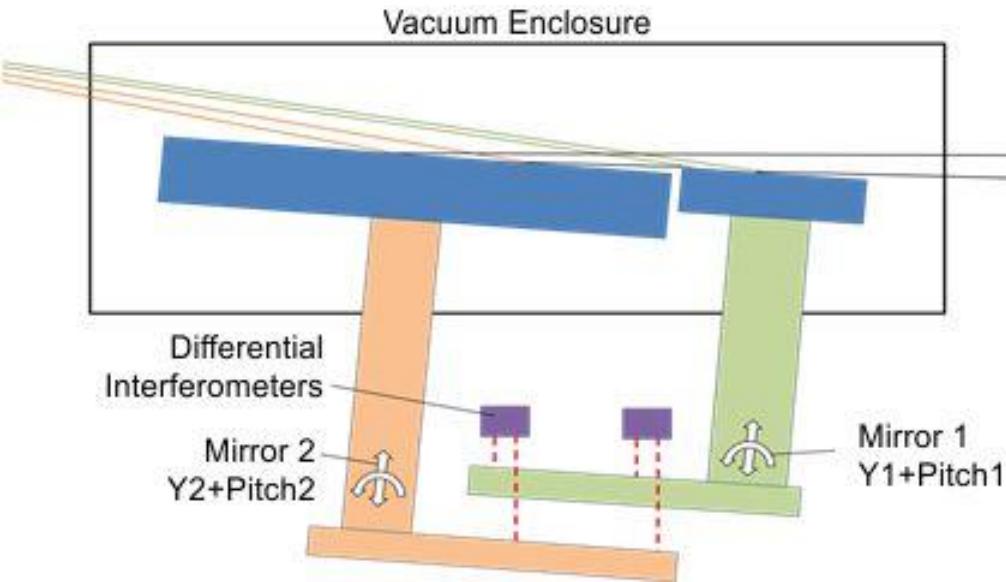
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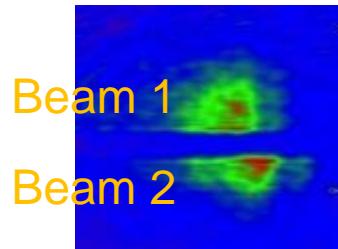
Split & Delay Basic Design Concept:

SLAC

- Two mirror device that splits the beam across the trailing edge of the first mirror
- Second mirror position and angle set to overlap beams in the interaction region

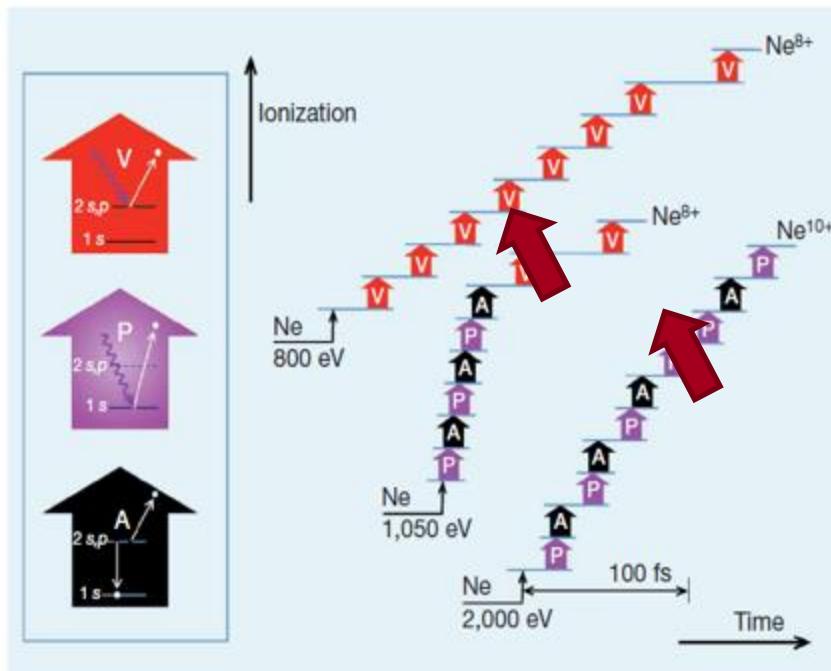


- Delay range 0 – 200 fsec
- Step size ~ fsec
- Available at all SXD beamlines



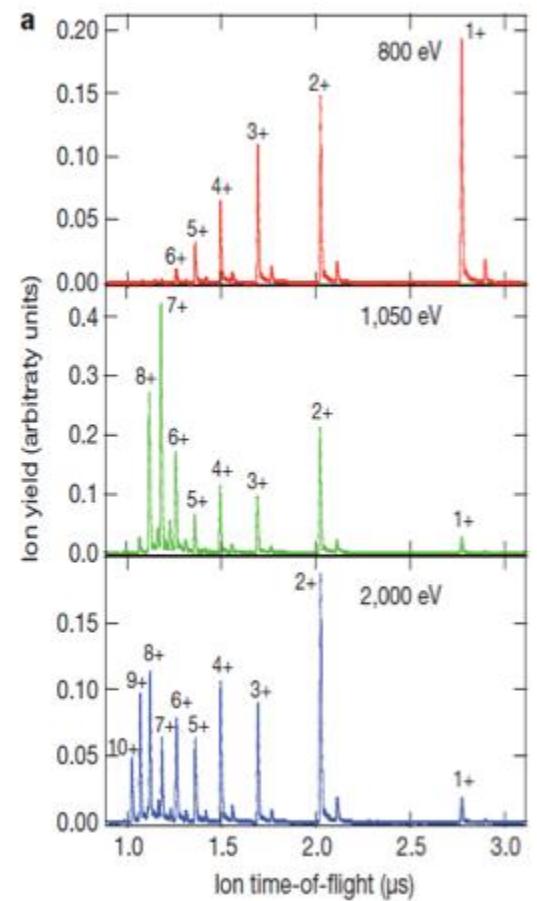
Atomic photoionization in extreme x-ray pulses

SLAC



Sequential, excitation energy dependent processes:
V – Valence ionization
P – Core level ionization
A – Auger process

Ne ion tof data



Young, et al, Nature, 466 p56 (2010)

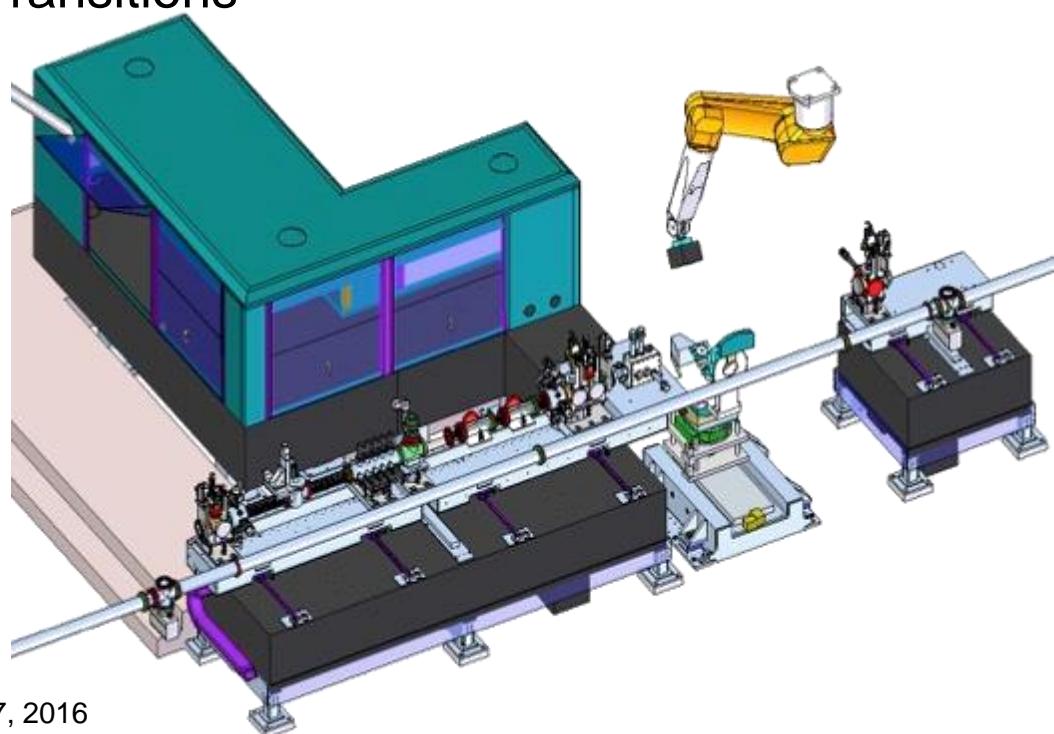
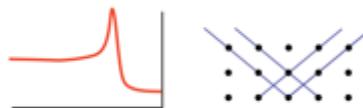
XPP

