Future Science Opportunities Enabled by X-ray Free Electron Lasers

Bill Schlotter

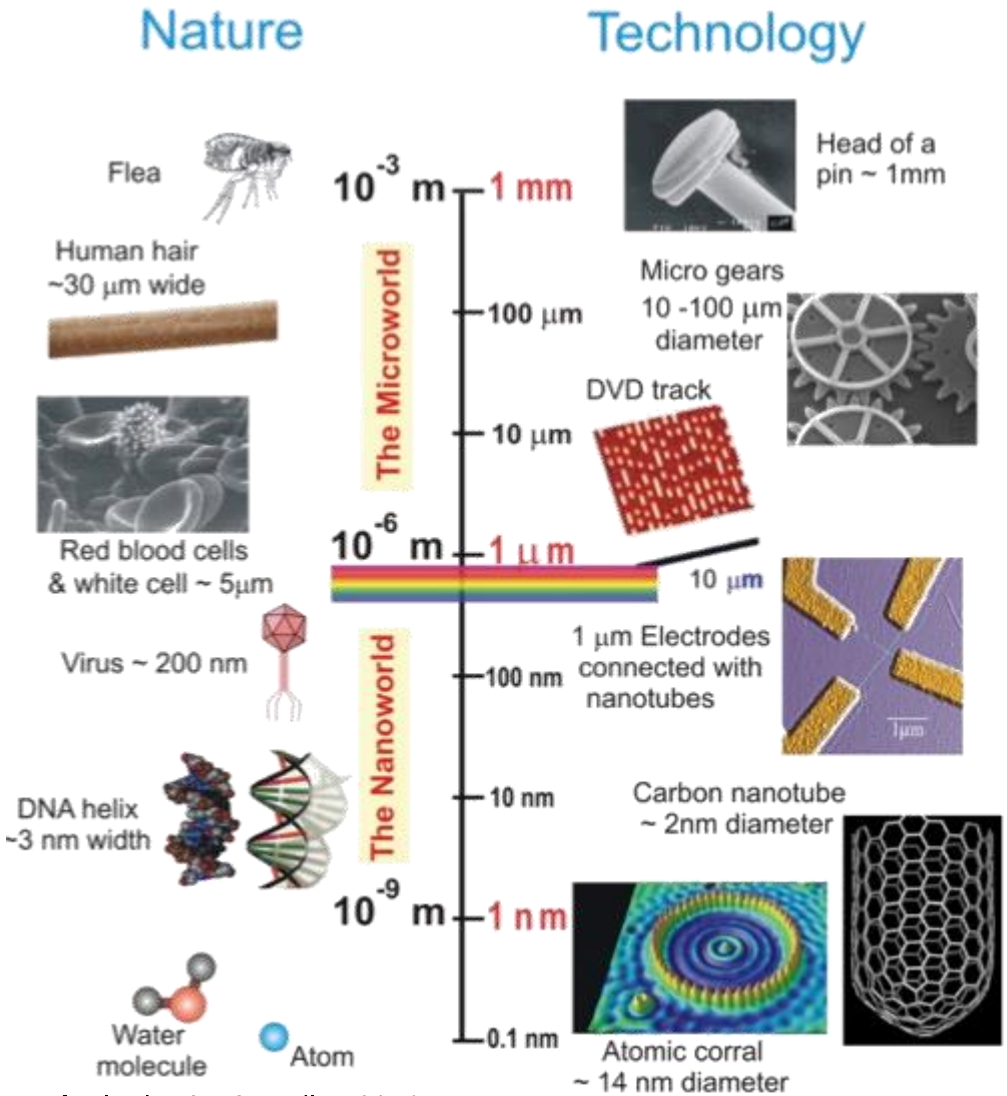
Linac Coherent Light Source, SLAC

Thursday, April 7, 2015

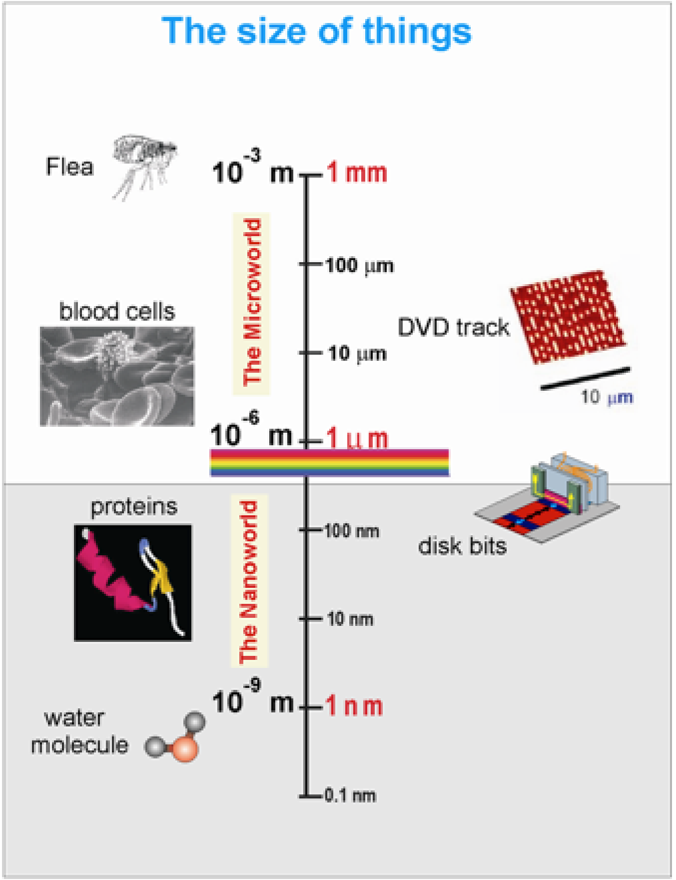
Outline

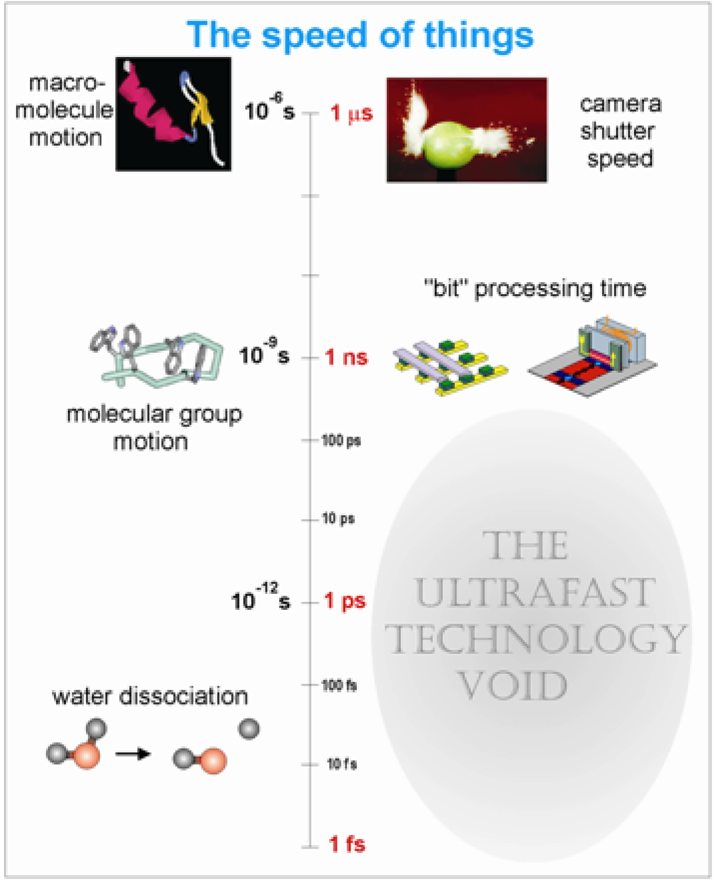
- X-ray Science and Methods
- Soft and Hard X-ray Free Electron Lasers
- A Tour of LCLS with some science examples
  - Soft X-ray Instrument for Materials (CXI)
  - Coherent X-ray Imaging (CXI)
- The LCLS-II upgrade
- Further Reading

How do we see the nanoworld?



Relevant Time and Length Scales

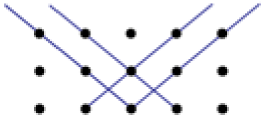
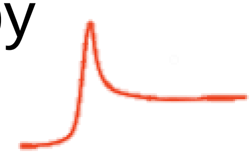




1 light picosecond = 0.3 mm

Jo Stohr, LCLS, SLAC

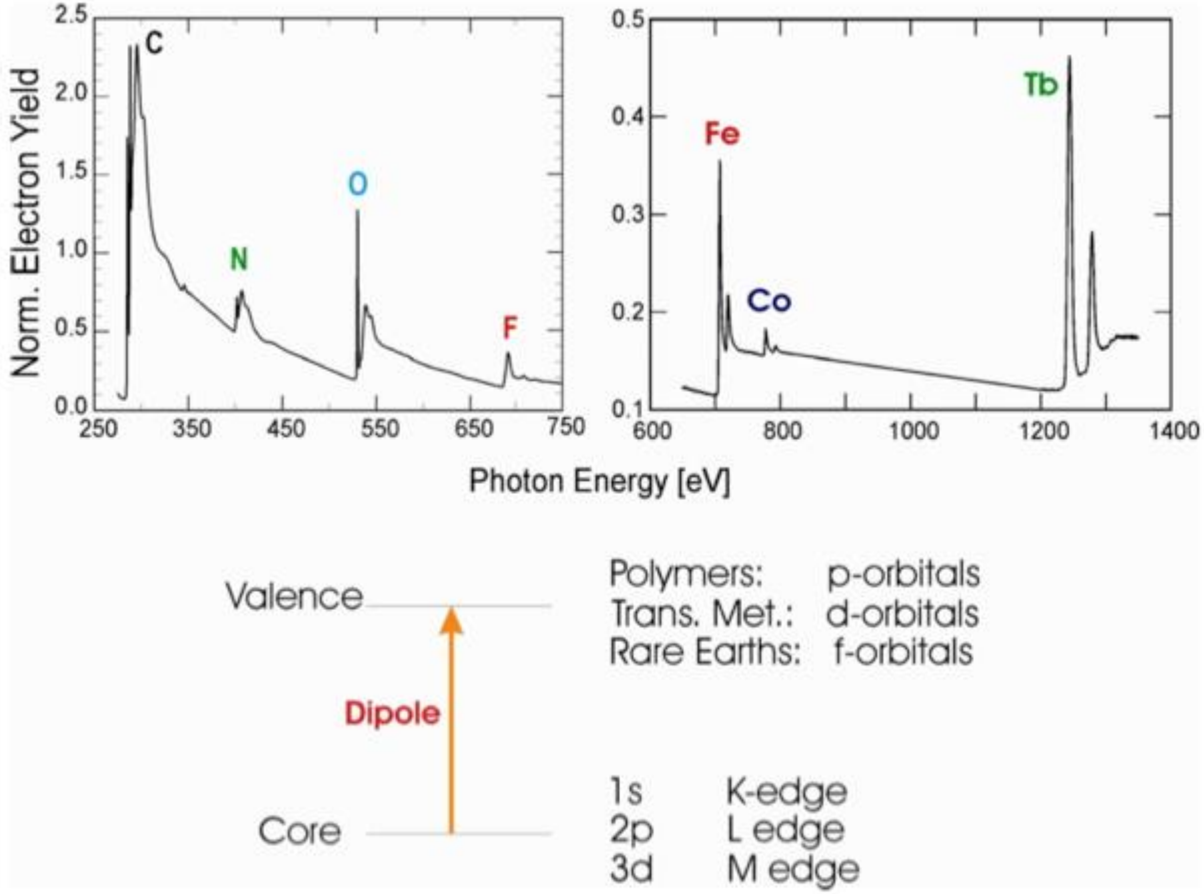
Why do we use x-rays?

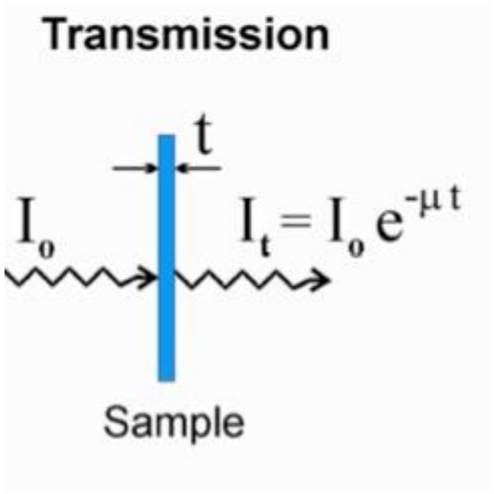
Capability	Technique
Access to atomic length scales	Scattering 
Capture texture exactly and access bulk	Imaging 
Element and chemical sensitivity	Spectroscopy 

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

X-ray Absorption Spectroscopy

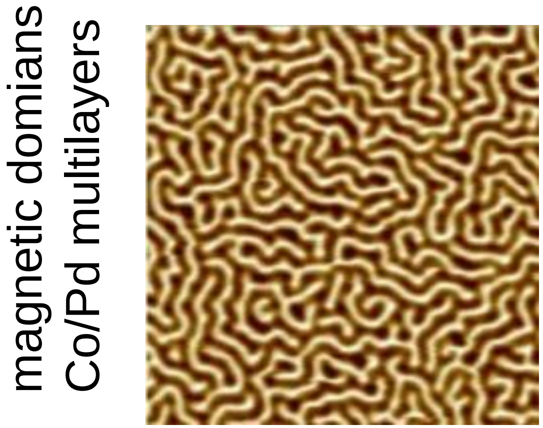
Element Specific Sensitivity and Contrast

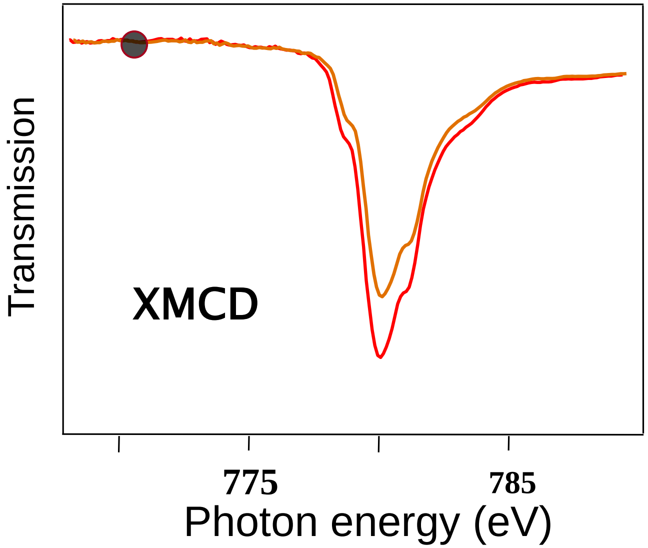


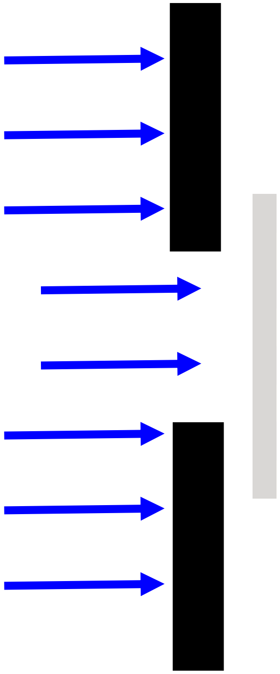


Resonant Coherent Scattering

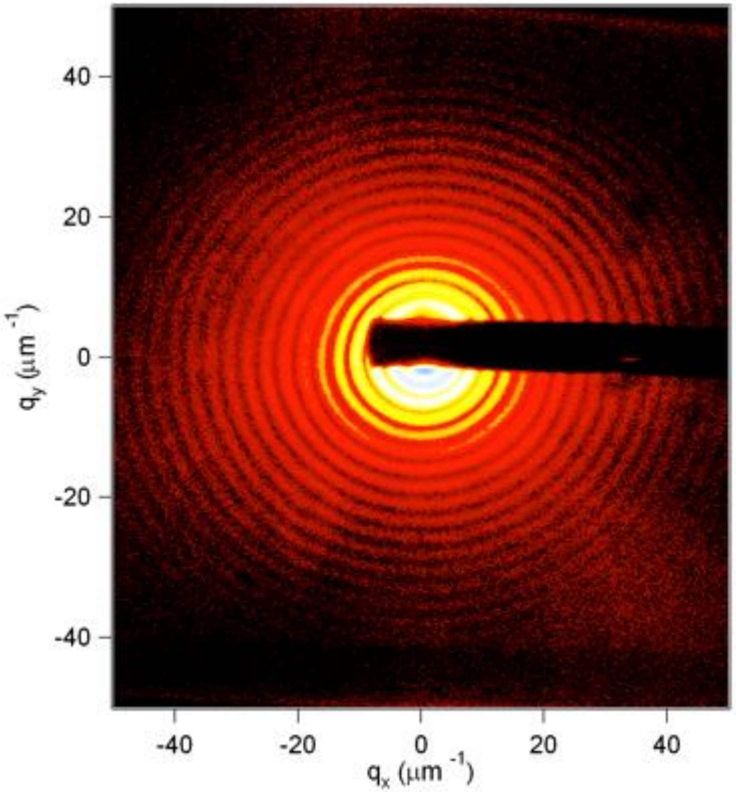
•Perpendicular Magnetization
•X-Ray Magnetic Dichroism