X-ray Pump Probe

Science Program

- Condensed Phase Photochemistry
 - Charge Transfer Reactions
 - Photosynthetic Reactions/Photovoltaics
- Lattice Dynamics and Phase Transitions
 - Order/Disorder
 - Metal/Insulator
 - Vibrational Dynamics

First Light: July 2010
Energy : 4keV-10 keV

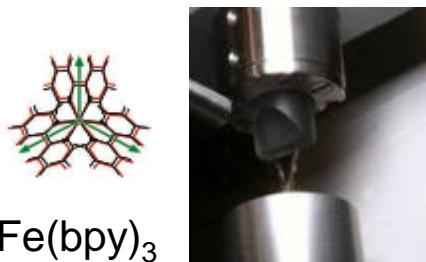


X-ray Pump Probe

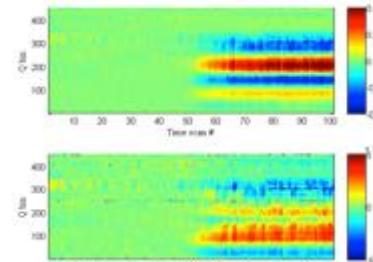
SLAC

XPP: How do the atoms in materials and chemical complexes respond to excitations?

Femtochemistry



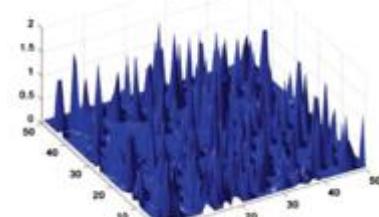
$\text{Fe}(\text{bpy})_3$



Haldrup et al. in preparation

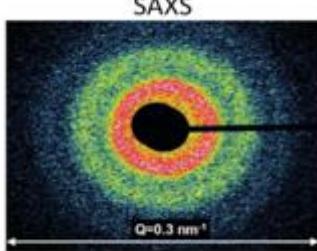
Structural and Temporal correlations

WAXS

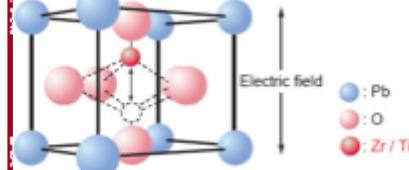


Gutt et al. (2012). Phys. Rev. Lett. **108**, 024801

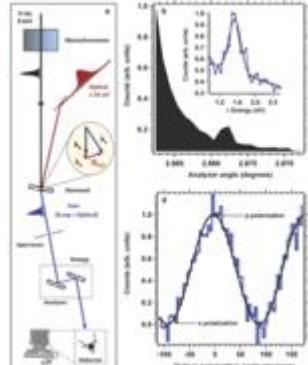
SAXS



Solid state physics

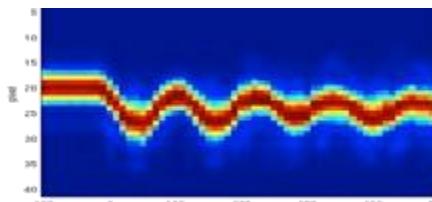


Nonlinear optics



Glover et al. (2012), Nature **488**, 7413

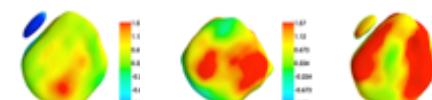
Nanostructures



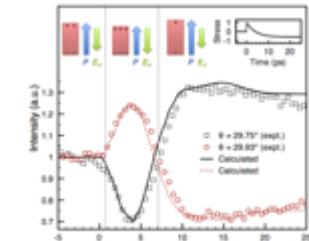
t=0 ps

t=360ps

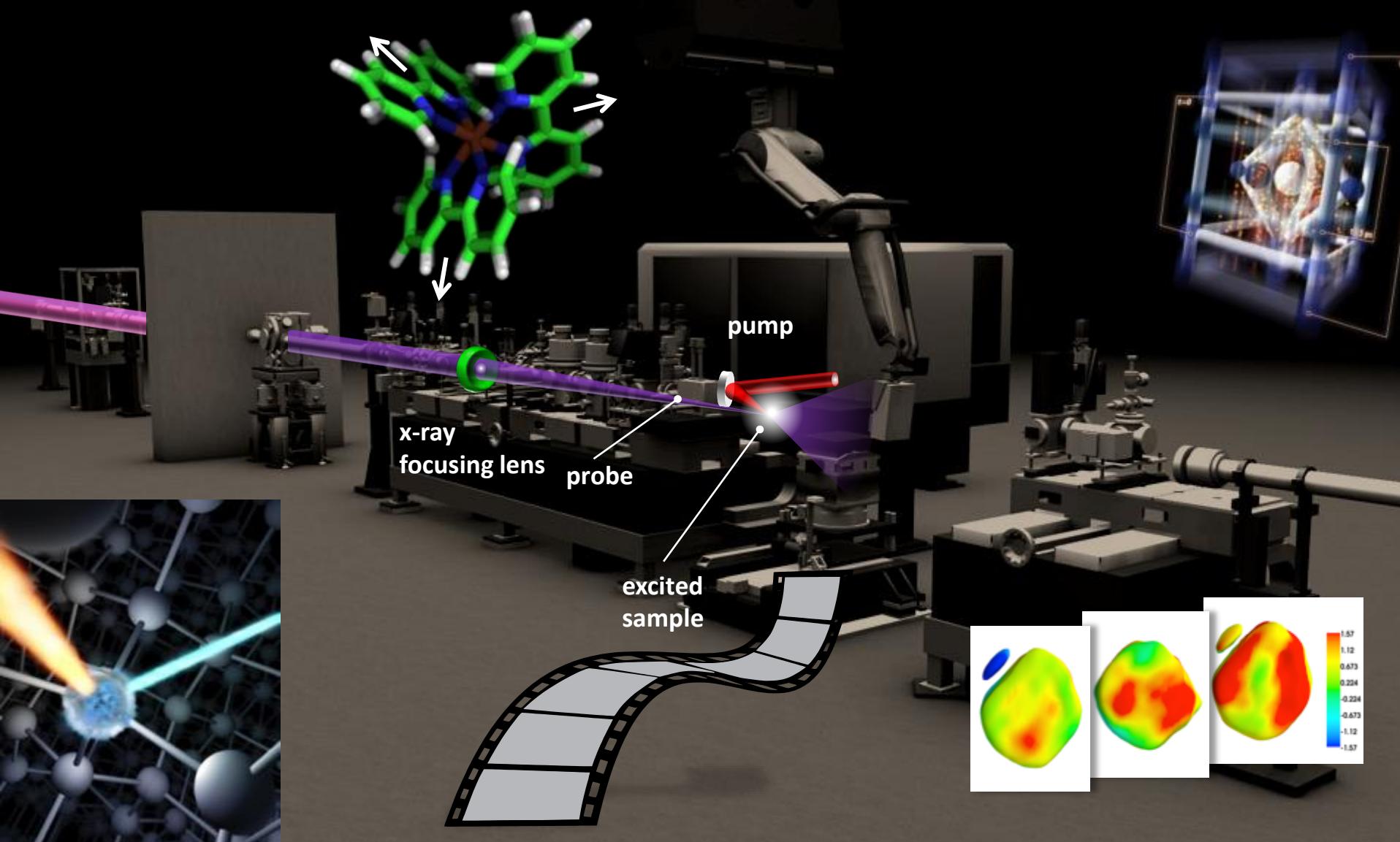
t=370ps



Clark et al., Science **341**, 56 (2013)

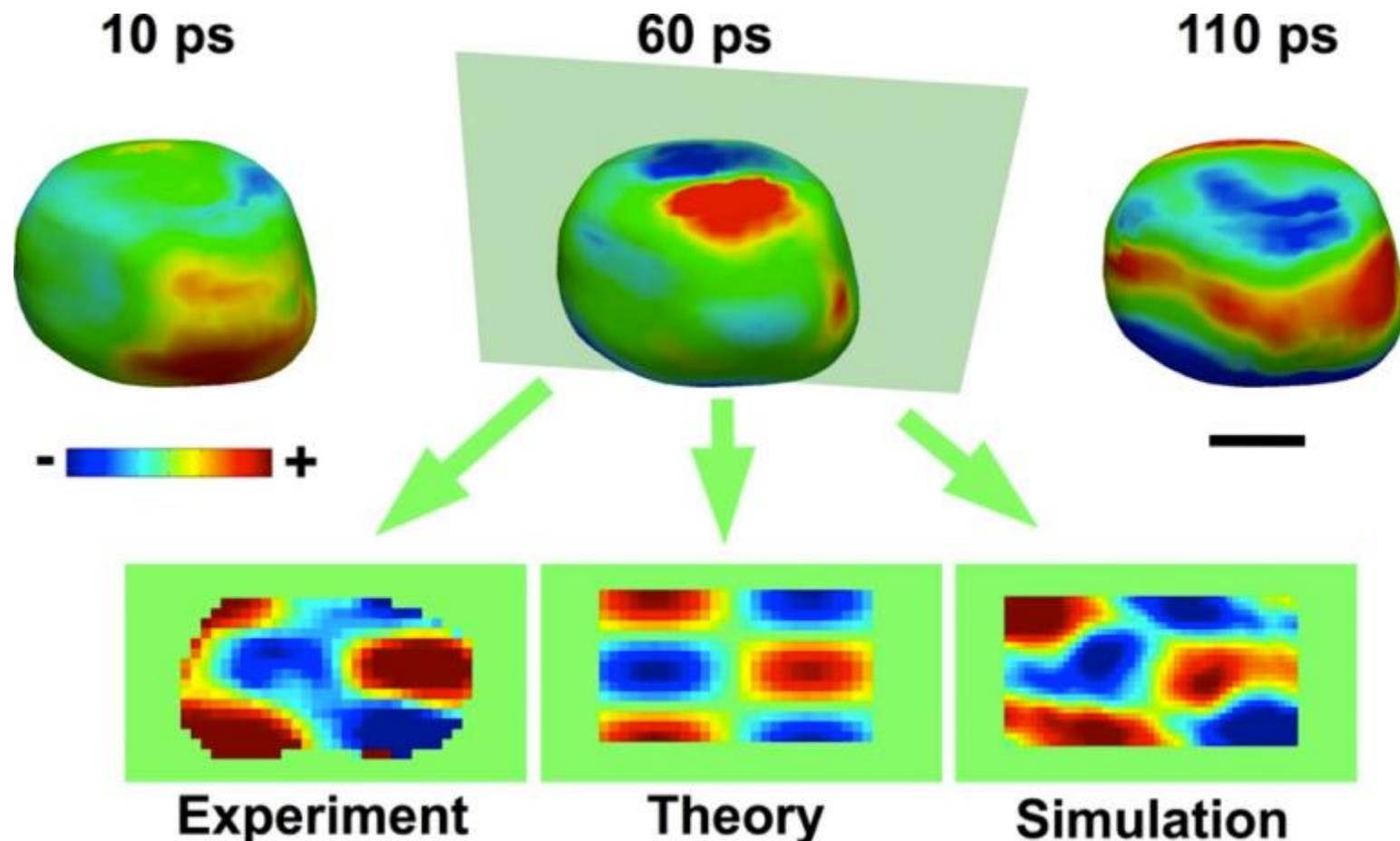


Daranciang et al. (2012). Phys. Rev. Lett. **108**.087601



Imaging phonons in nanocrystals

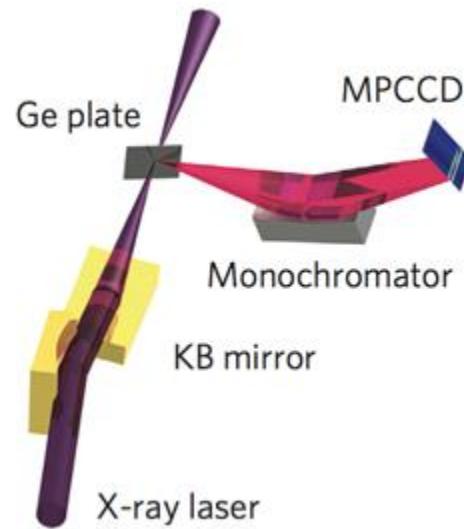
SLAC



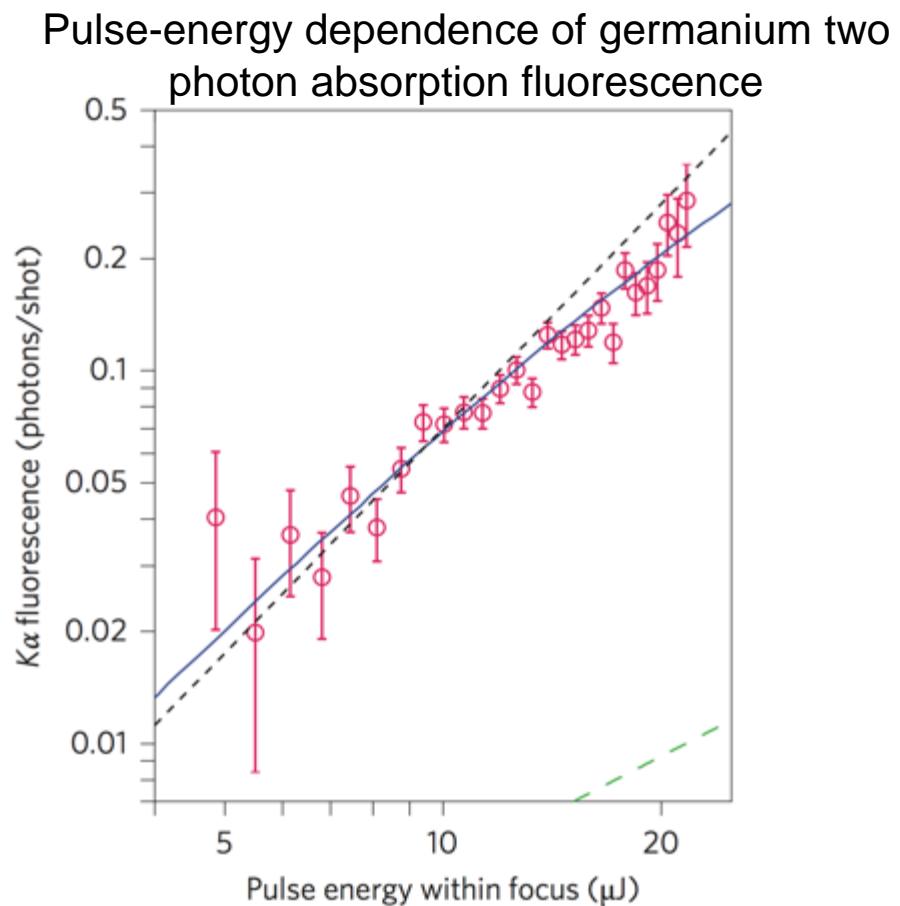
X-ray two-photon absorption at SACLA

SLAC

First observation of a third order nonlinear process with hard x-rays.