Non-Resonant



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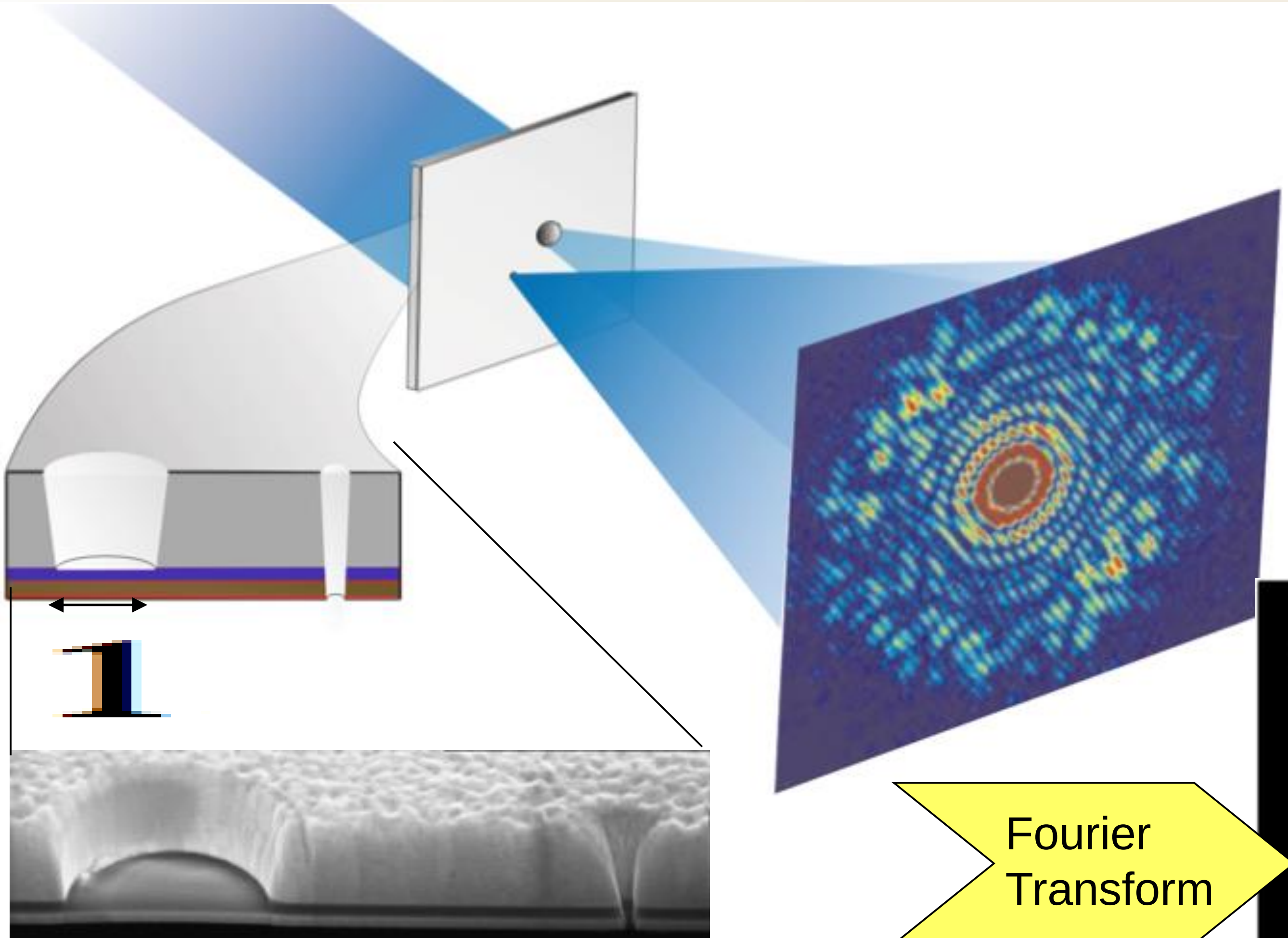
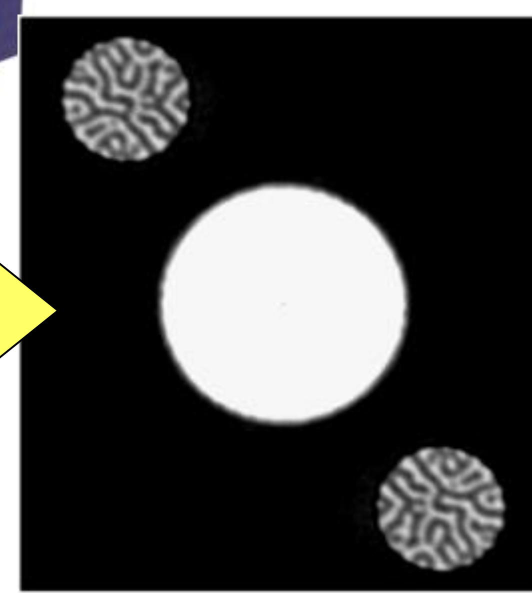
Fourier Transform Holography



Autocorrelation

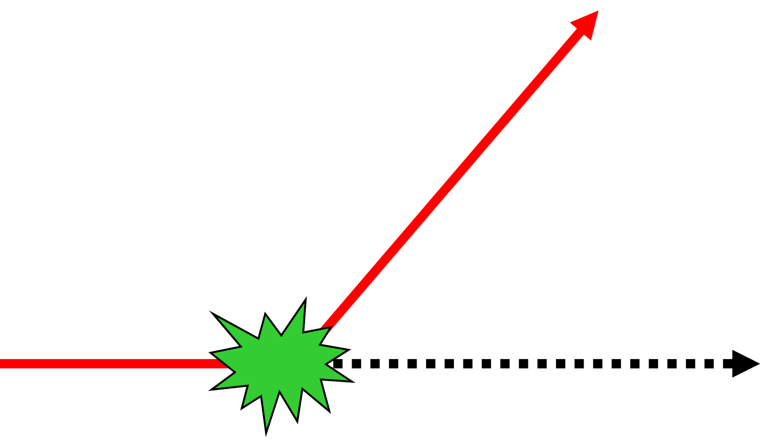


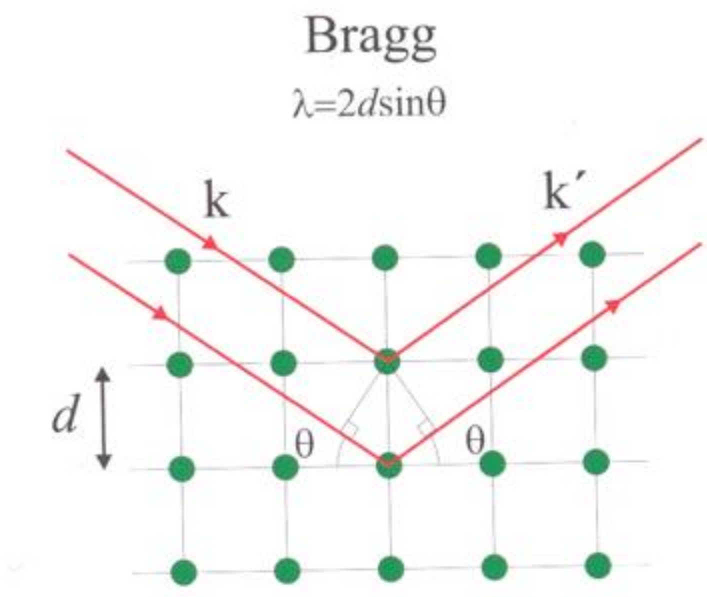
Nature **432**, p885 Dec. 16, 2004

X-ray Scattering & Diffraction

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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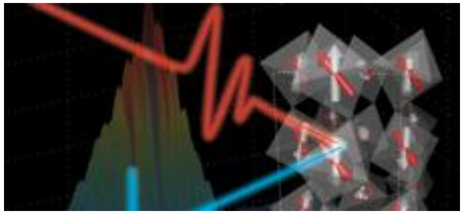
X-rays provide element specificity and atomic resolution…

➢ Ultrashort X-ray Pulses

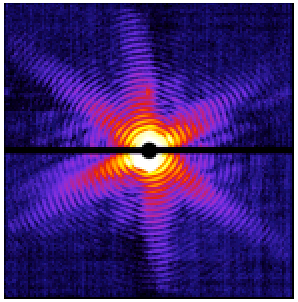


- Study ultrafast (femtosecond) dynamics
- Out-run damage to samples

➢ 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 FLASH-II	SC SC	1.2	0.03–0.3	$(1-500)\times 10^{a}$	2005 2015
	XFEL	SC	17.5	3–25 0.2–3	$(1-2800)\times 10^{b}$	2017
Italy	FERMI-FEL1 FERMI-FEL2	NC	1.5	0.01–0.06 0.06–0.3	10–50	2012 2014
Japan	SACLA	NC	8	4–15	30–60	2011
Korea	PAL-XFEL	NC	10 3	1–20 0.3–1	60	2016
Switzerland	SwissFEL	NC	5.8 3	2–12 0.2–2	100	2017
USA	LCLS LCLS-II LCLS-II	NC NC SC	16 16 4	0.25–11 1–25 0.2–5	120 120 10^6	2009 2020 2020

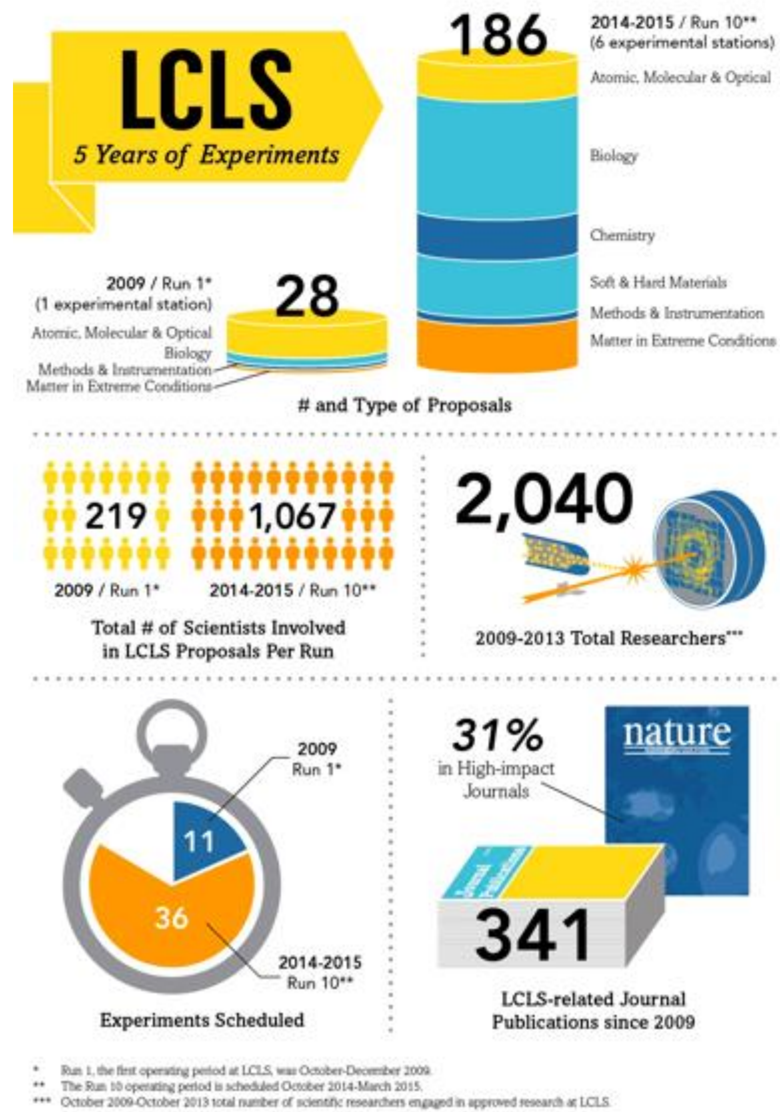
[a]Pulsed mode operation at 10 Hz, with each macropulse providing up to 500 bunches.
[b]Pulsed mode operation at 10 Hz, with each macropulse providing up to 2800 bunches.

VUV: below 0.2 keV
Soft X-ray: 0.2-2.0 keV
Hard X-ray: 4-25keV

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

How does LCLS work?

- 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

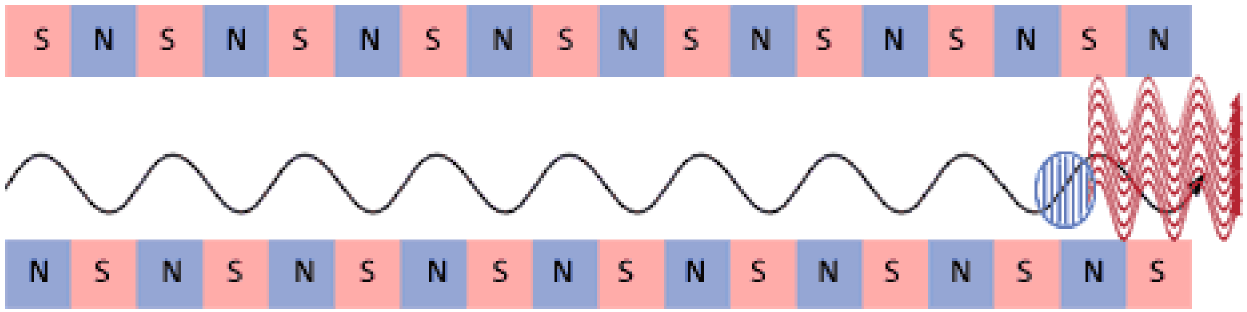


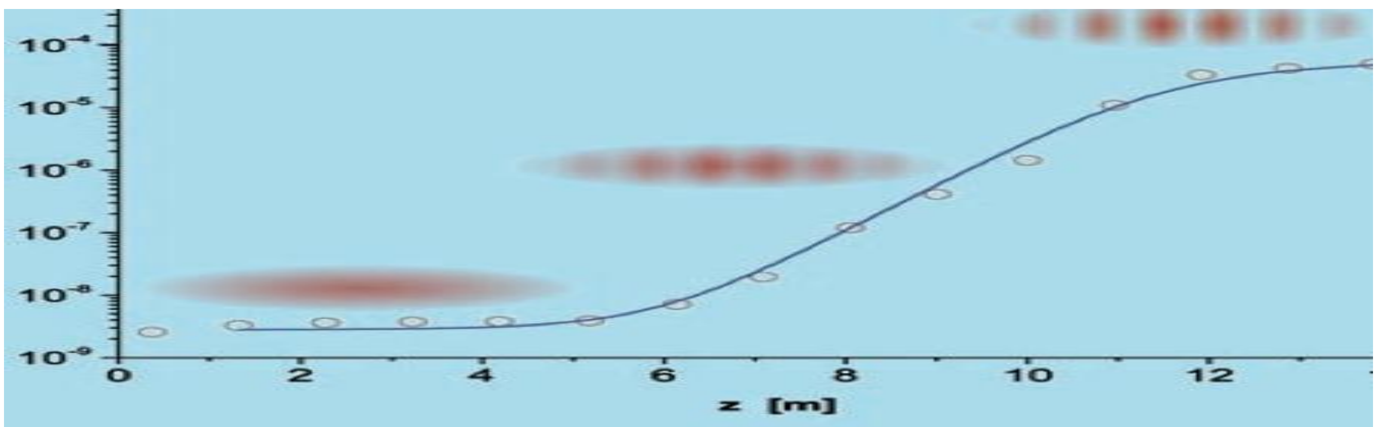
A tour of the LCLS

LCLS from Above

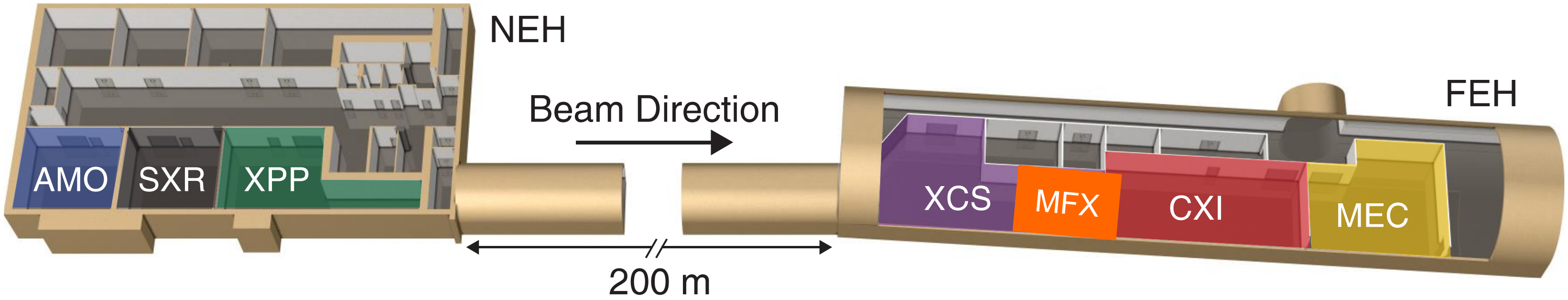
132 meters of FEL Undulator

Self Amplified Spontaneous Emission





LCLS Experimental Instruments



- 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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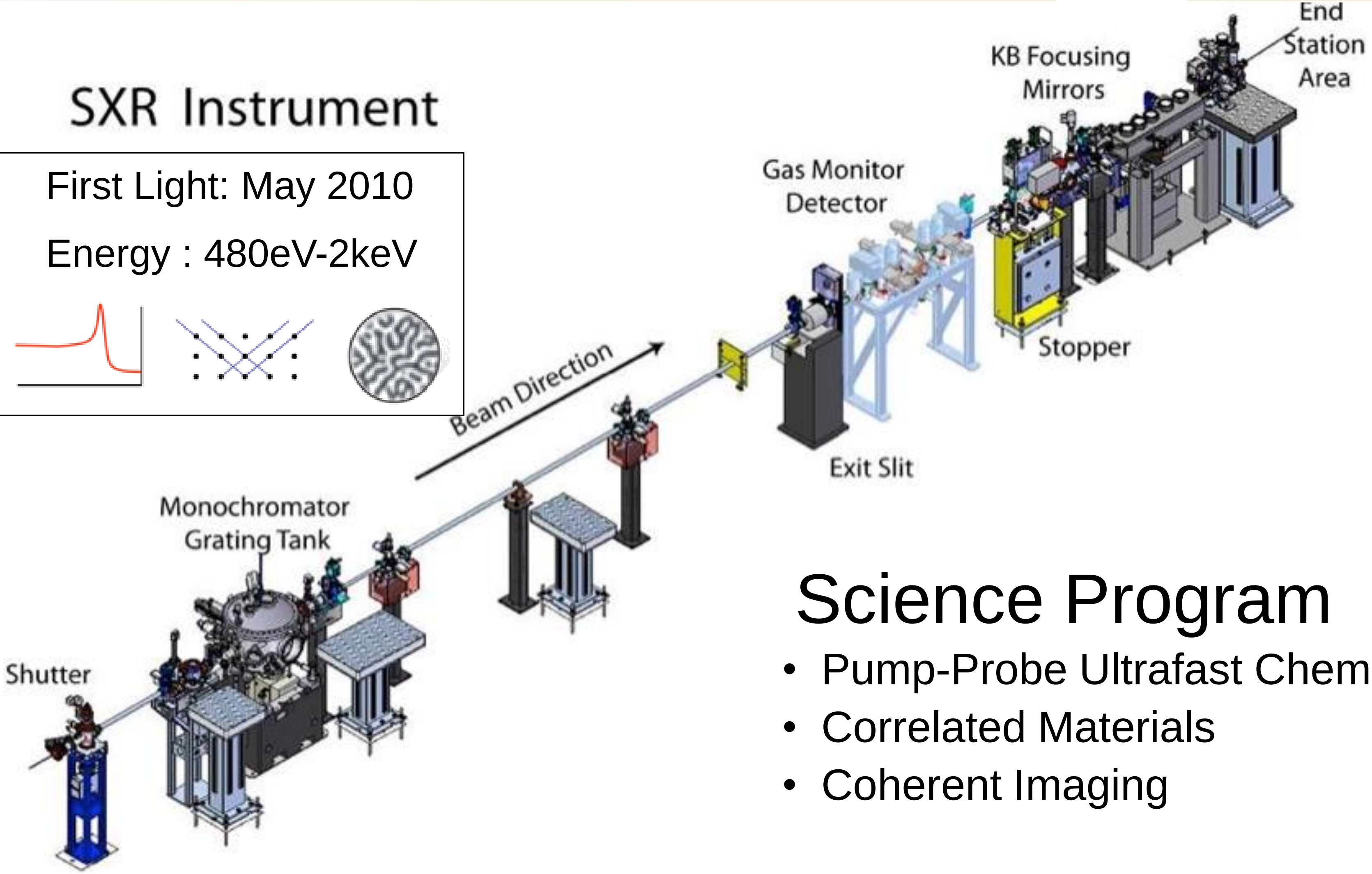
SXR Instrument