K. Tamasaku, et al., Nature Photonics (2014)



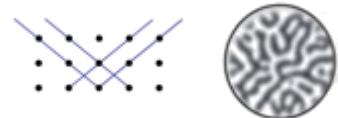
MEC

Matter in Extreme Conditions

MEC Instrument Layout in Hutch 6

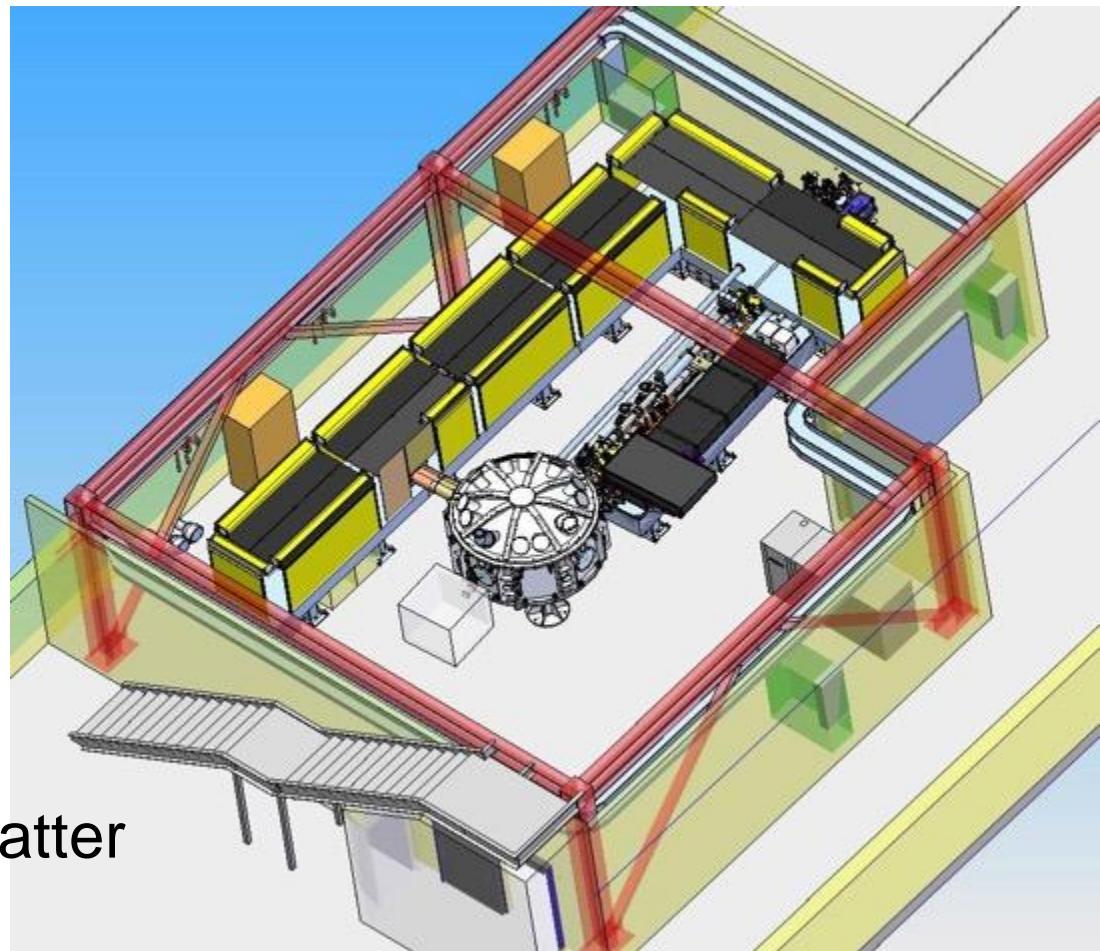
SLAC

First Light: January 2012
Energy : 4 keV-9 keV

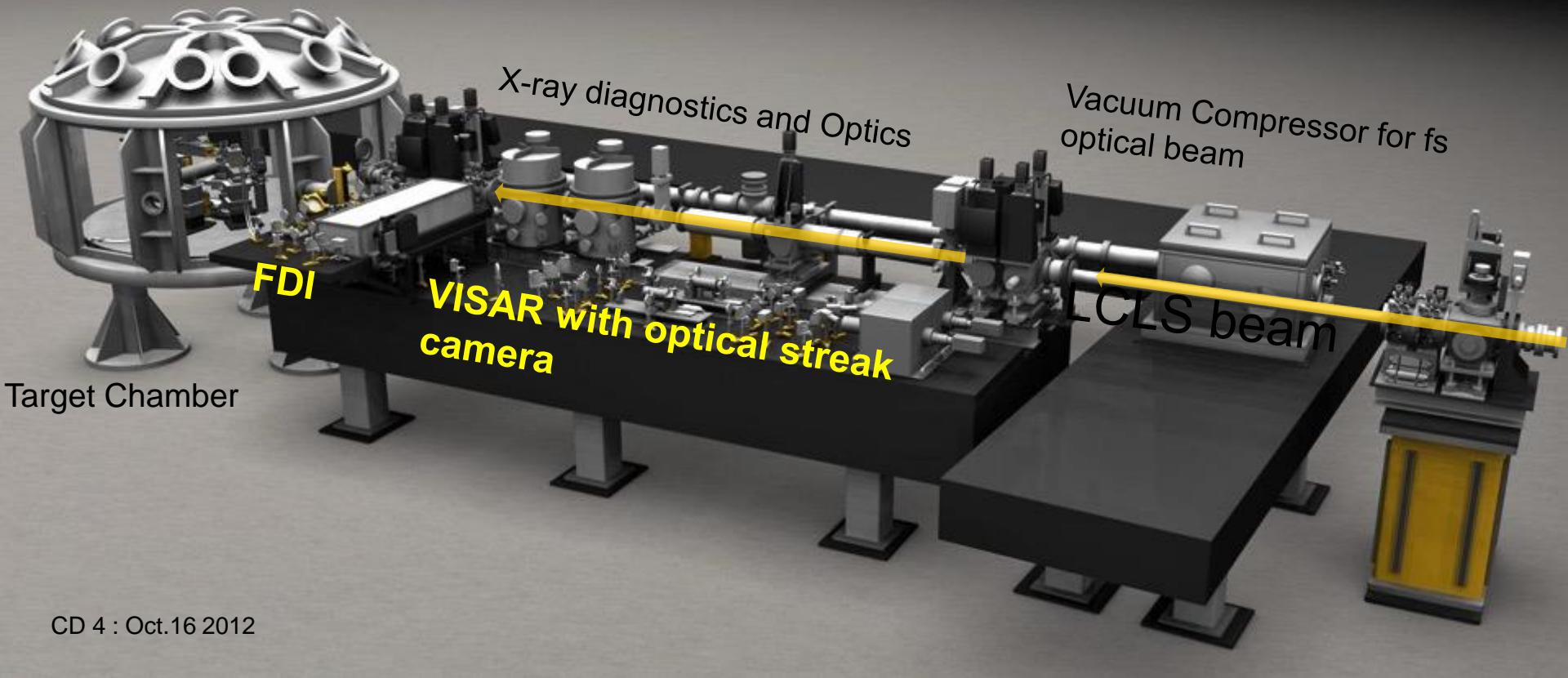


Science Program

- High Pressure
- Shock phenomena
- Warm Dense Matter
- High Energy Density Matter