First Light: May 2010

Energy : 480eV-2keV

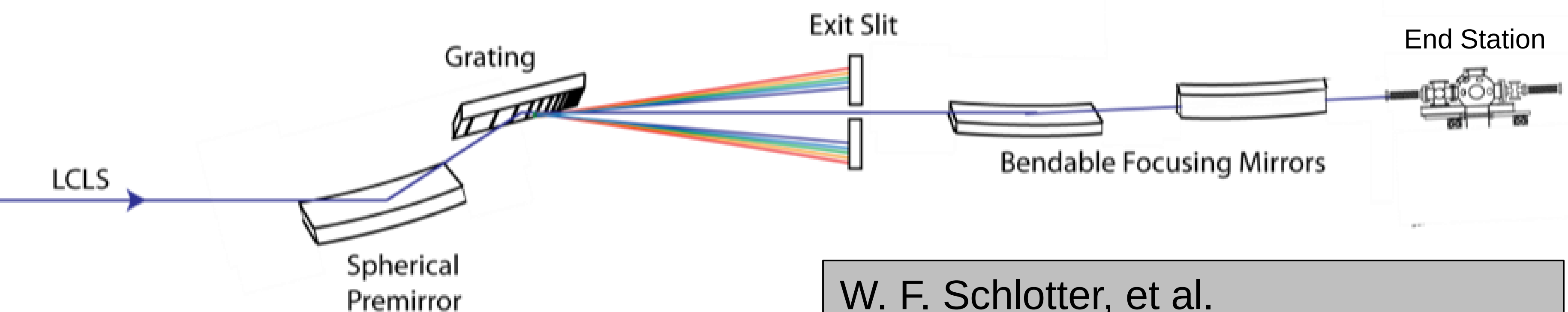


Science Program

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

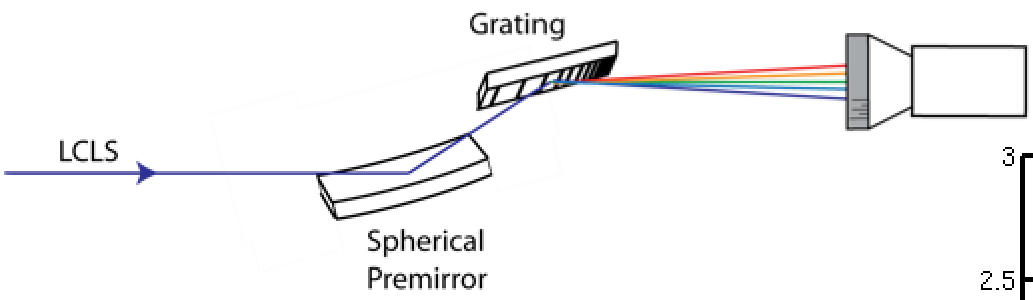
The SXR Instrument at LCLS

- Soft X-rays (250-2000eV)
- Pulse Energy 10^{12} photons/pulse
- Varied Line Spacing Plane Grating Mono
  - E/ΔE ~3000
- KB Focusing
  - 10x10μm is nominal focus spot size.
  - Bendable KB allows for spot sizes up to ~1mm
- Optical Pump Laser (Synchronizable with x-rays to ~280 fs)

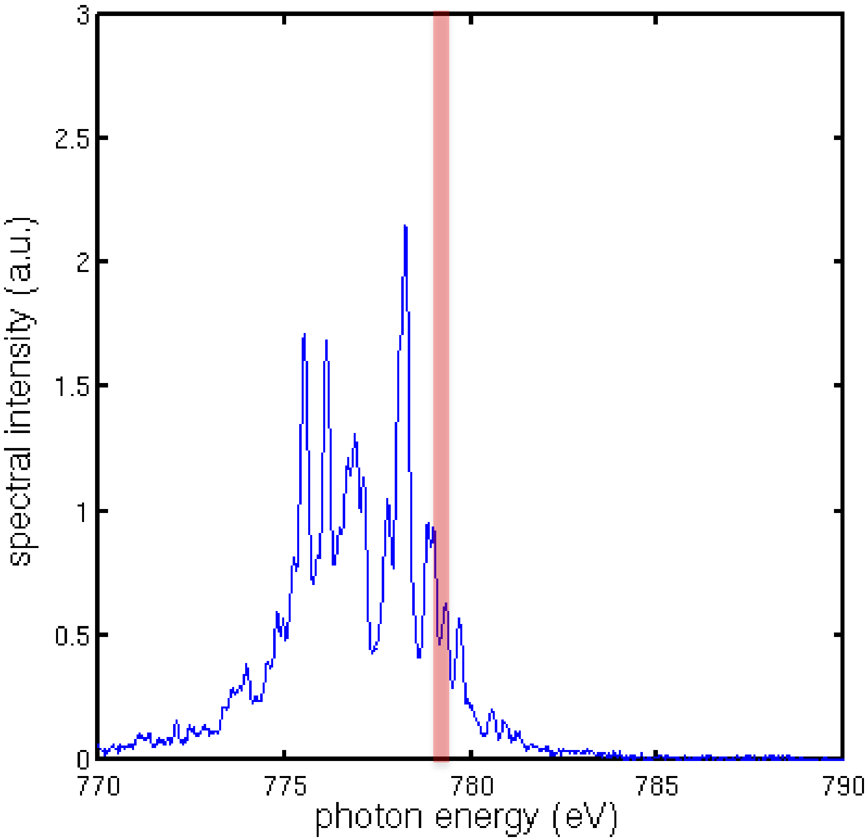


W. F. Schlotter, et al.
Rev. Sci. Instrum. 83, 043107 (2012)

Spectrometer + Monochromator

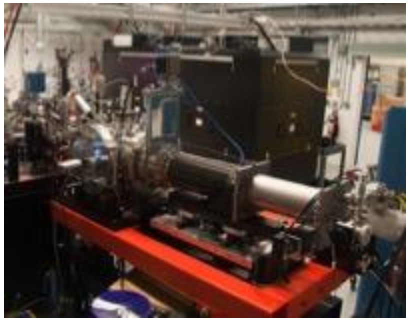


Spectrometer allows for an entire spectrum to be acquired from a single FEL pulse



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

Commissioned SXR End Stations

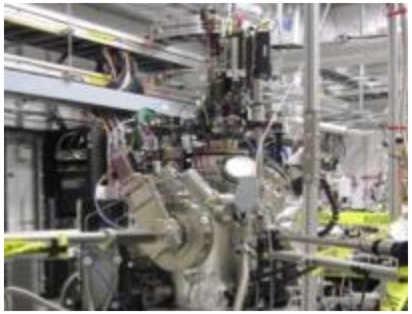


Resonant Coherent Imaging Station

Coherent scattering from fixed target and structured samples

Surface Science End Station

Ultrafast surface chemistry



Soft X-ray Scattering

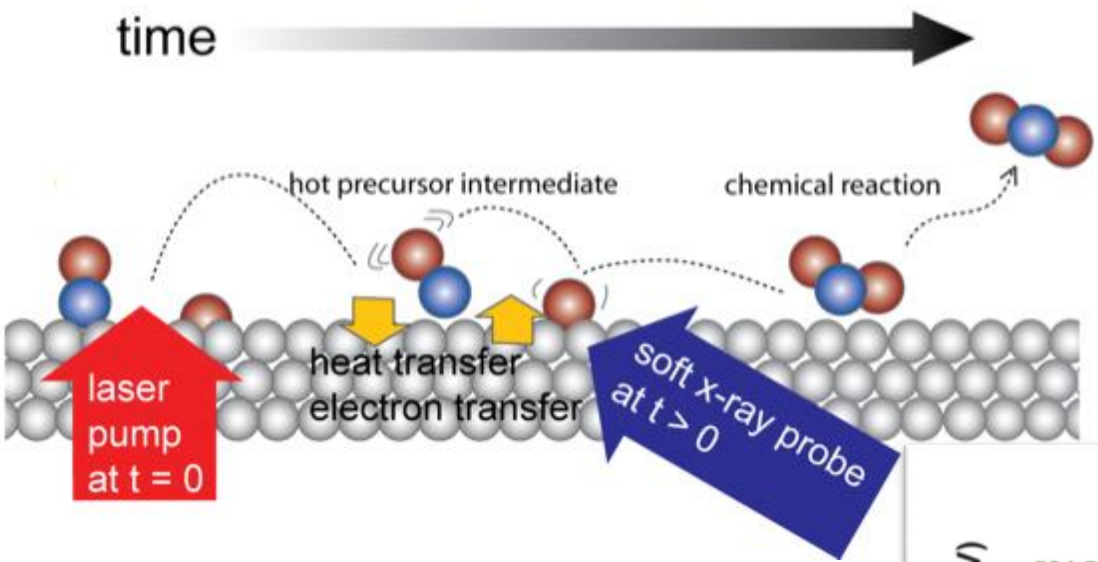
Resonant and non-resonant diffraction

Liquid Jet End Station

Photochemistry in solution

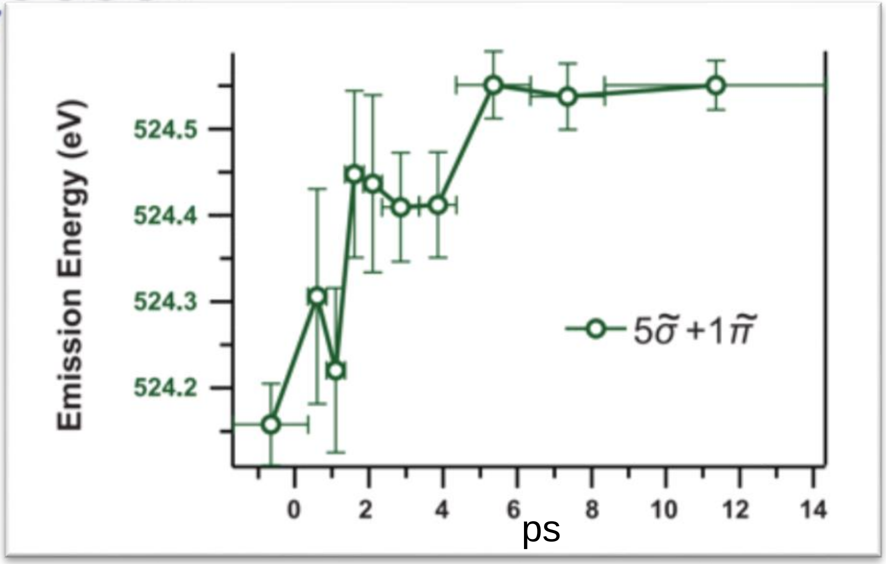
Watching surface bonds break in real-time at LCLS:

Transient weakly bound state observed in desorption process



Bond formation of carbon monoxide on a ruthenium substrate

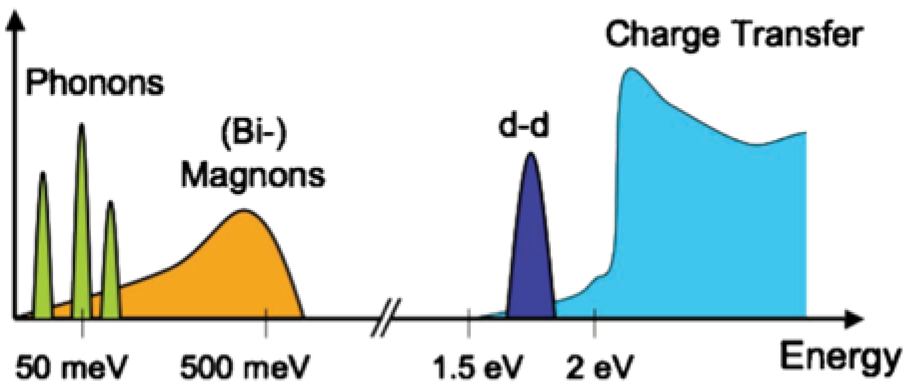
Electronic structure changes consistent with a weakening of the CO interaction with the substrate but without notable desorption.



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

What can be done with X-ray Emission

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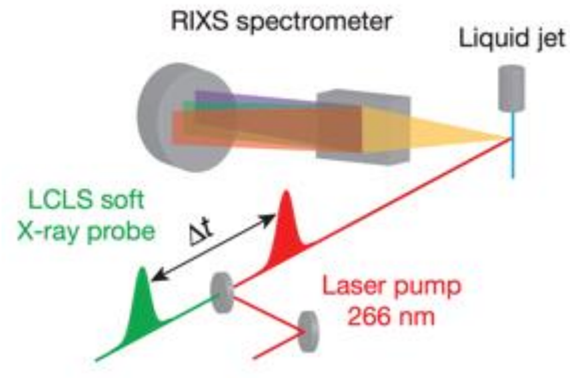
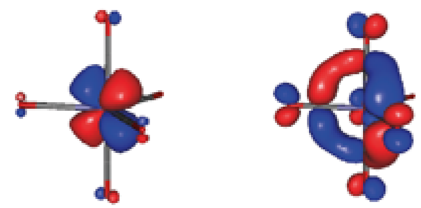
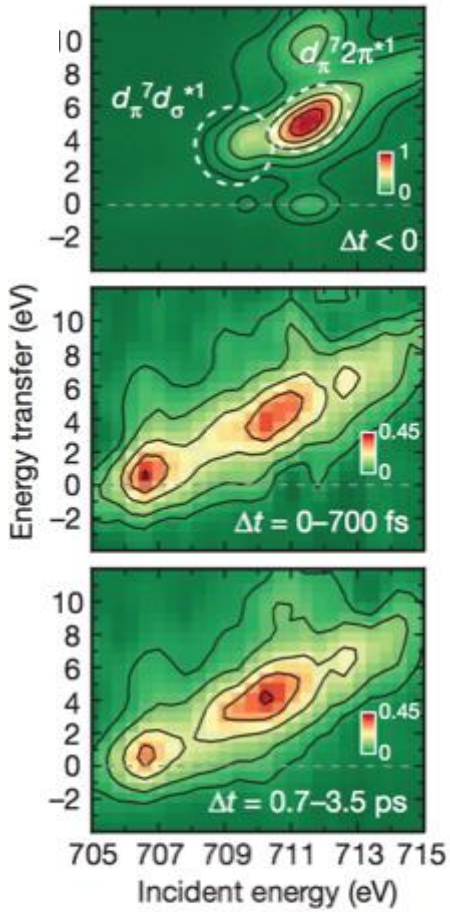
- Soft X-ray RIXS maps molecular orbitals & their evolution
- Element-specific: transition-metals & ligands
- Local chemical structure & bonding
- Current limitations:
  - Sensitivity - observe only large molecular changes, in model complexes, at high concentrations
  - Limited time information - average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

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



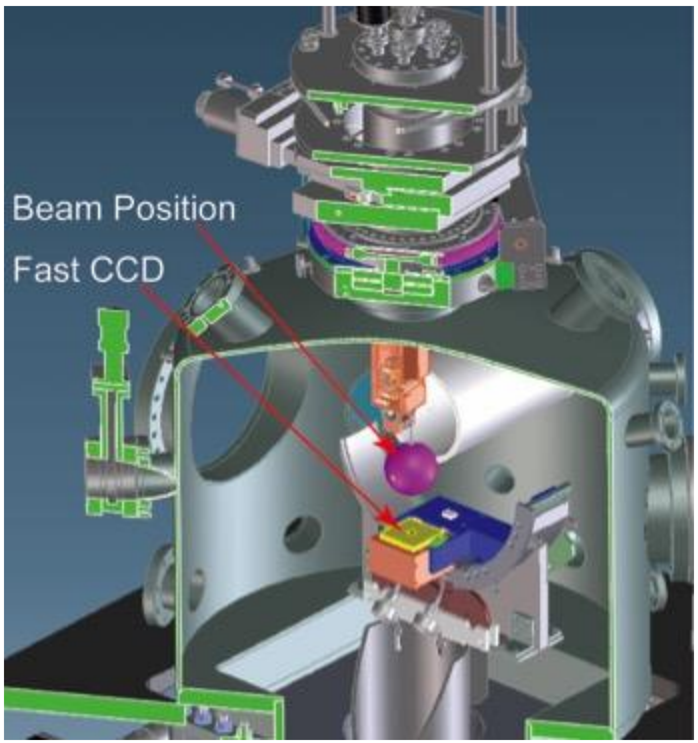


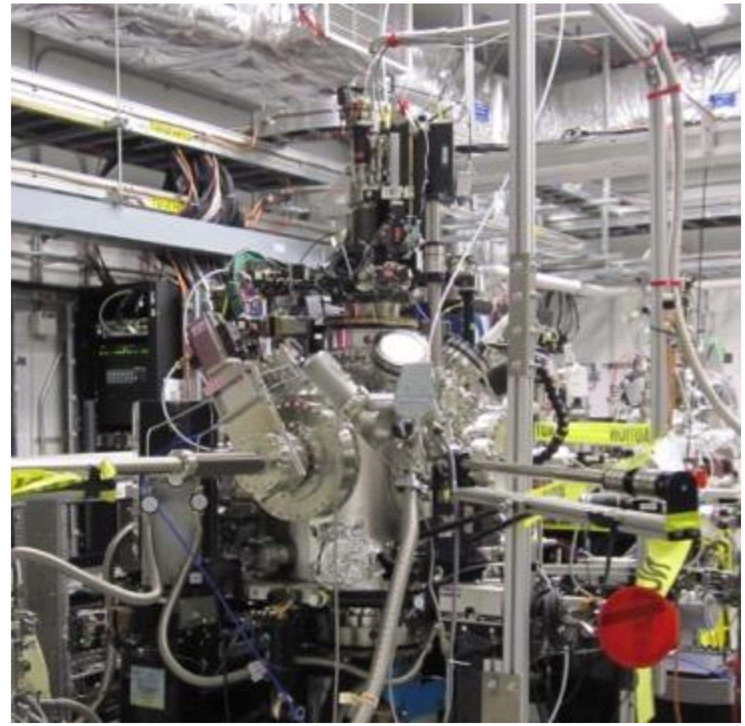


P. Wernet et al., *Nature*, 520, **78** (2015)

Resonant Soft X-ray Scattering

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





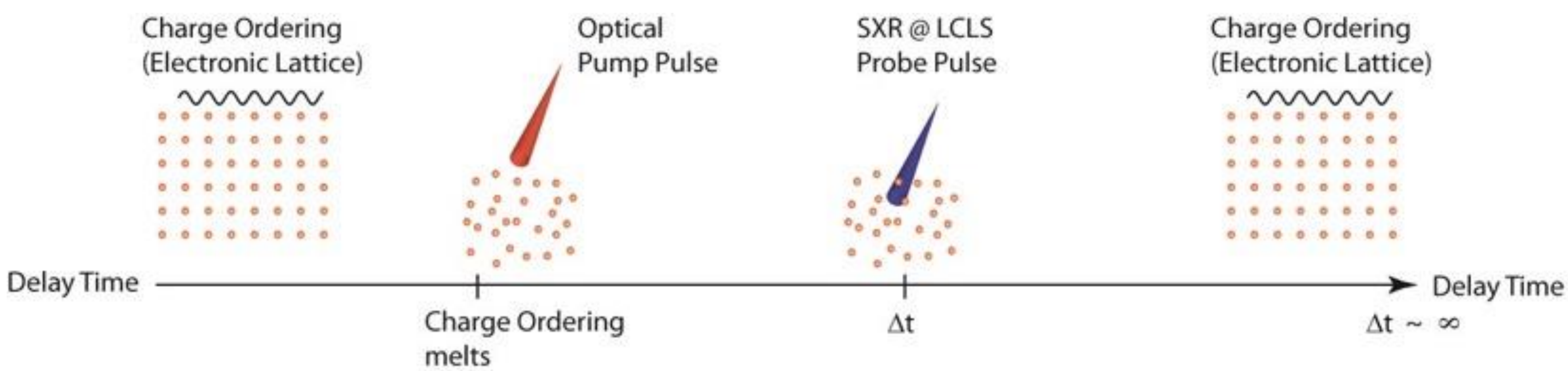
Fast CCD

In-vacuum diffractometer

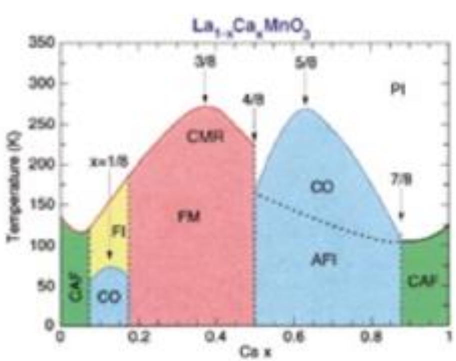
Cryo sample environment

D. Doering, *et al.*, Rev. Sci. Inst., **82**, 073303 (2011);

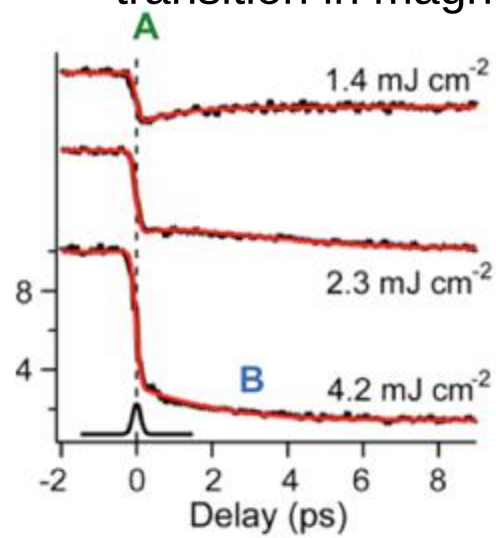
Probing Long Range Order with Soft X-rays

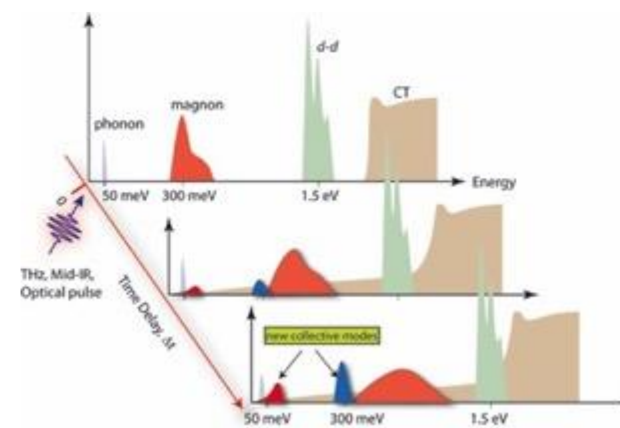


Correlate:
charge-order insulating and ferromagnetic metallic phases



Laser induced phase transition in magnetite

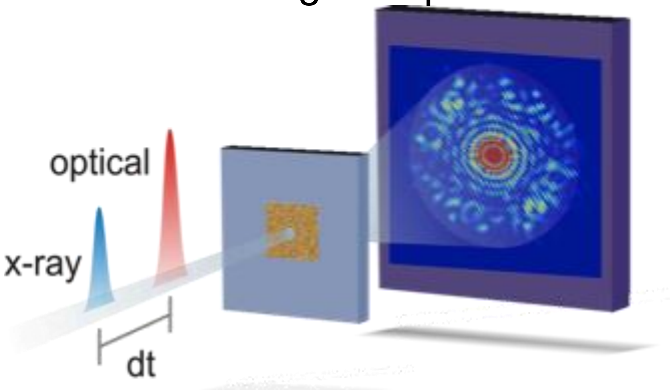


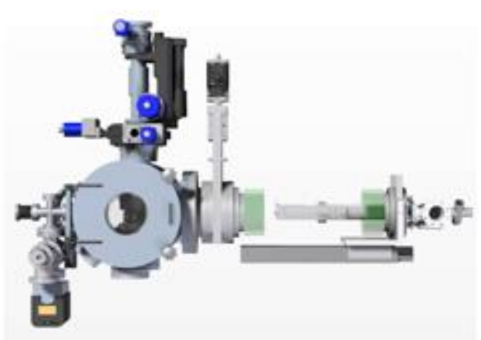


Wei-Sheng Lee

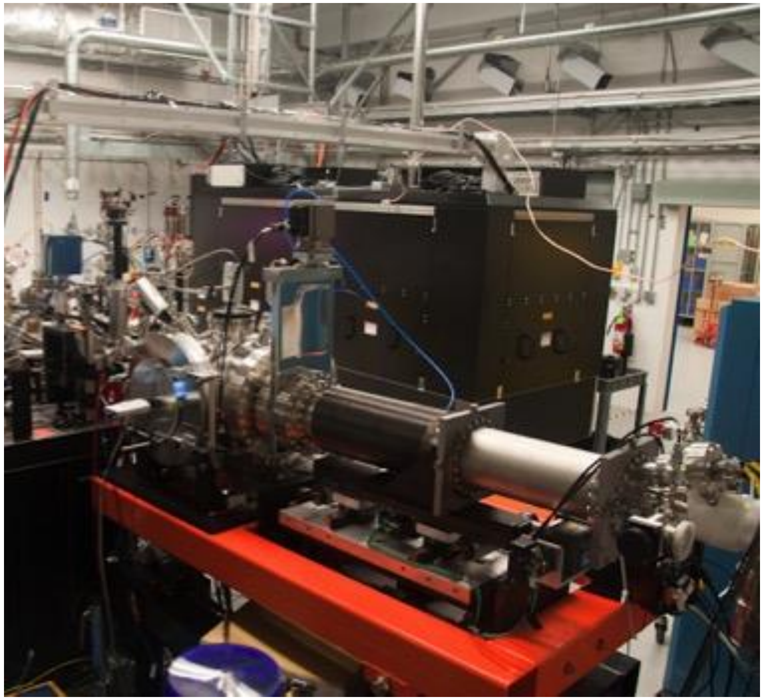
Resonant Coherent Imaging

- **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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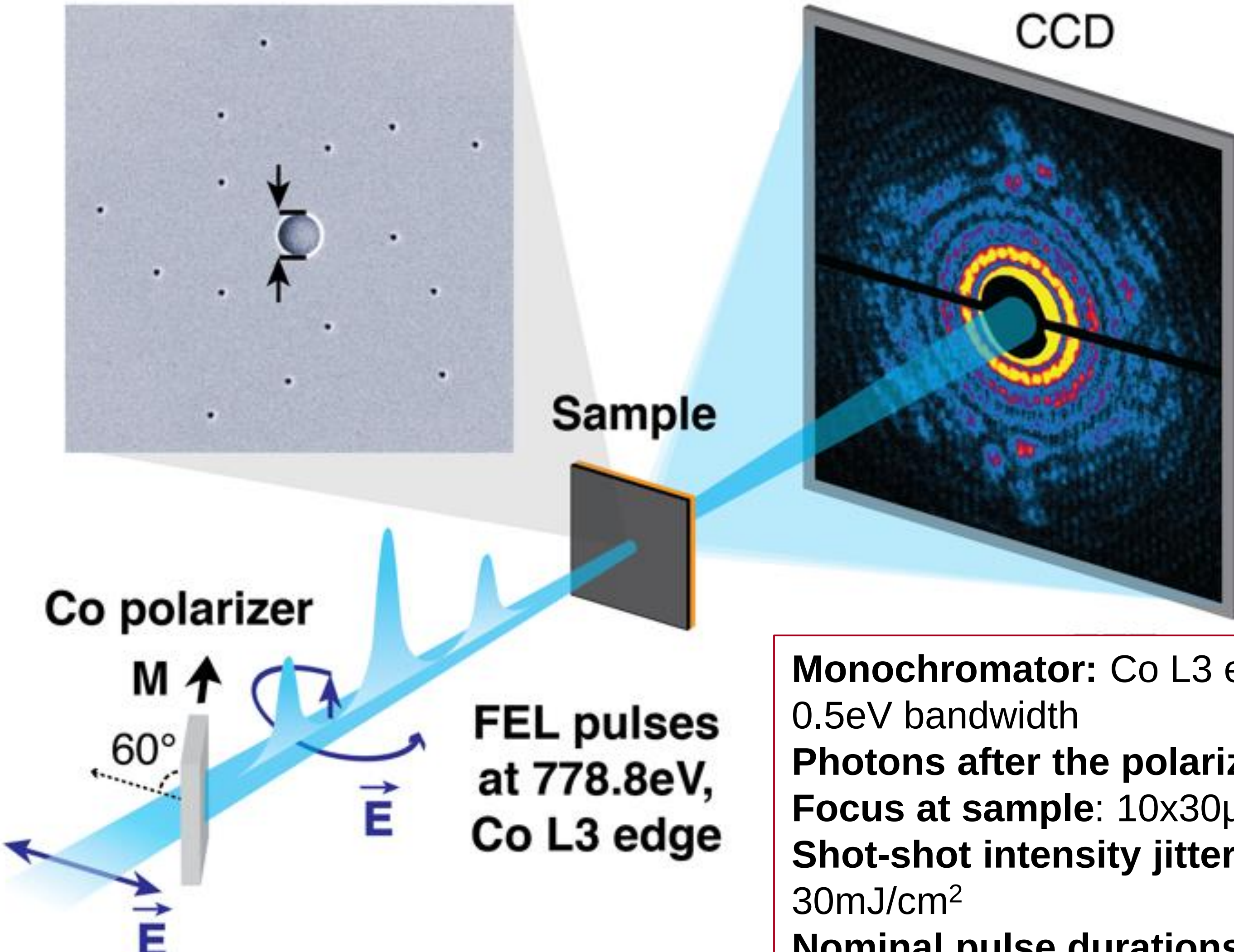
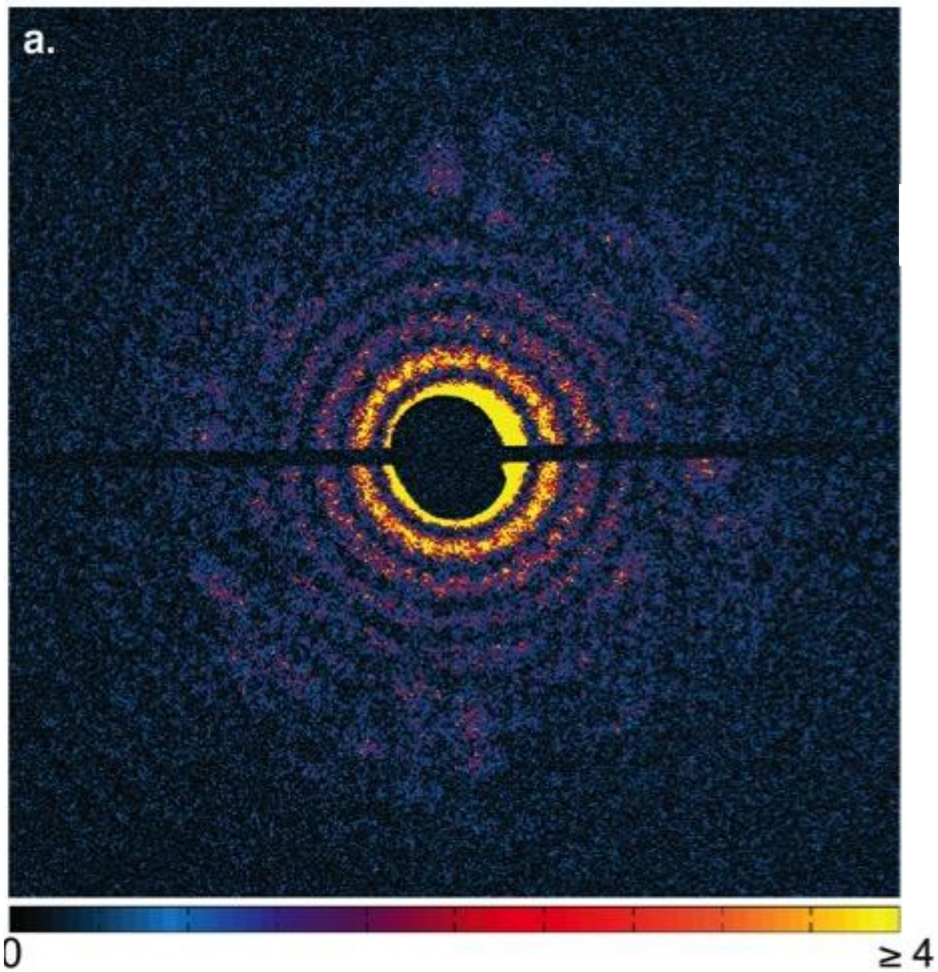


T. Wang, et al, *PRL* 108, 267403 (2012)

Monochromator: Co L3 edge (778.8eV) with 0.5eV bandwidth
Photons after the polarizer: $1x10^9$ photons/pulse
Focus at sample: $10x30µm^2$
Shot-shot intensity jitter: Fluences from 1 to $30mJ/cm^2$
Nominal pulse durations: 80fs and 360fs

80 fs single-shot Hologram with spatial multiplexing

SLAC

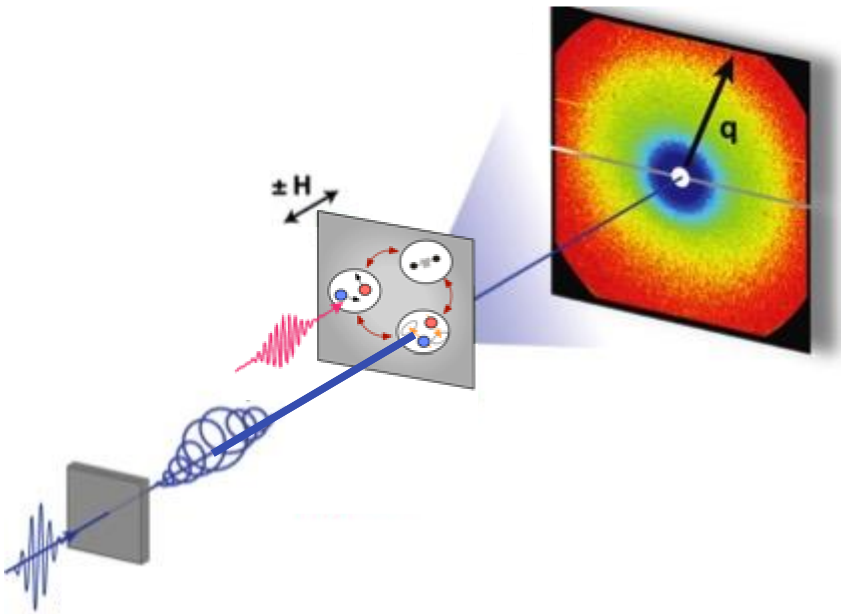


1.5 x 10^5 detected photons in hologram

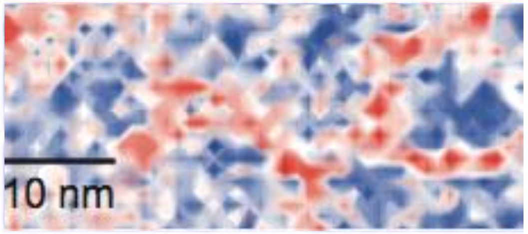
T. Wang, et al, *PRL* 108, 267403 (2012)