MEC Instrument optics and diagnostics



CD 4 : Oct.16 2012

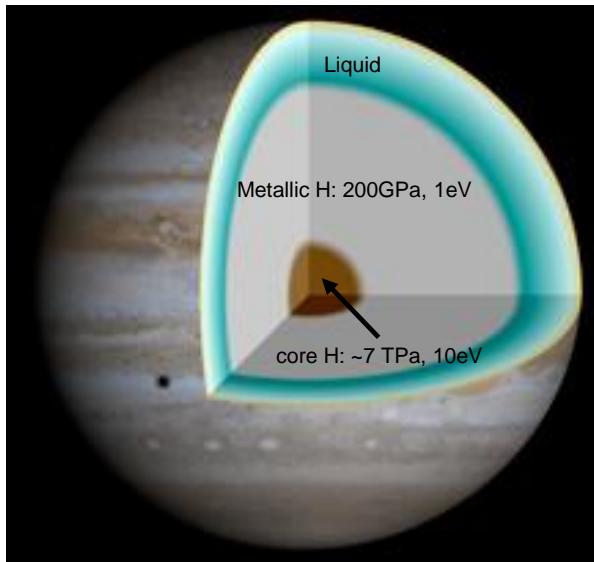
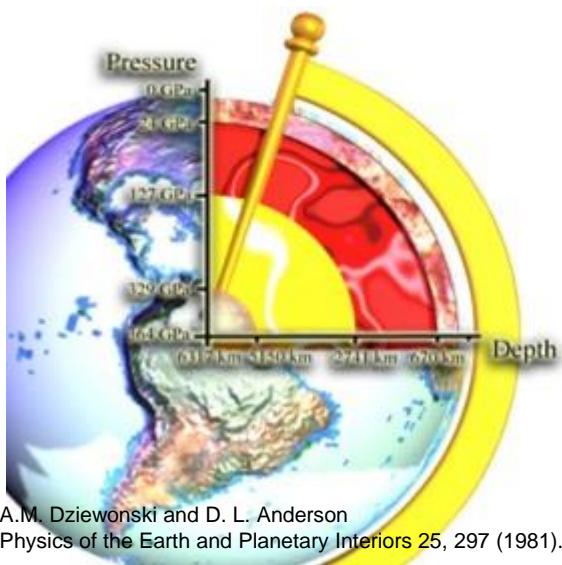
Photon energy: 2keV - 10keV fundamental ($\sim 10^{12}$ photons)
up to 24keV in third harmonic (10^{10} photons)

Pulse length : 60fs - 30fs (<10fs with penalty in photons)

bandwidth : 0.3% in SASE

Matter in Extreme conditions

SLAC

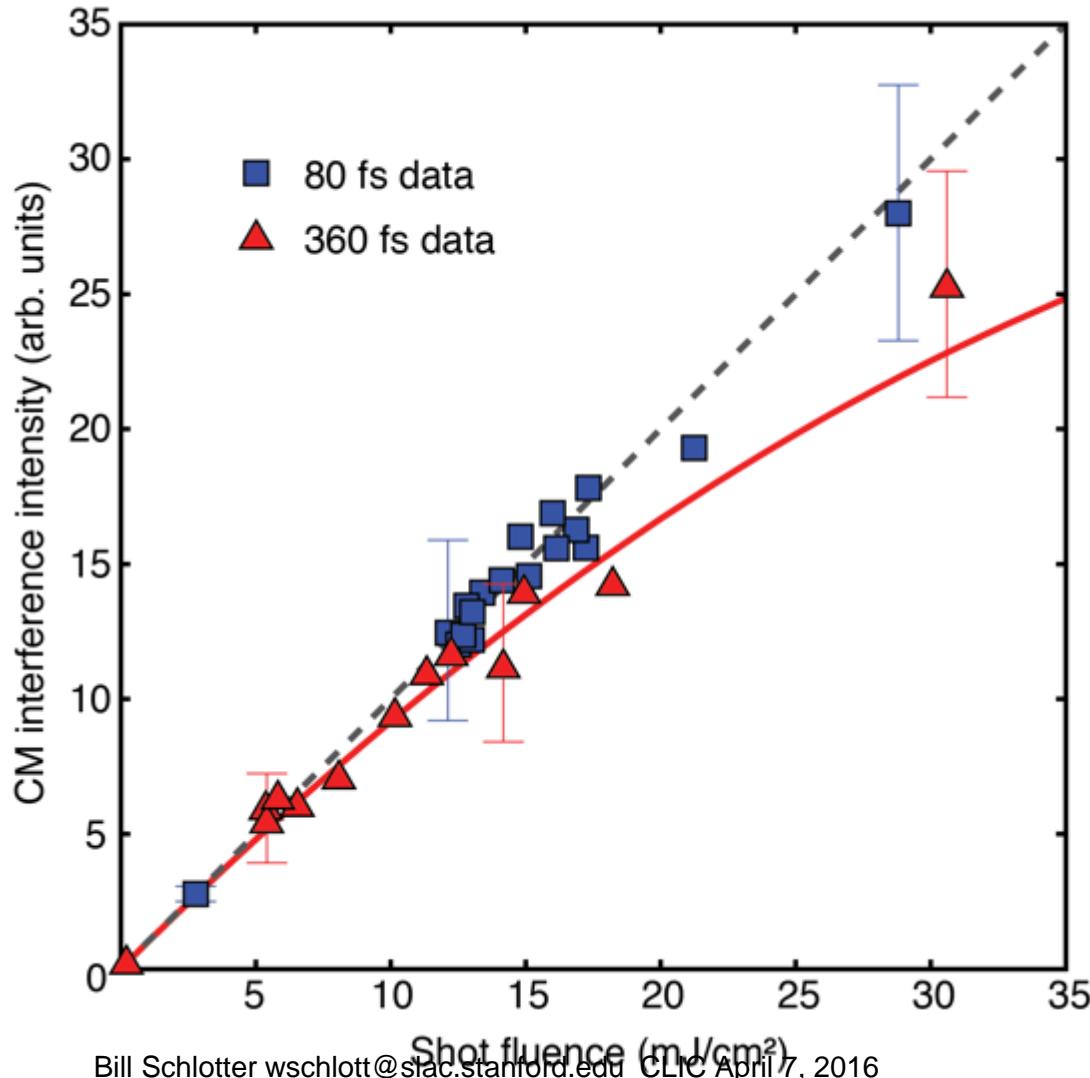


- Matter in extreme conditions is extremely interesting state
 - Solid or near solid density: Pressure typically tens GPa – a few of TPa
 - Heated to $1,000 \text{ K} < 1,000,000 \text{ K}$
 - Inside the Earth, structure of large planet, planetary impact phenomena...
 - High Energy Density Physics, Warm Dense Matter, High Pressure Physics