Optical control of nanoscale spin order in $Fe_{66}Co_{10}Gd_{24}$

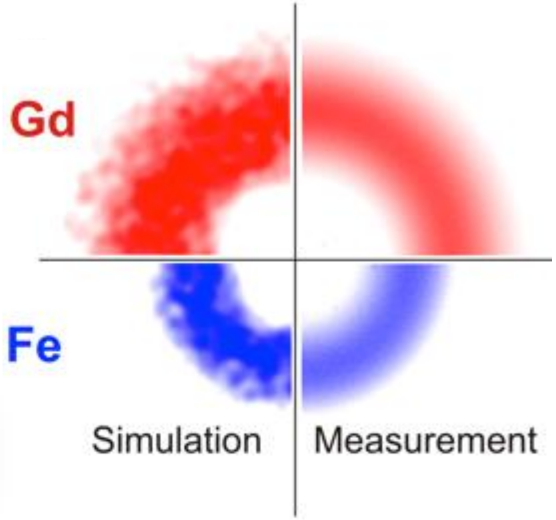
Diffraction



Real Space



Scattering Pattern

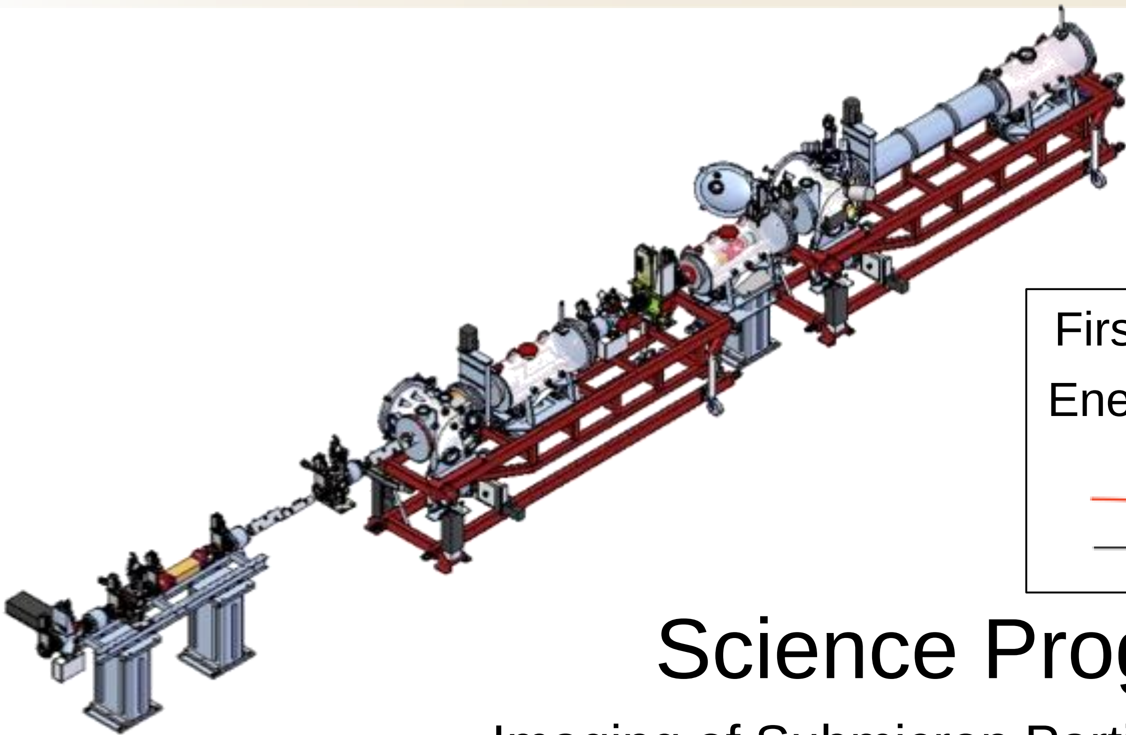


C. Graves, et al., Nature Materials, **12** 293 (2013)

CXI

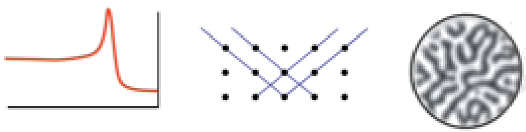
Coherent X-ray Imaging

CXI: Coherent X-ray Imaging



First Light: December 2010

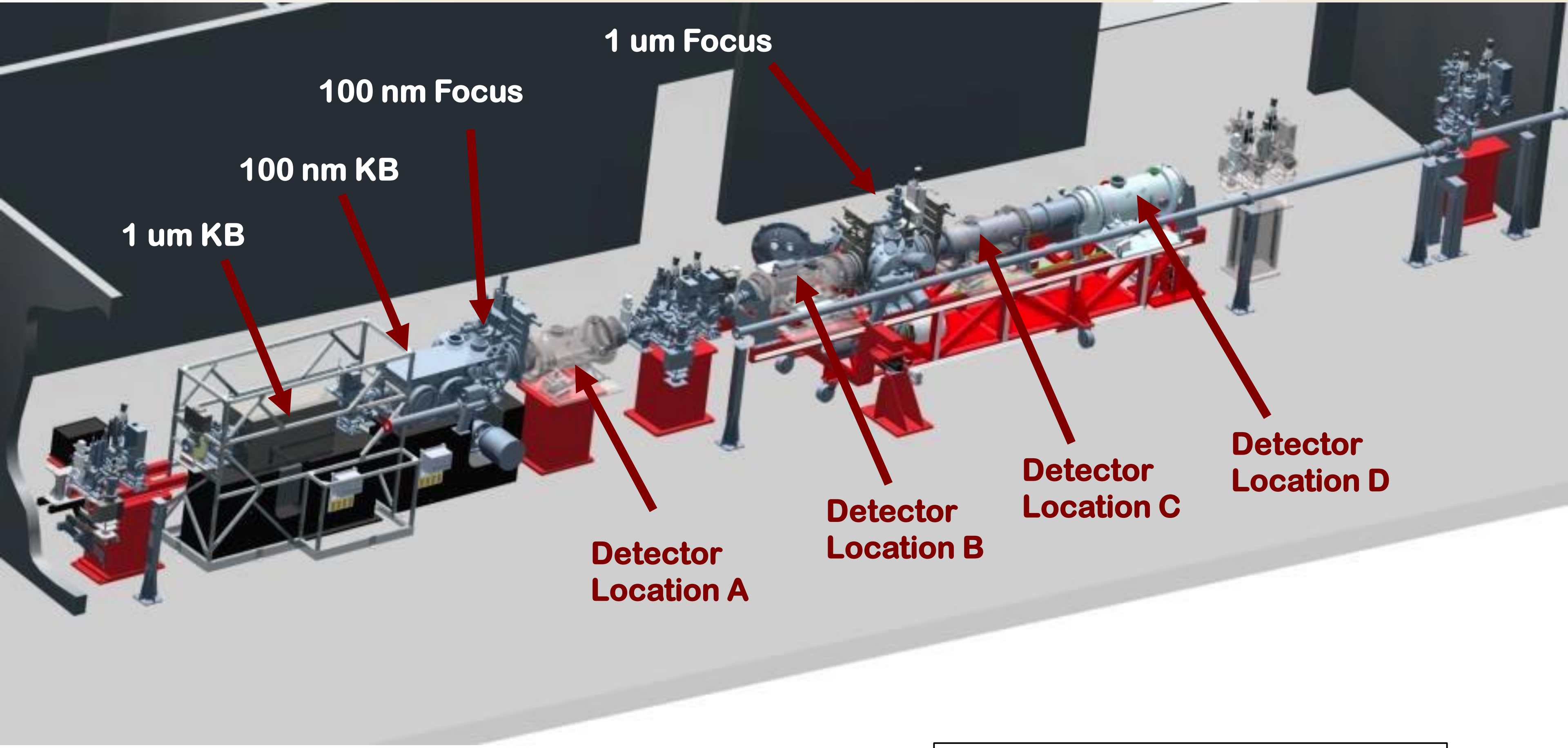
Energy : 4 keV-10 keV



Science Program

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

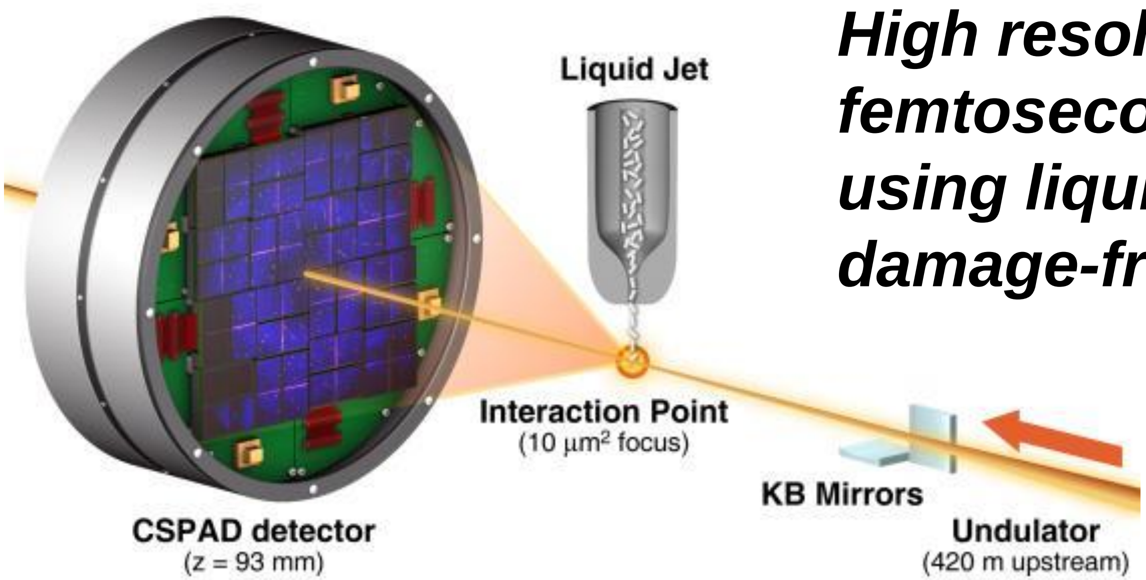
CXI Instrumentation Description



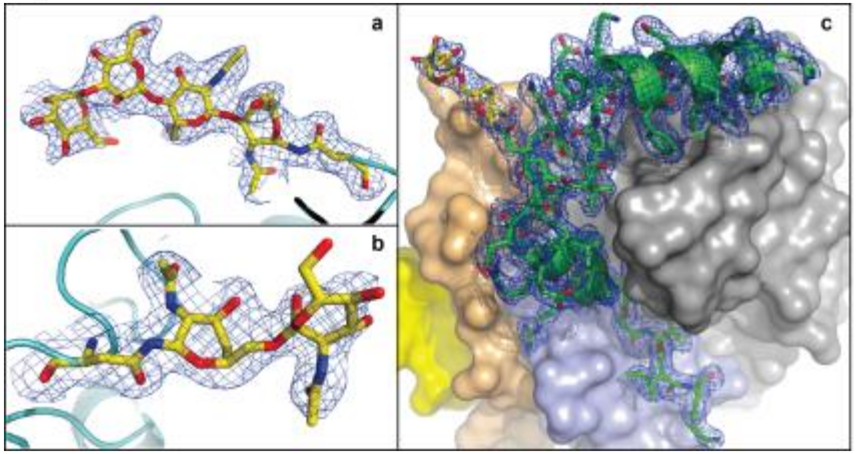
First Light: December 2010

Energy : 4 keV-10 keV

Nano-crystalography at LCLS



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



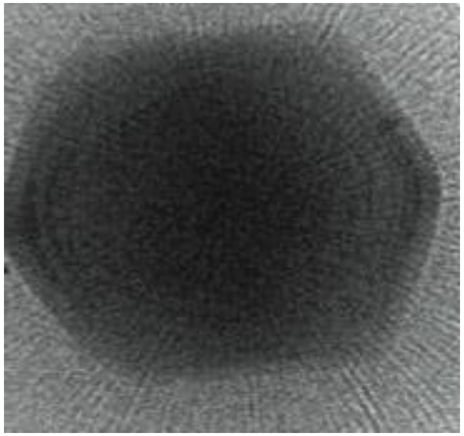
In-vivo grown crystal of a glyco-protein

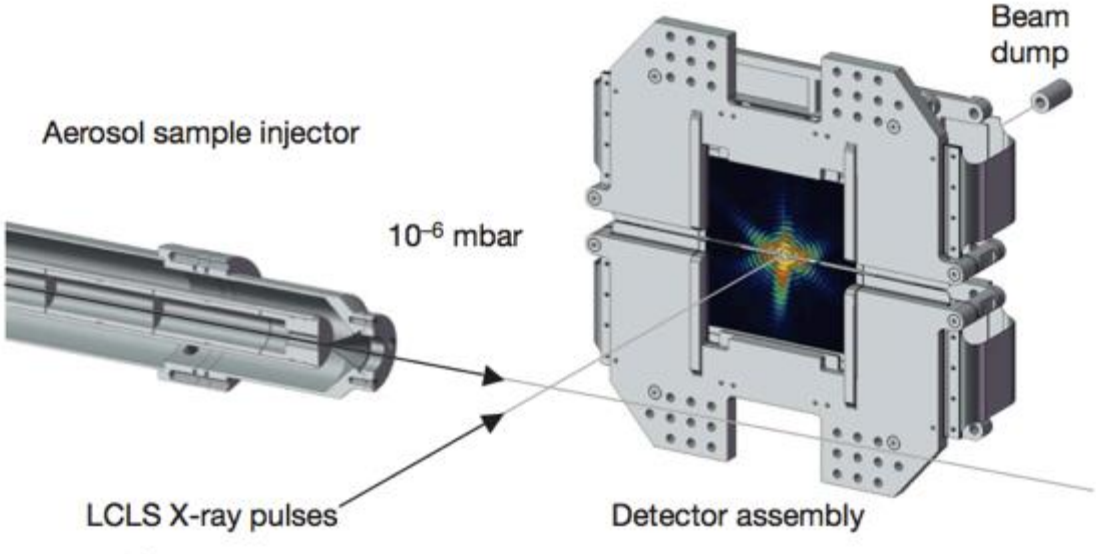
Redecke *et al*, Science **339**, 6116 (2012)

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

Imaging of the Mimi Virus

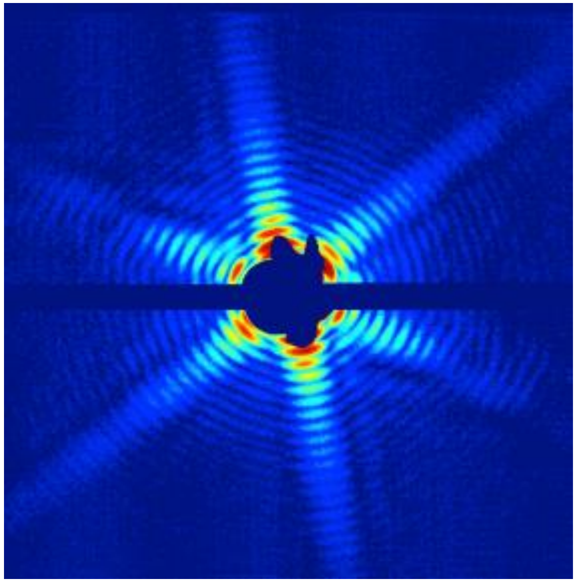
- Mimi Virus is the largest known virus (0.5 um)
- It is too big for cryo-electron microscopy
- It does not crystalize because of dense outer fibrils

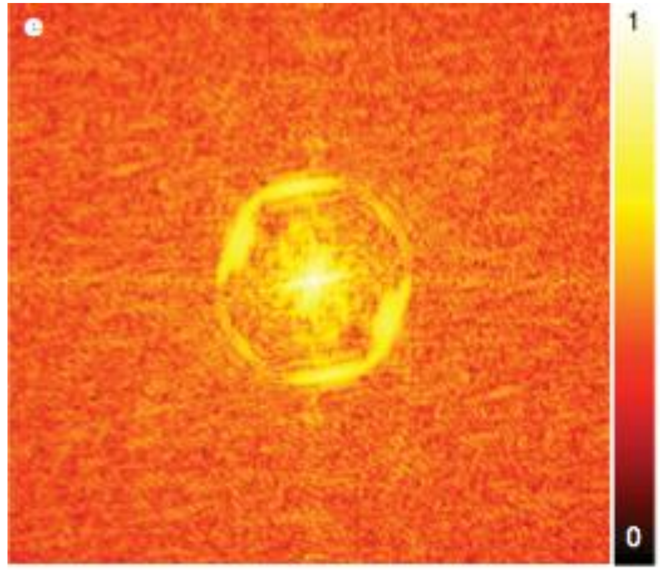


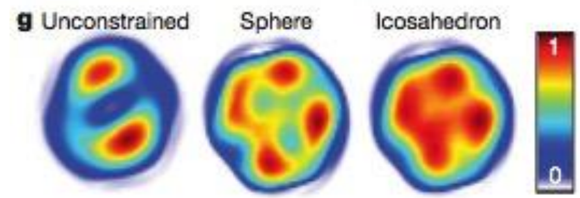


M. Seibert, et al, *Nature* 470, p78 (2011)

Mimi Virus







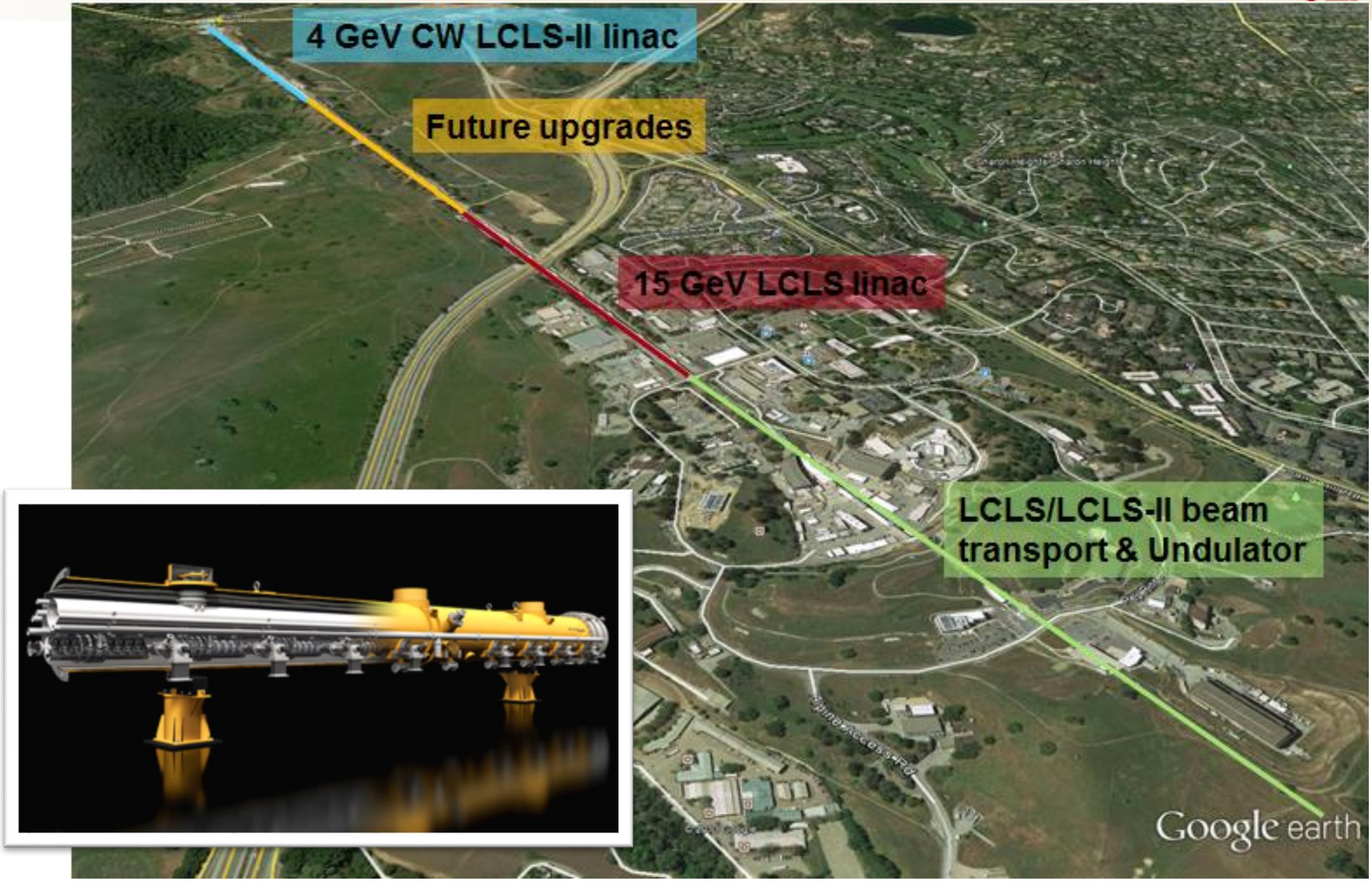
Energy: 1.8 keV
Photons per pulse: 1.2×10^{12} photons/pulse
Focus at sample: 10 µm
Nominal pulse durations: 70 fs

Demonstrates that short XFEL pulses can outrun sample damage

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

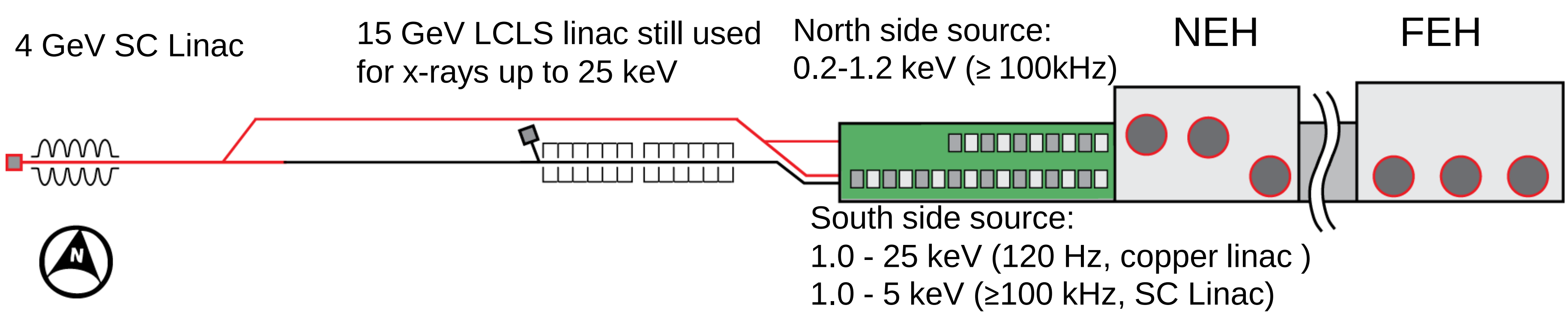
LCLS-II

LCLS-II Upgrade
Use 1st km of SLAC linac tunnel for Super Conducting linac



LCLS-II Project Scope

Accelerator	**<u>Superconducting linac</u>**: 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)

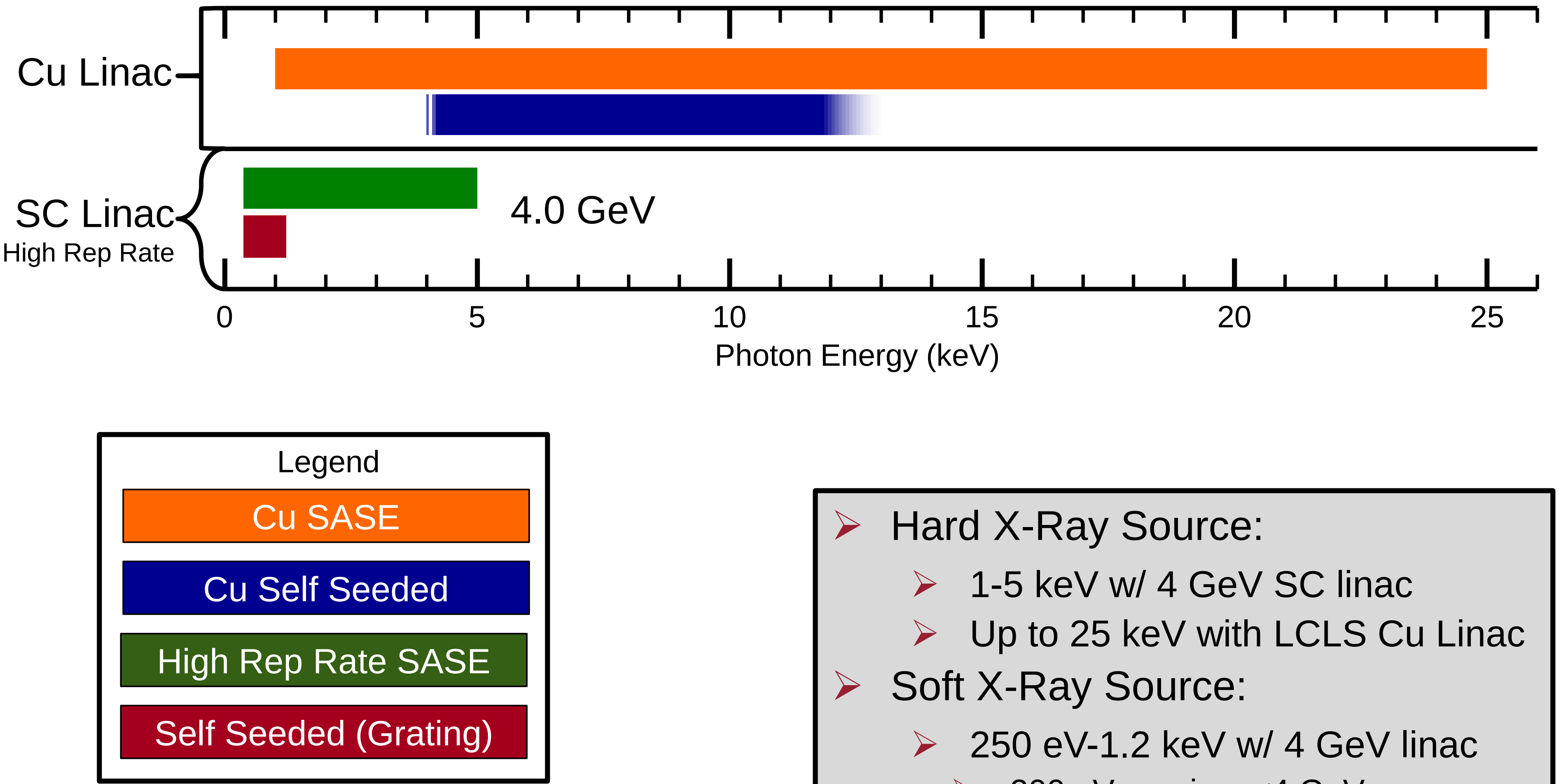


LCLS-II

	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

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

LCLS-II Operating Energy Range

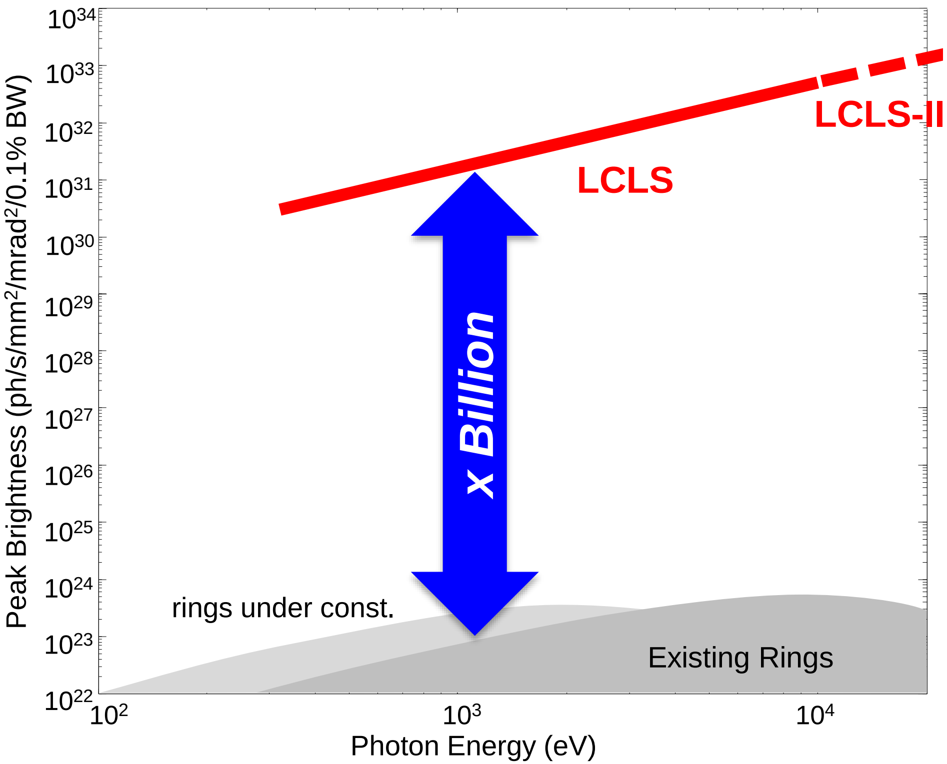


- Hard X-Ray Source:
  - 1-5 keV w/ 4 GeV SC linac
  - Up to 25 keV with LCLS Cu Linac
- Soft X-Ray Source:
  - 250 eV-1.2 keV w/ 4 GeV linac
    - 200 eV requires <4 GeV

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

- 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


Contributors

*corresponding author

LCLS Strategic Facility Document (July 2015)


LCLS STRATEGIC FACILITY DEVELOPMENT PLAN

July 2015

1

- 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

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

Linac Coherent Light Source: The first five years

Christoph Bostedt,* Sébastien Boutet, David M. Fritz, Zhirong Huang, Hae Ja Lee, Henrik T. Lemke,† Aymeric Robert, William F. Schlotter, Joshua J. Turner, and Garth J. Williams‡

SLAC National Accelerator Laboratory, 2575 Sand Hill Road, Menlo Park, California 94025, USA

(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.

DOI: 10.1103/RevModPhys.88.015007

CONTENTS

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†Current address: Paul Scherrer Institut, CH-5232 Villigen, Switzerland.
‡Current address: Brookhaven National Laboratory, PO Box 5000, Upton, NY 11973, USA.

- 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 a 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

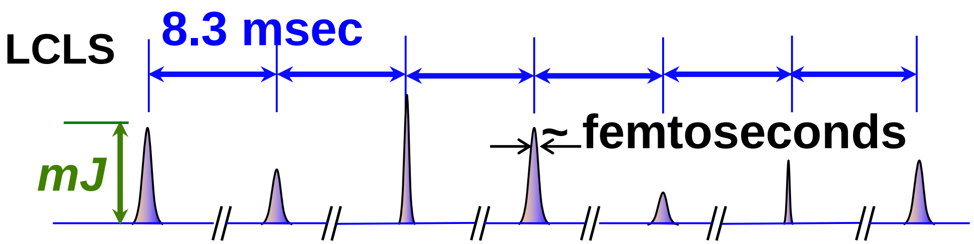
The Linac Coherent Light Source (LCLS), SLAC National Accelerator Laboratory, is supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Contract No. DE-AC02-76SF00515.

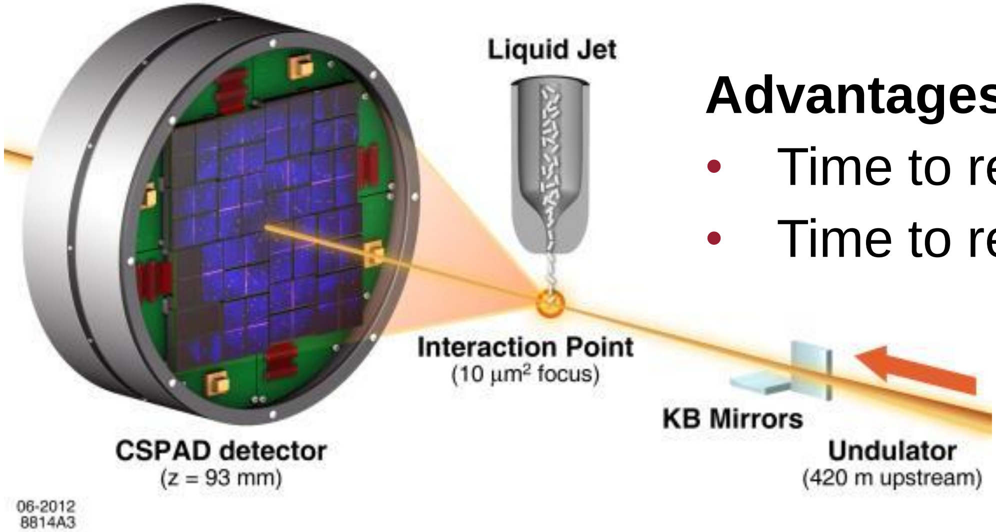
END
Backup Slides

How we detect x-rays at LCLS?

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



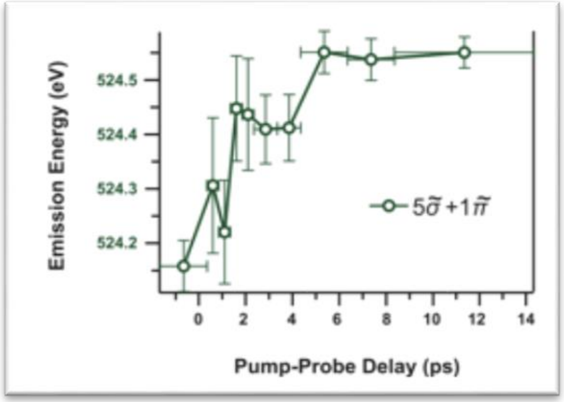


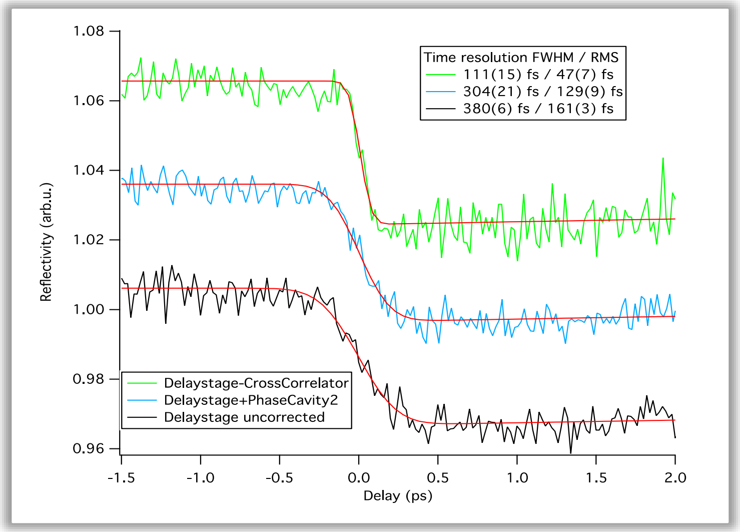
Advantages of single shot mode

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

Limitations to single shot data collection at 120Hz

- 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

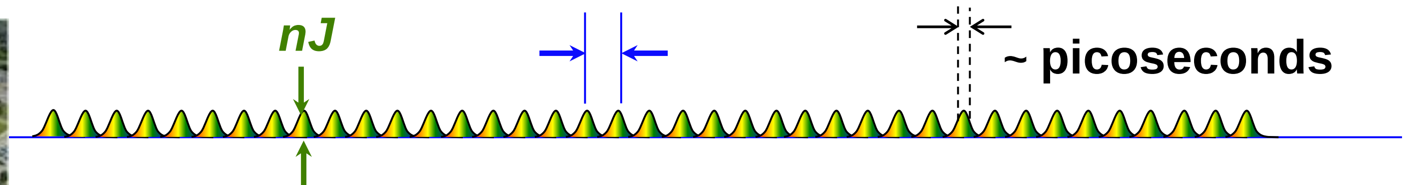




Accumulation Data Collection

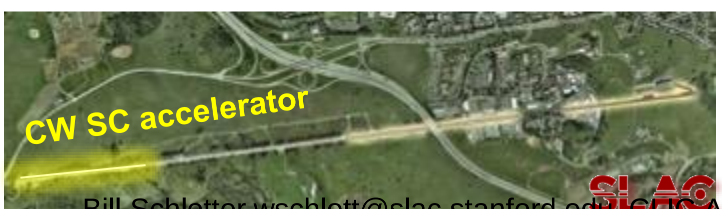
- To the extent each x-ray pulse is the same, we can accumulate the detected photons over many pulses
- But this is exactly how experiments are done at storage ring sources

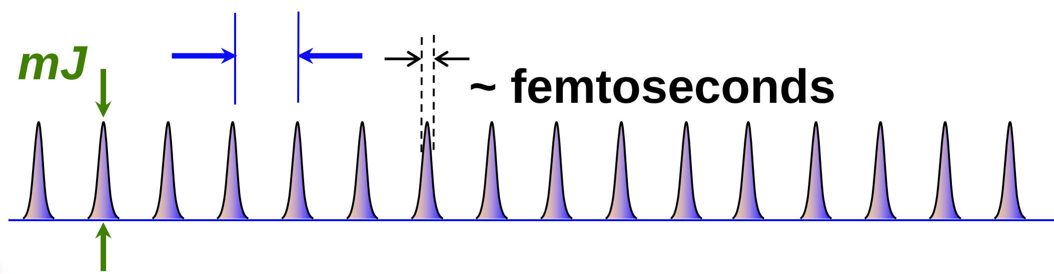
storage ring X-ray source (NSLS-II)

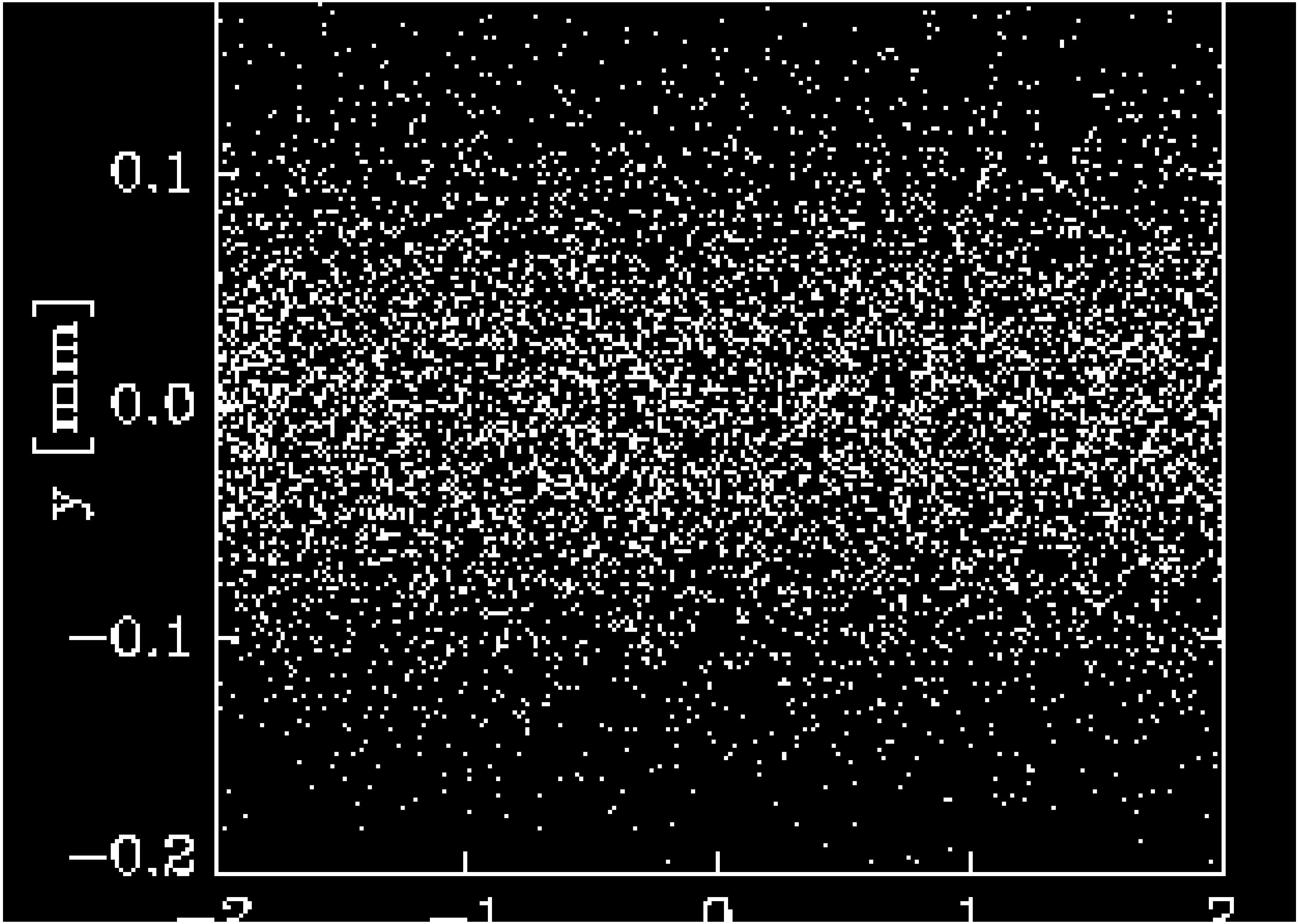


- Combining the mJ, fs pulses of an FEL with the stability of a storage will revolutionize x-ray experiments.