LCLS Instrument Backup SXR,CXI

Avoiding demagnetization during the x-ray pulse

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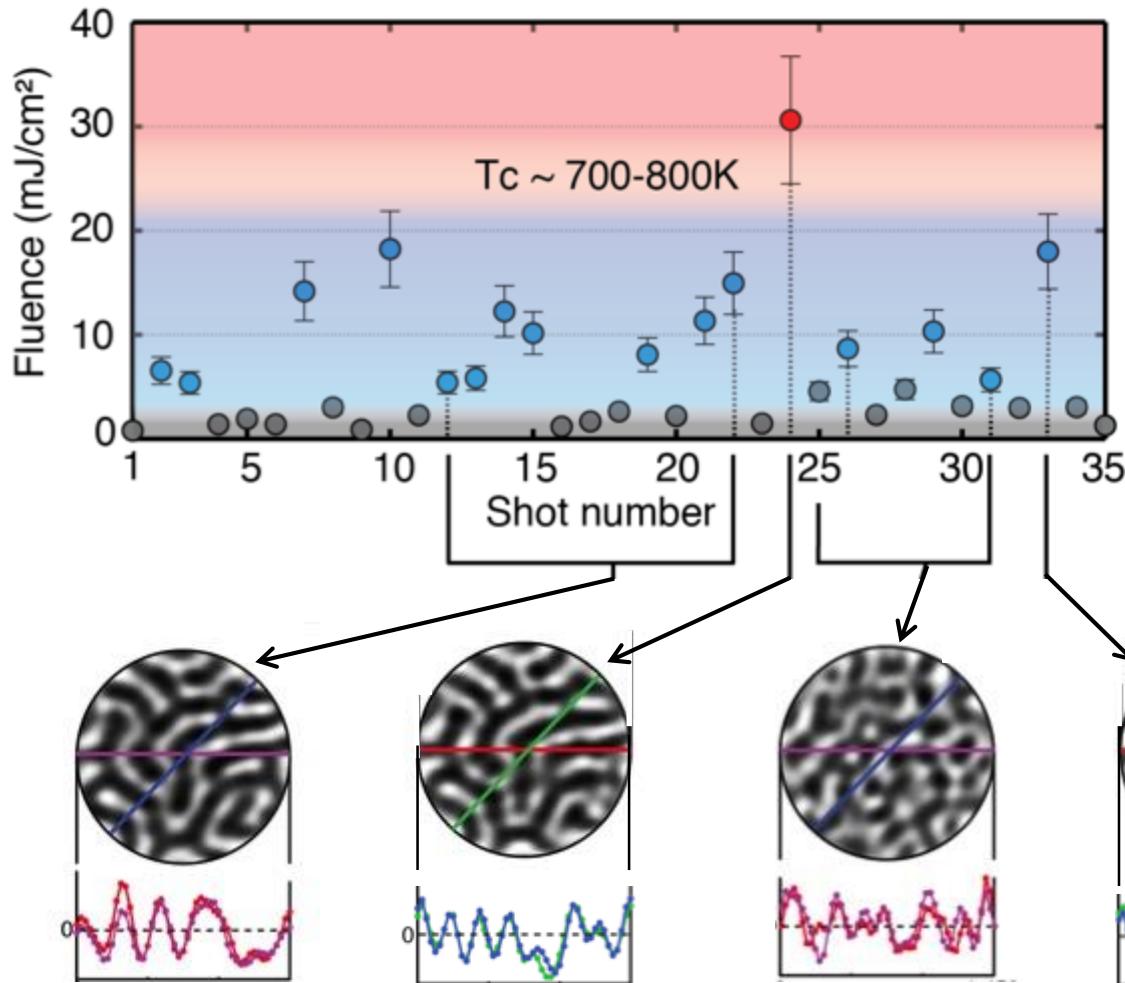


Illumination with $20\text{mJ}/\text{cm}^2$:

- Comparable energy deposited with an optical pulse will result in a reduction of magnetization (red curve)
- Front of 360 fs pulse excite the electronic systems which thermalize to the lattice within 100fs thus reducing the magnetization
- 80 fs pulses are fast enough to outrun demagnetization

After effects of heating: damage thresholds

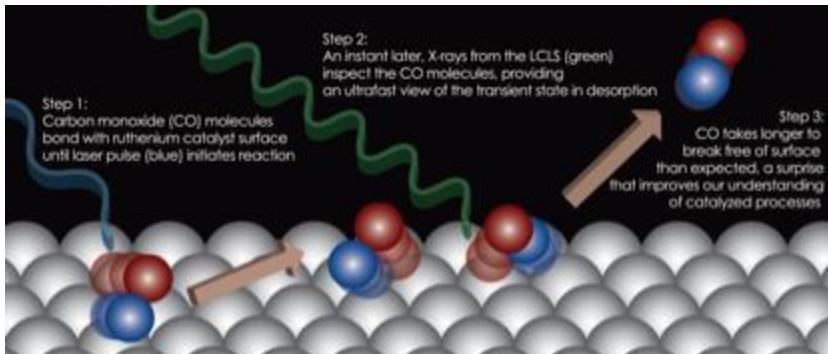
SLAC



- Sequential imaging on a single sample possible but limited to 50nm resolution
- Irreversible damage above $\sim 30\text{mJ/cm}^2$

Watching surface bonds break in real-time: Transient weakly bound state observed in desorption process

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Experiment:

- An ultrafast laser pulse heats the metal surface and initiates the process of converting CO to CO₂.
- Snapshots of the electronic states of oxygen are captured in x-ray spectra.

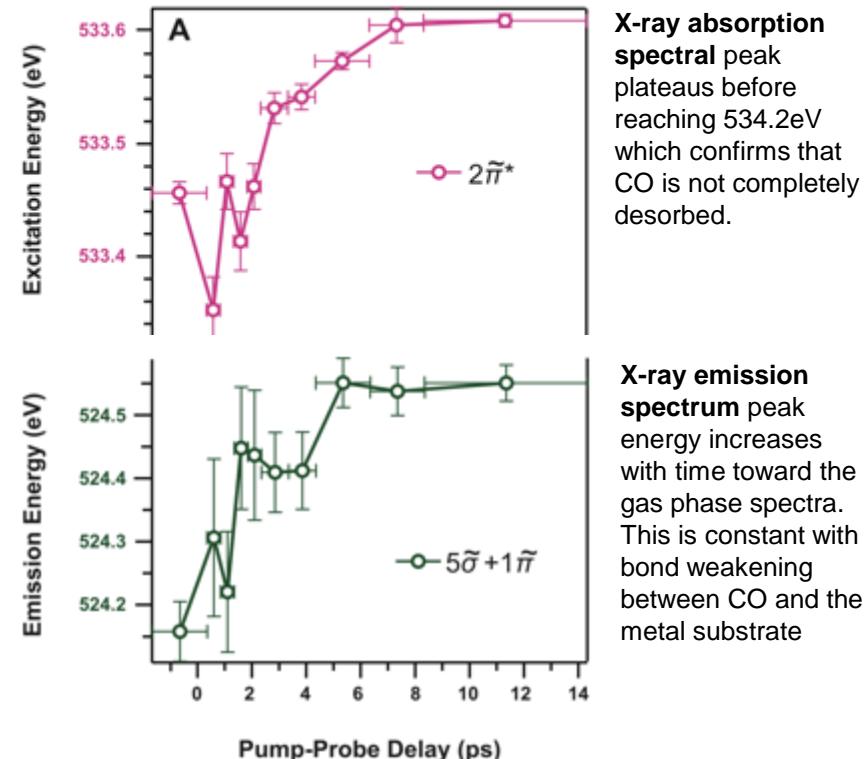
Nilsson Group, Surface Science End Station
M. Dell'Angela, *et al.*, Science **339** 6125 (2013)
M. Beye, *et al.*, Phys. Rev. Lett. **110** 186101 (2013)

Bill Schlotter wschlott@slac.stanford.edu CLIC April 7, 2016

Results:

- CO enters a transient state where it is weakly bonded yet not completely desorbed.

Spectral Peak Energy vs. Delay



CXI Primary Science Areas

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- Structural Biology
 - Serial Femtosecond Crystallography
 - Laser induced Dynamics
 - Coherent Diffractive Imaging
 - Protein Crystal Screening Program
- Nanoparticle Studies and Imaging
 - Clusters
 - Aerosols
- High Field Hard X-ray Physics
 - 100 nm focus is unique capability
 - **Produces the highest x-ray power density in the World**
 - Non-linear x-ray studies
- Material Science
 - Nanoparticle studies and imaging
 - Laser induced phase transitions
- AMO Science with Hard X-rays



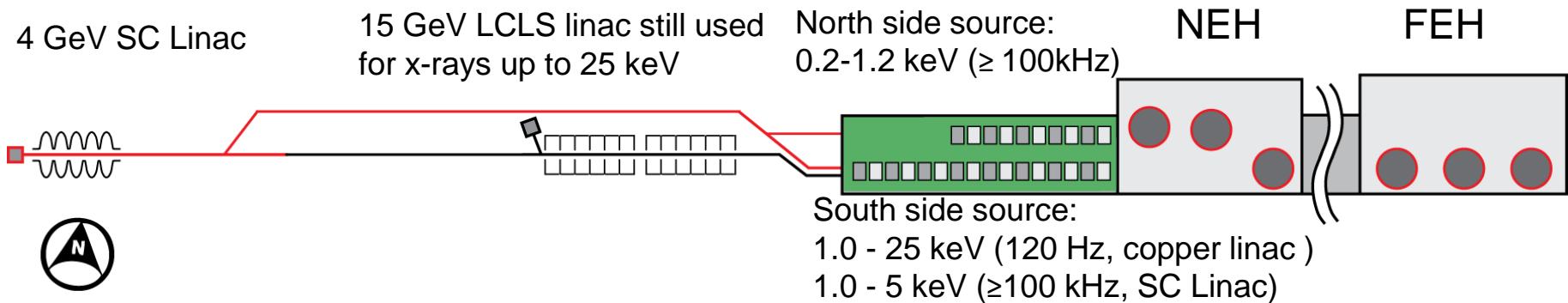
LCLS II

Backup

LCLS-II Upgrade Project Scope

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| | |
|---|--|
| Accelerator | Superconducting linac: 4 GeV |
| Undulators in existing LCLS-I Tunnel | New variable gap (north) New variable gap (south), replaces existing fixed-gap und. |
| Instruments | Re-purpose existing instruments (instrument and detector upgrades needed to fully exploit) |



Development of Science Drivers LCLS-II Science Opportunities Workshops

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Science opportunities
workshops held at SLAC
in February, 2015

Workshop Registrants

| | |
|---------------------------|------------|
| Chemistry | 165 |
| Materials Physics | 264 |
| Life Sciences | 149 |
| MEC Breakouts | 116 |
| Unique Registrants | 410 |

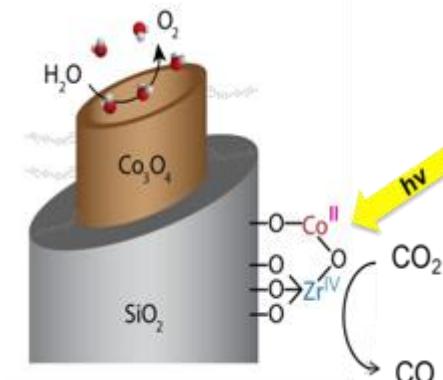
Chemistry: Photo and heterogeneous catalysis

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Predictive understanding of catalysis

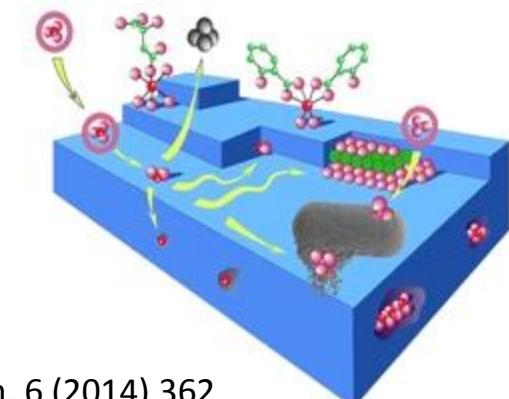
LCLS-II Science Opportunity

- Understand the fundamental processes that occur on metal surfaces during catalytic reaction conditions in order to design new, efficient, and selective catalysts
- Provide a robust structure-function relationships for materials in electronic excited states
- Understanding and predicting photon driven phenomena



Significance and Impact

- Light harvesting & charge separation are fundamental to understanding natural & artificial photo-catalytic systems
- Interfacial chemistry and charge-transfer in real time & under reactive conditions



Strengths of SRF source

- High average power at high rep rate (moderate peak power)

Chemistry: Charge migration and redistribution

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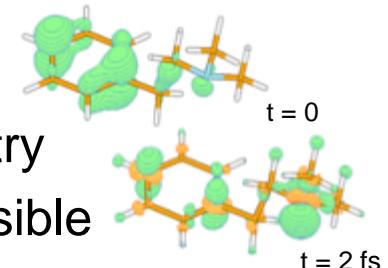
Follow molecular transformations & bond formation

LCLS-II Science Opportunity

- Map electron dynamics on sub-angstrom and sub-femtosecond scales and reveal coupled electronic and nuclear motion in molecules

Significance and Impact

- Charge migration initiates all charge transfer chemistry
- Dynamics on fundamental time scale have been invisible before this



Strengths of SRF source

- Coherent bandwidth and pulse intensity are essential for transient impulsive electronics
- 2-color (element selectivity)
- High rep rate for rare events and coincidences

Materials Physics: Revealing interactions among degrees of freedom in high temperature SC cuprates

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LCLS-II Science Opportunity

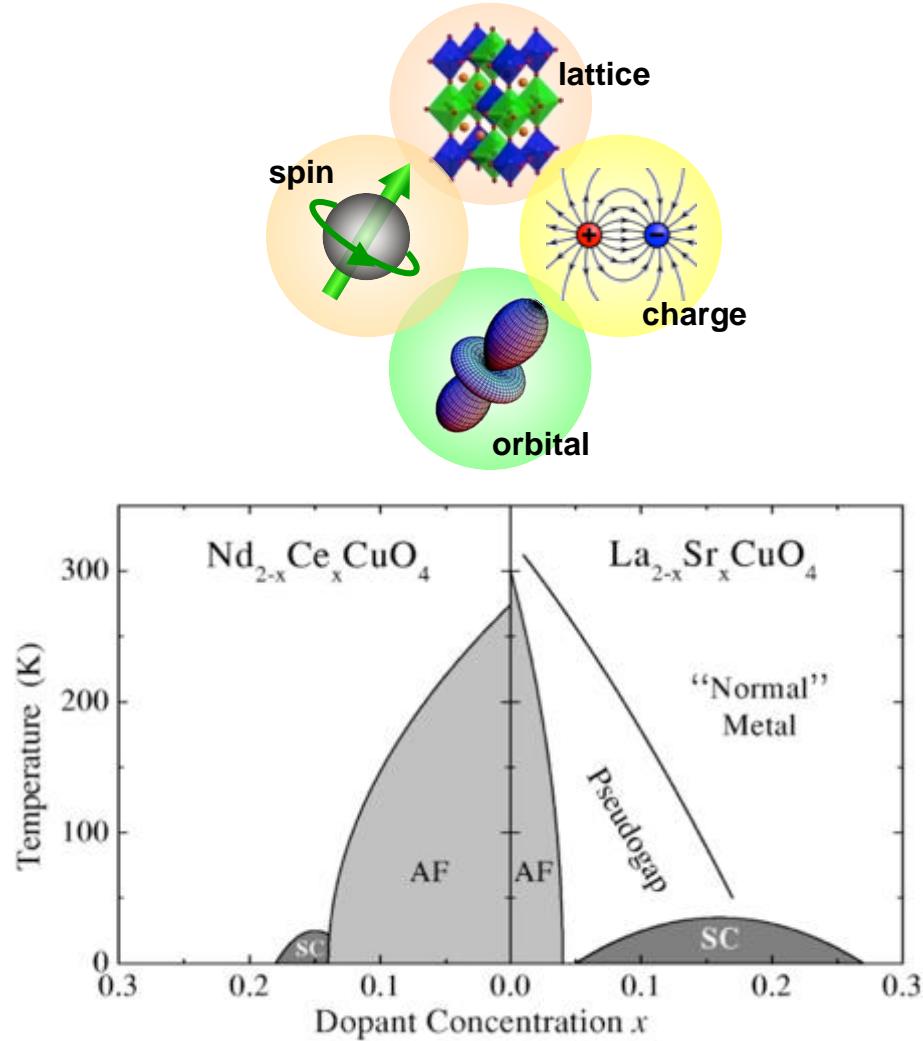
- Magnetic, lattice, and charge degrees of freedom are strongly intertwined makes it difficult to understand the mechanism of HTSC.