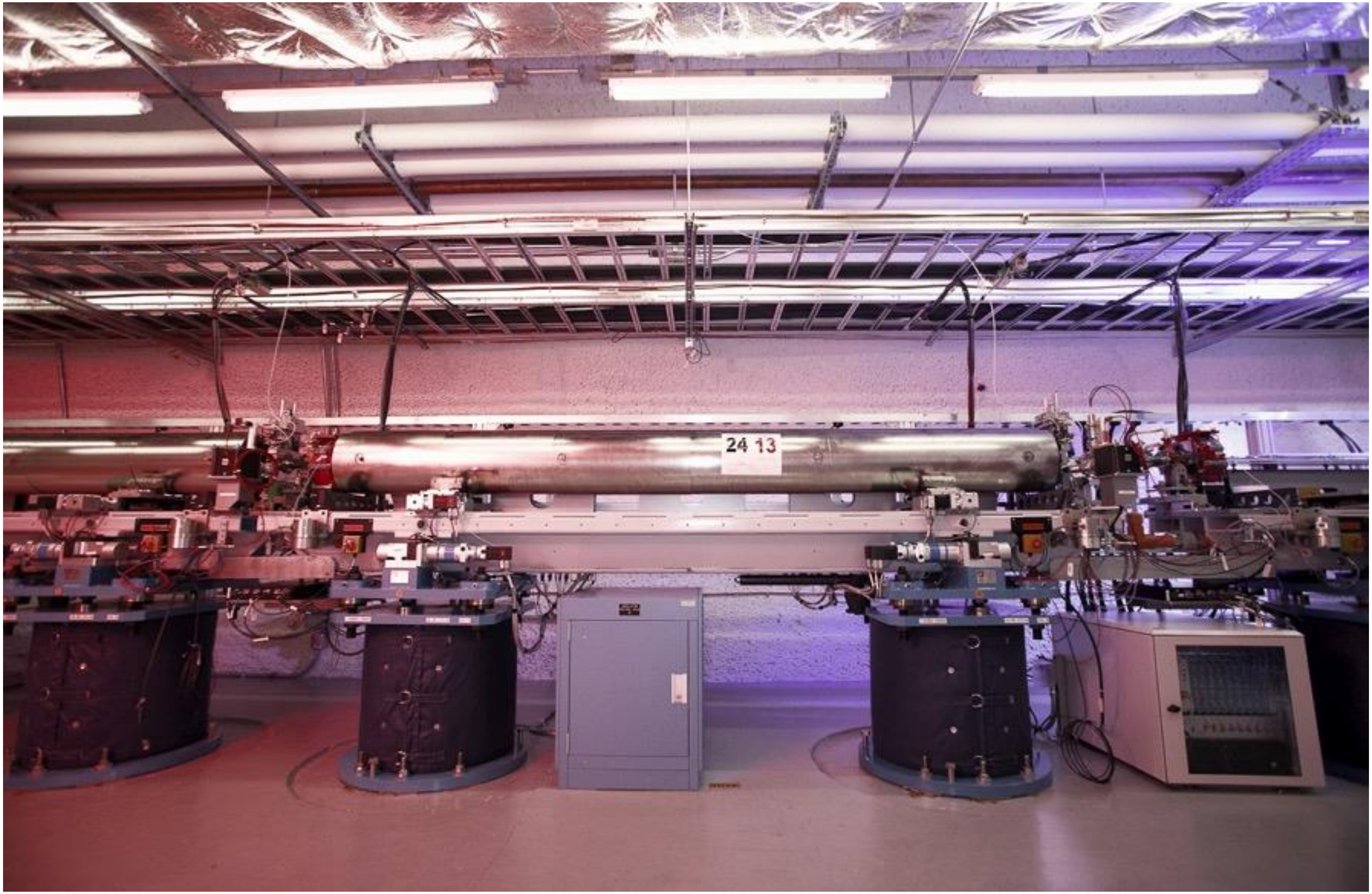
2019 LCLS-II



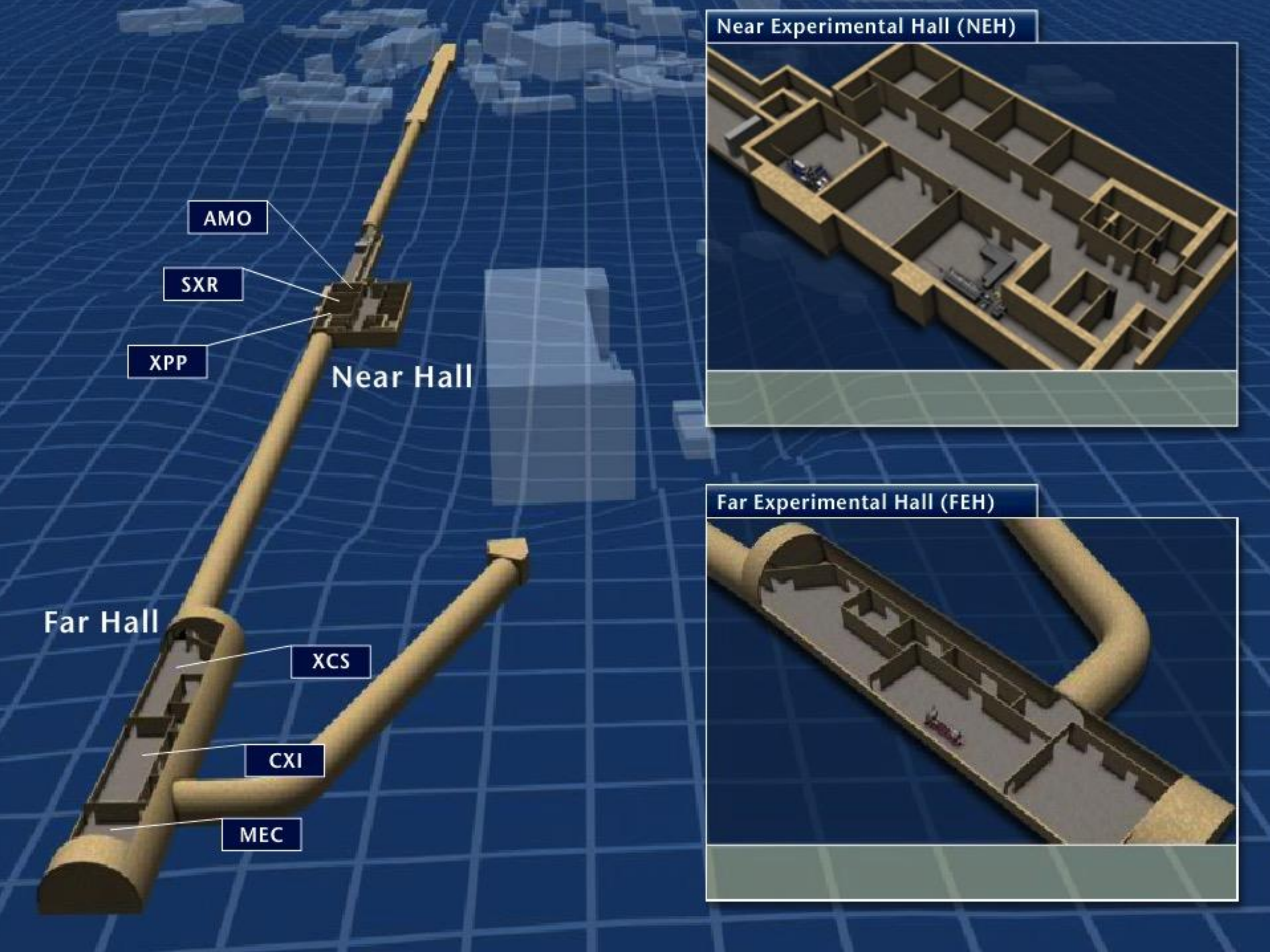




S. Reiche UCLA



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


AMO
SXR
XPP
Near Hall
Far Hall
XCS
CXI
MEC
Near Experimental Hall (NEH)
Far Experimental Hall (FEH)

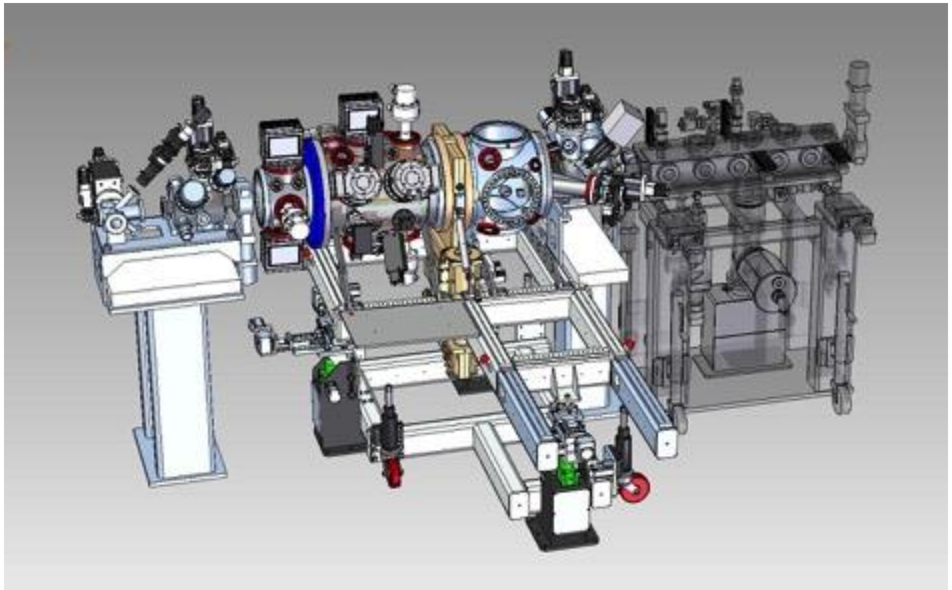
LCLS Instrument Backup AMO,XPP,MEC

AMO

Atomic, Molecular & Optical Physics

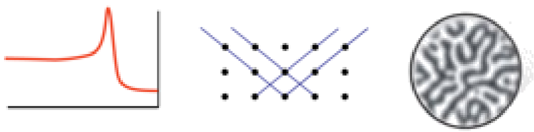
- Intense x-ray interactions with atoms and molecules
  - Non-linear x-ray interactions
- Ultrafast chemical dynamics of molecular gases
- Soft X-ray imaging
- Structure and evolution of clusters

AMO: Atomic, Molecular and Optical Physics



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

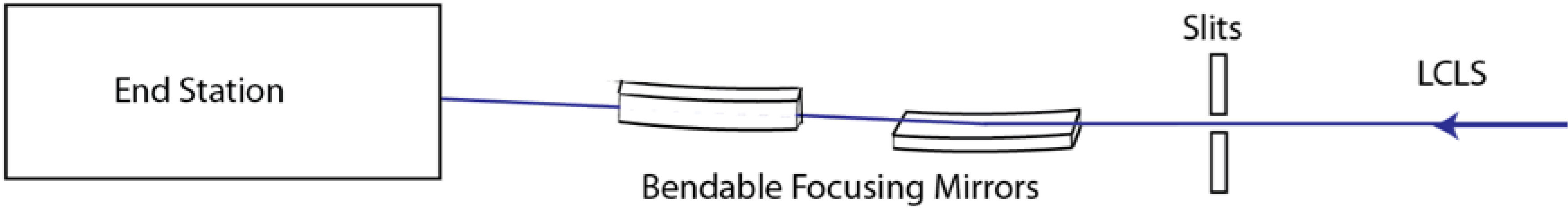
Machine and Instrumentation Development

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

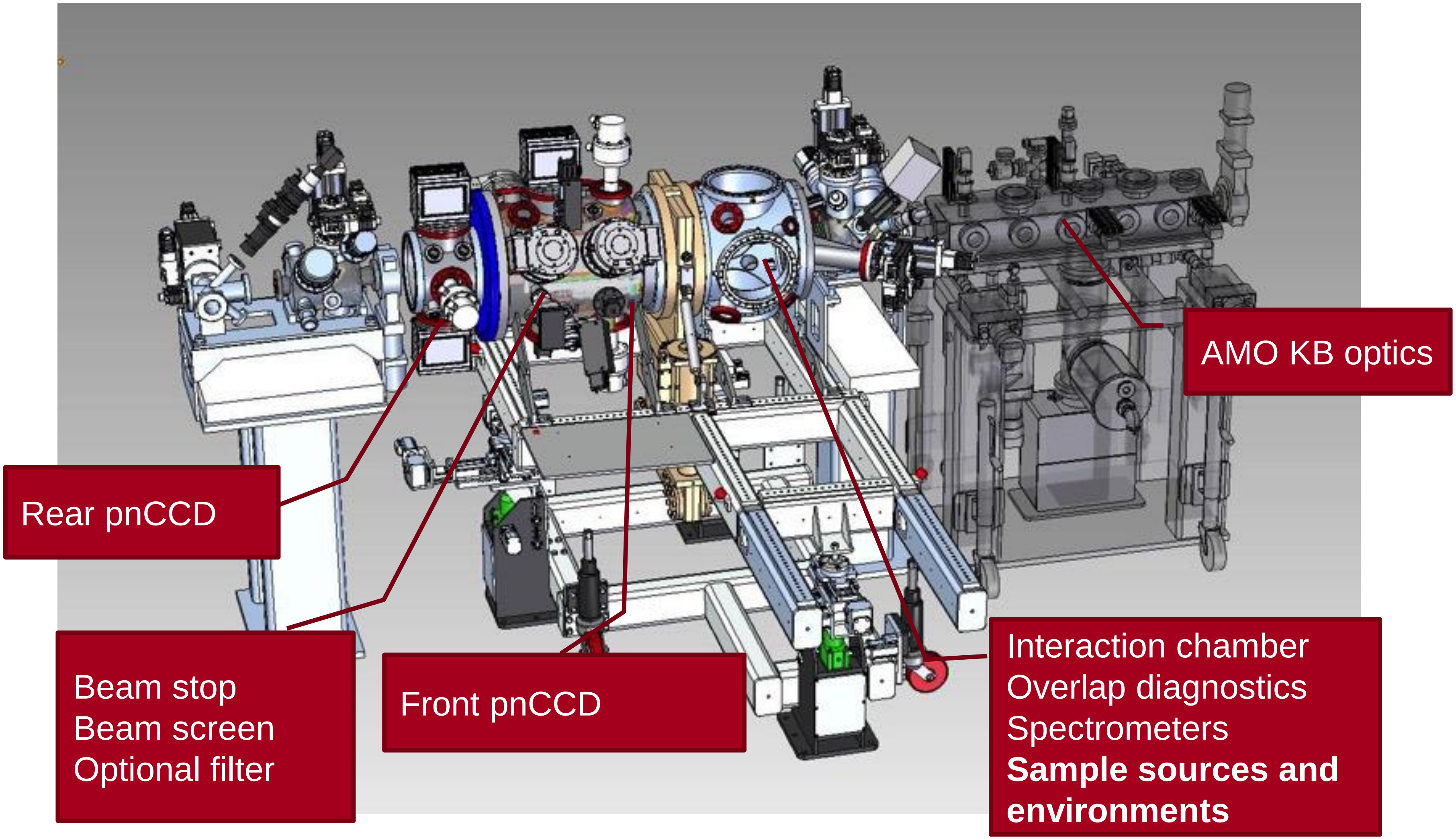
Read About First Experiments: http://wcm.aps.anl.gov/lcls/

The AMO Instrument

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



AMO Instrument: LAMP

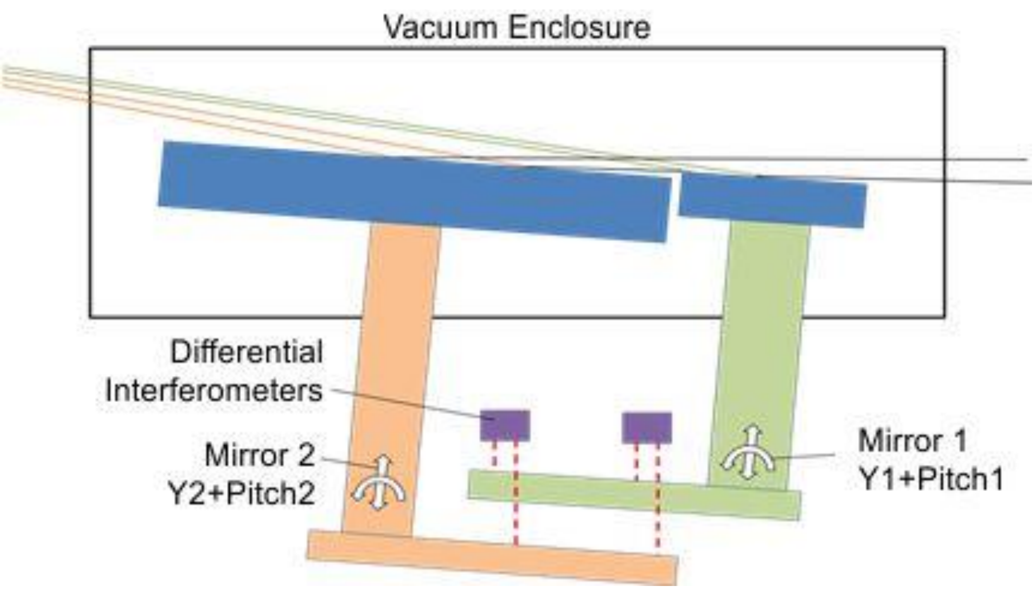


Collaboration with Nora Berrah (WMU)

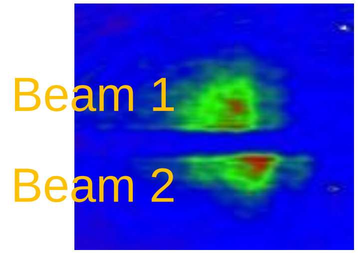
Inspired by CAMP

Split & Delay Basic Design Concept:

- 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



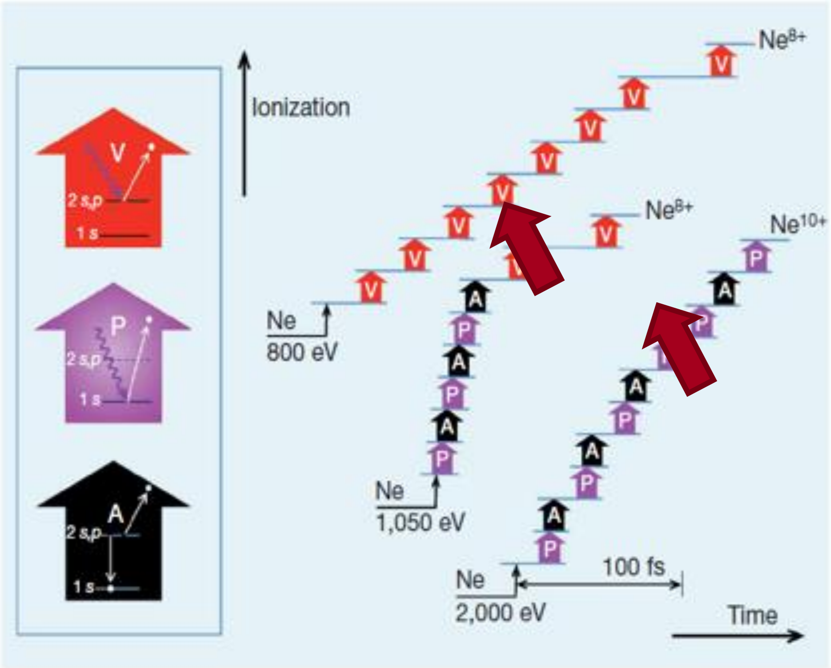
- Delay range 0 – 200 fsec
- Step size ~ fsec
- Available at all SXD beamlines



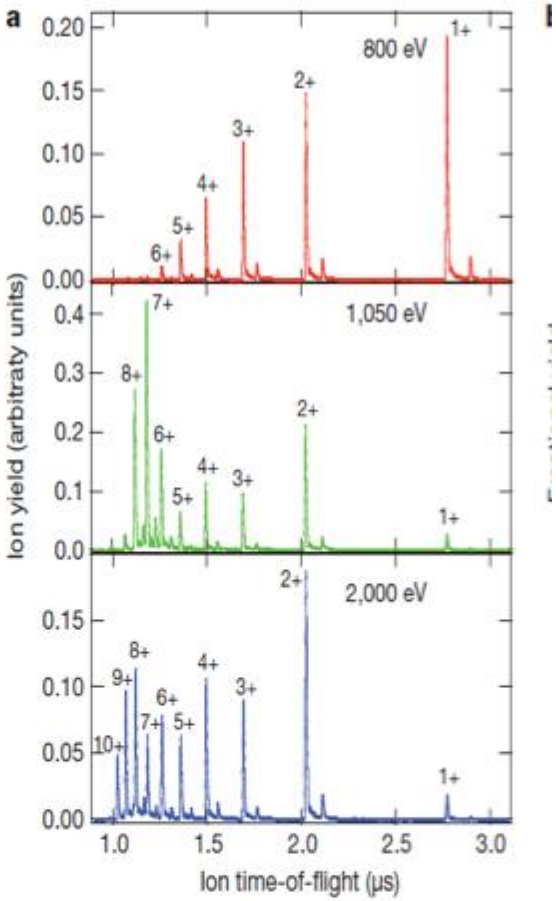
Schorb et al., Appl. Phys. Lett. (2012)

Collaboration with Nora Berrah (WMU)