Significance & Impact

- Clarify interactions among different degrees of freedom in high T_c cuprates, that may provide important clues to reveal its mechanism.
- Pathway to manipulate novel phase and perhaps lead to SC with even higher T_c .

Strengths of SRF source

- Time-resolved RIXS with Fourier-transform limited time and energy resolution.

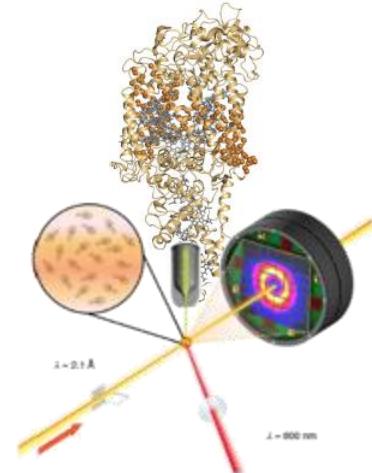


Life Sciences & Matter in Extreme Conditions at LCLS-II

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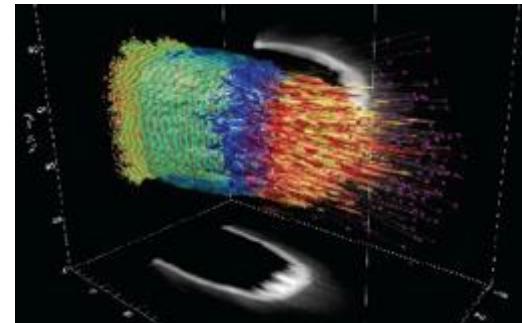
Life Science

- Small-scale structural dynamics at Å resolution
 - Serial nano-crystallography
- Large scale conformational dynamics
 - Molecular movies – single particle imaging (2-6 keV)
 - Solution scattering – fluctuation SAX



Matter in Extreme Conditions

- Warm & hot dense matter – lab. astrophysics
- Rapid compression, shock & impact physics
- Material weakening and hydrodynamic “flow” on ultrafast time scales



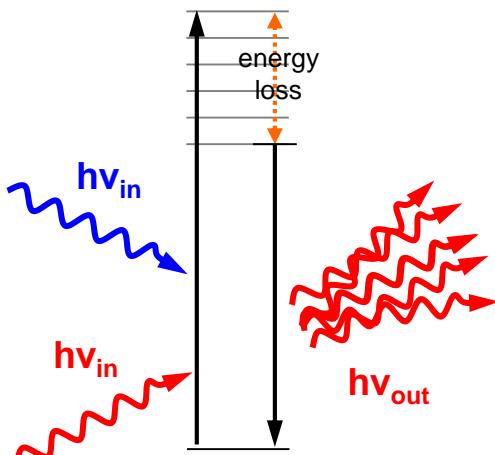
Other Backup

LCLS-II will enable completely new x-ray methods

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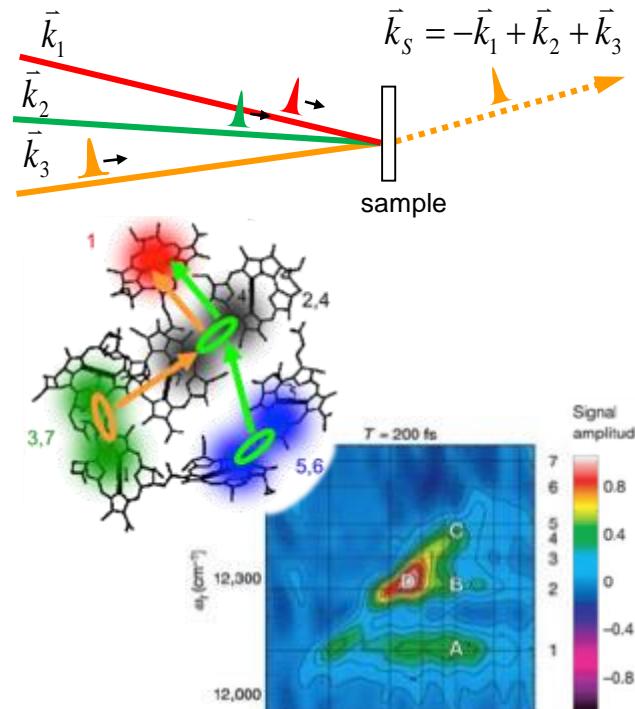
X-ray Lasers
today ↑ future

Time-resolved X-ray Raman, stimulated emission



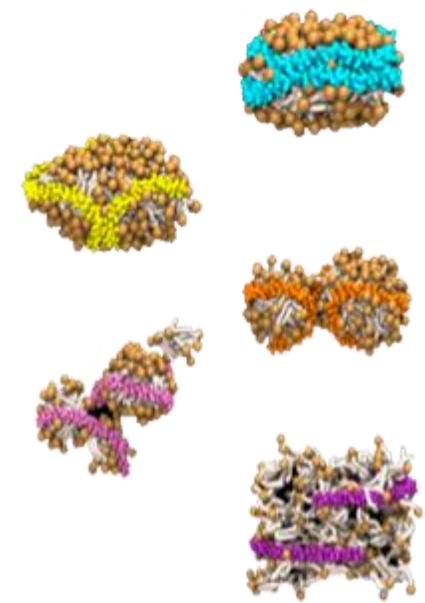
X-ray emission
spectrum

Multi-dimensional nonlinear spectroscopy



Pump-probe

Macromolecular assembly & dynamics

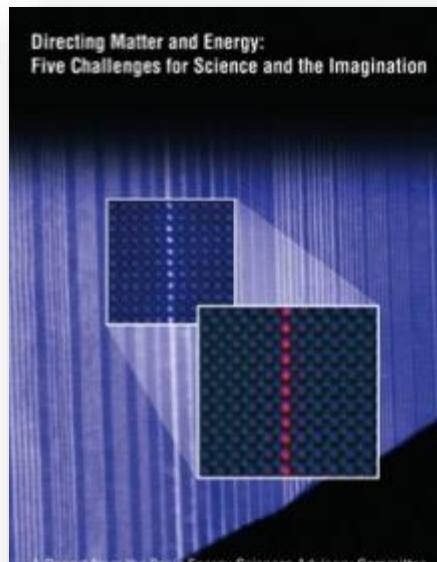


Structure of
single molecules

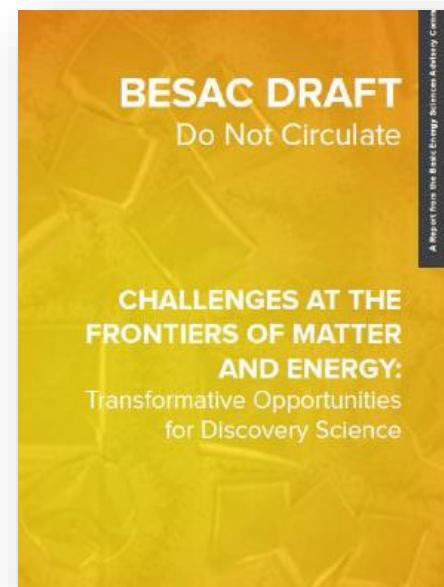
Guiding Scientific Themes

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Five Grand Challenges for Science and the Imagination (2007)



Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science (2015)



RIXS for Chemistry

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- RIXS experimental setup for studying liquids