Atomic photoionization in extreme x-ray pulses



Ne ion tof data



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

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

XPP

X-ray Pump Probe

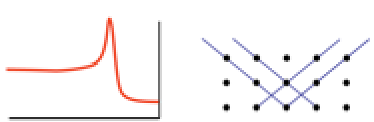
XPP: X-ray Pump Probe

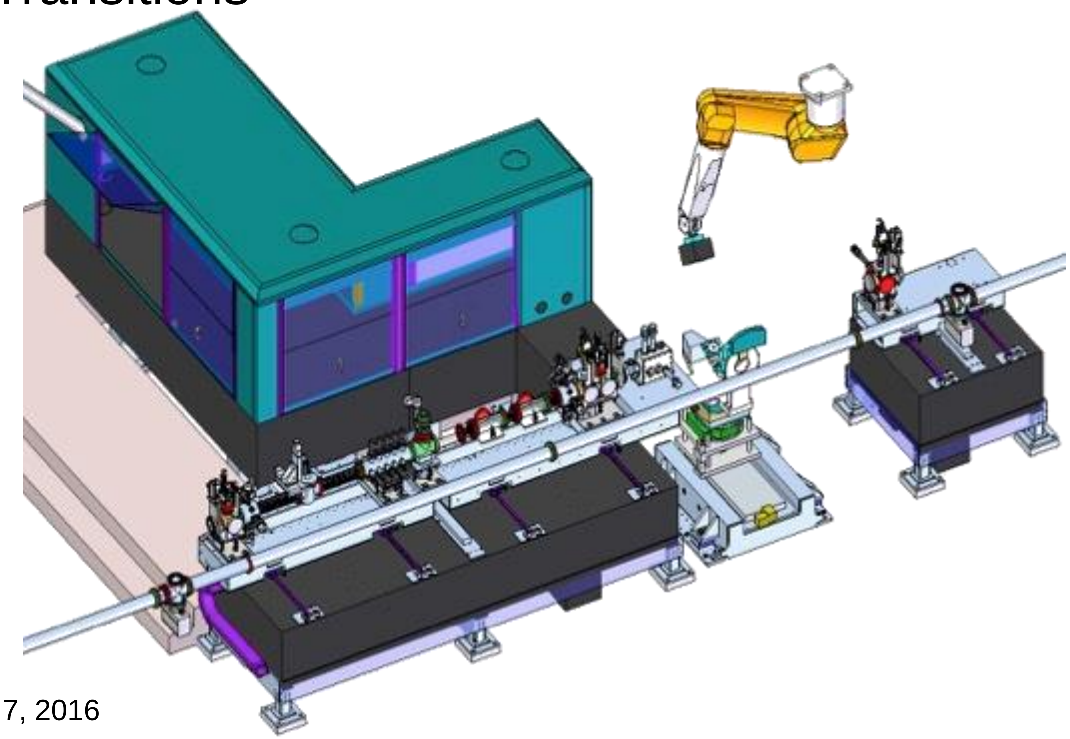
Science Program

- 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

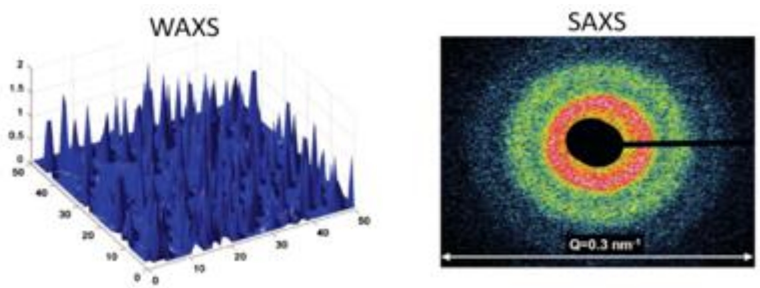




X-ray Pump Probe

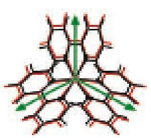
XPP: How do the atoms in materials and chemical complexes respond to excitations?

Structural and Temporal correlations

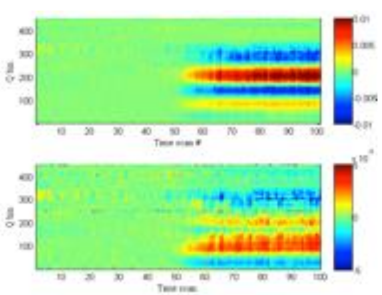


Gutt et al. (2012). Phys. Rev. Lett. **108**, 024801

Femtochemistry

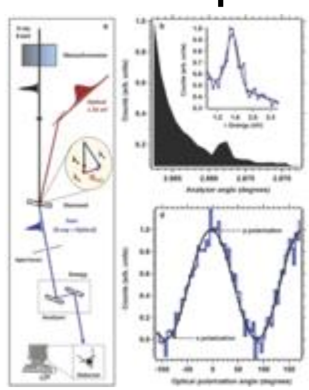


$Fe(bpy)_3$



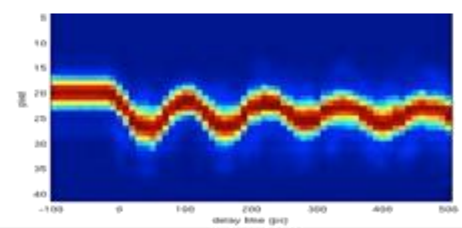
Haldrup et al. in preparation

Nonlinear optics



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

Nanostructures



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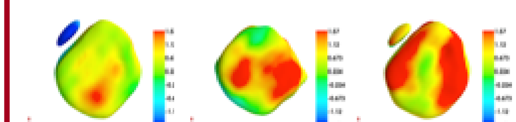
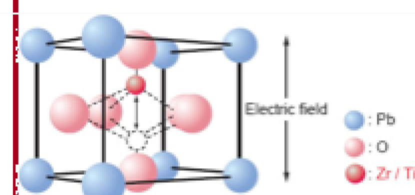
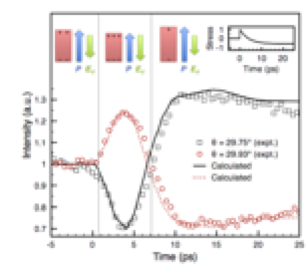


Clark et al., Science 341, 56 (2013)

Solid state physics





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

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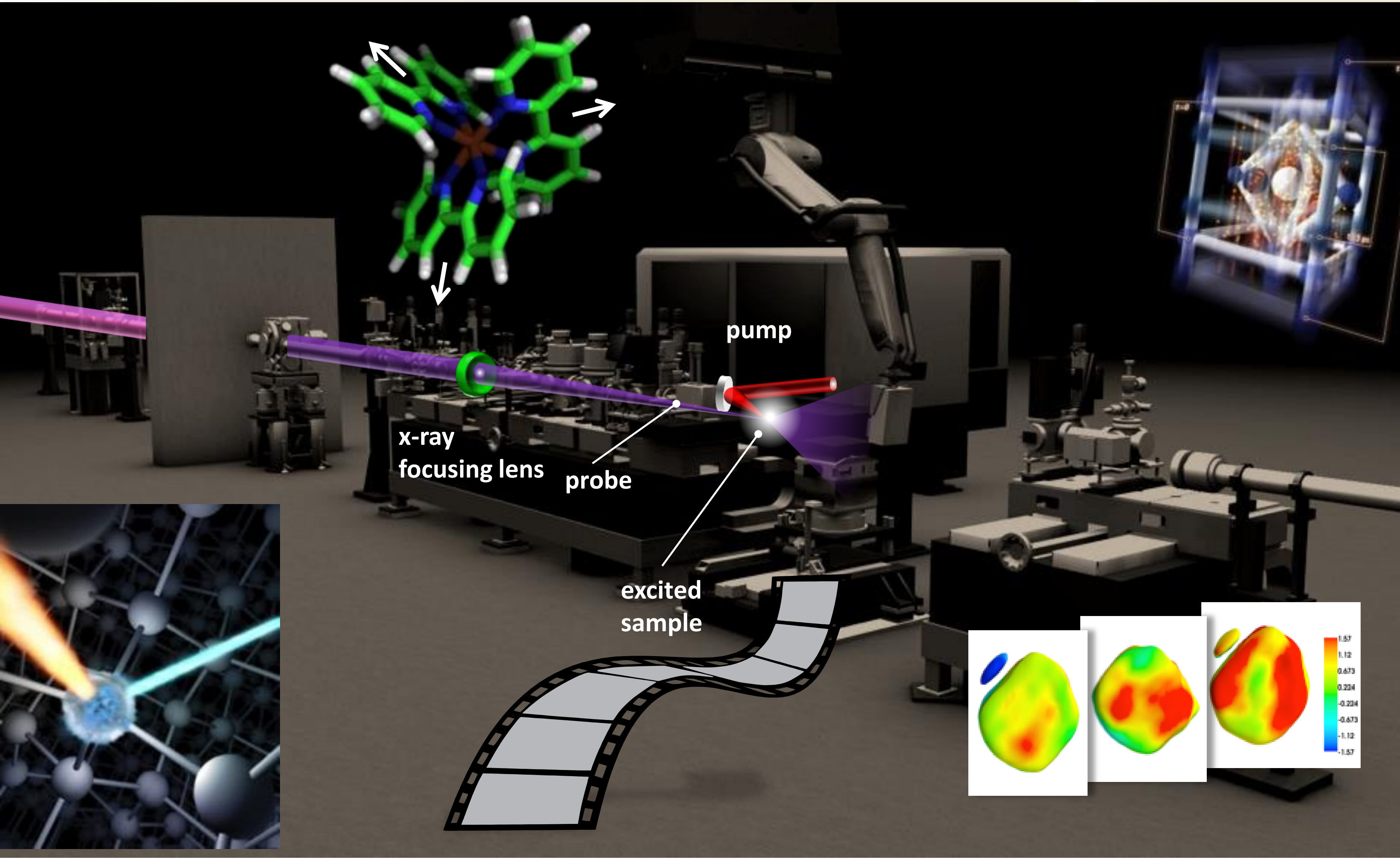
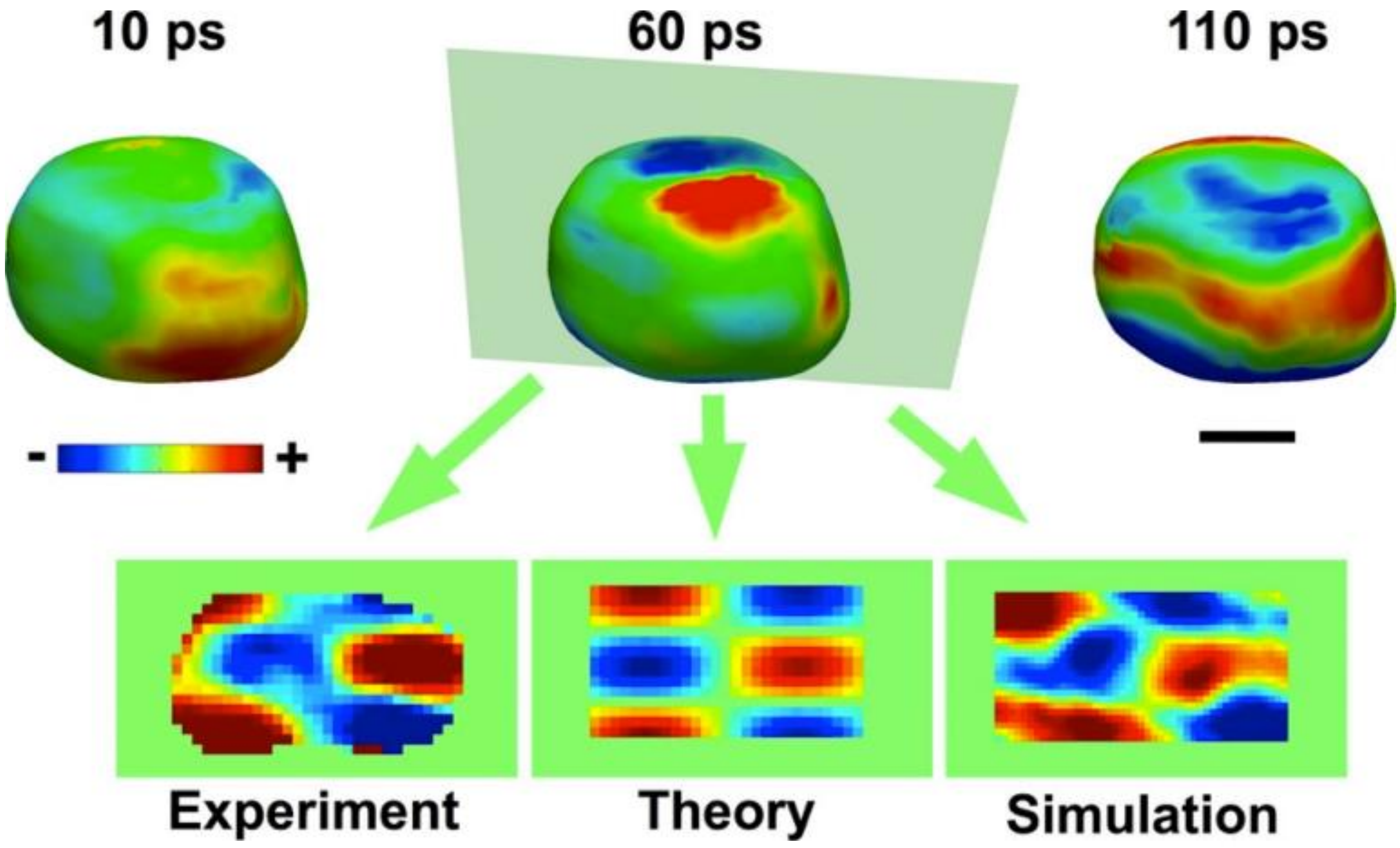

pump
x-ray
focusing lens
probe
excited
sample

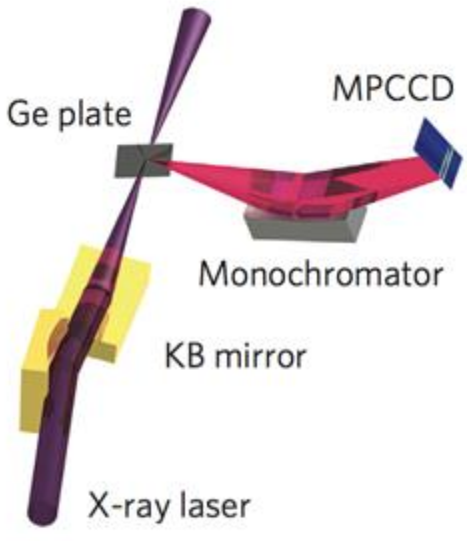
Imaging phonons in nanocrystals



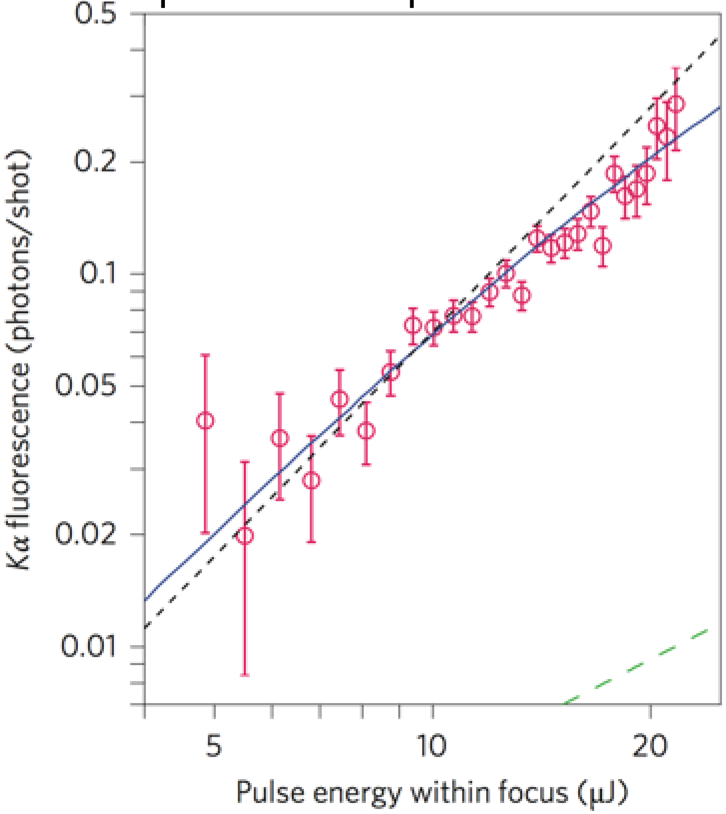
Clark et al., Science 341, 56 (2013)

X-ray two-photon absorption at SACLA

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



Pulse-energy dependence of germanium two photon absorption fluorescence



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

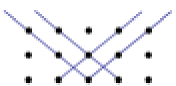
MEC

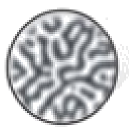
Matter in Extreme Conditions

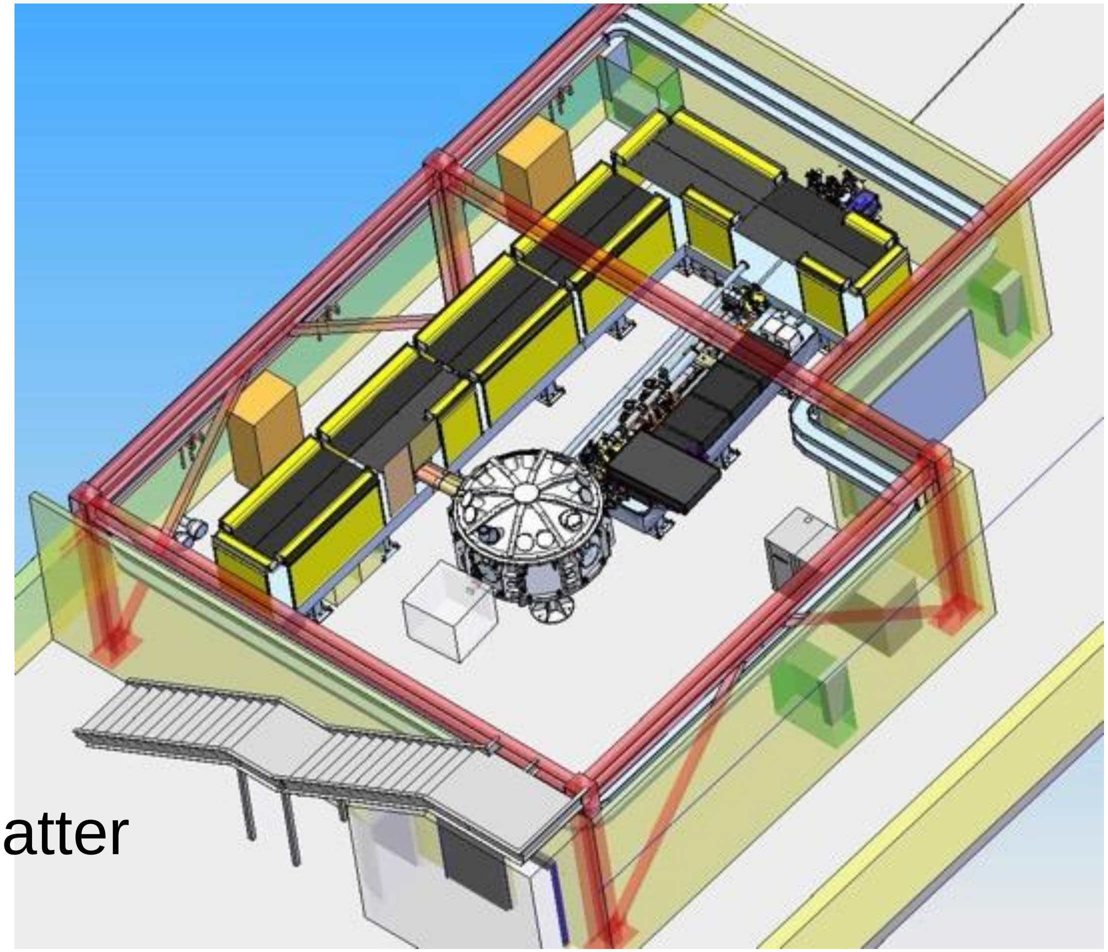
MEC Instrument Layout in Hutch 6

First Light: January 2012

Energy : 4 keV-9 keV



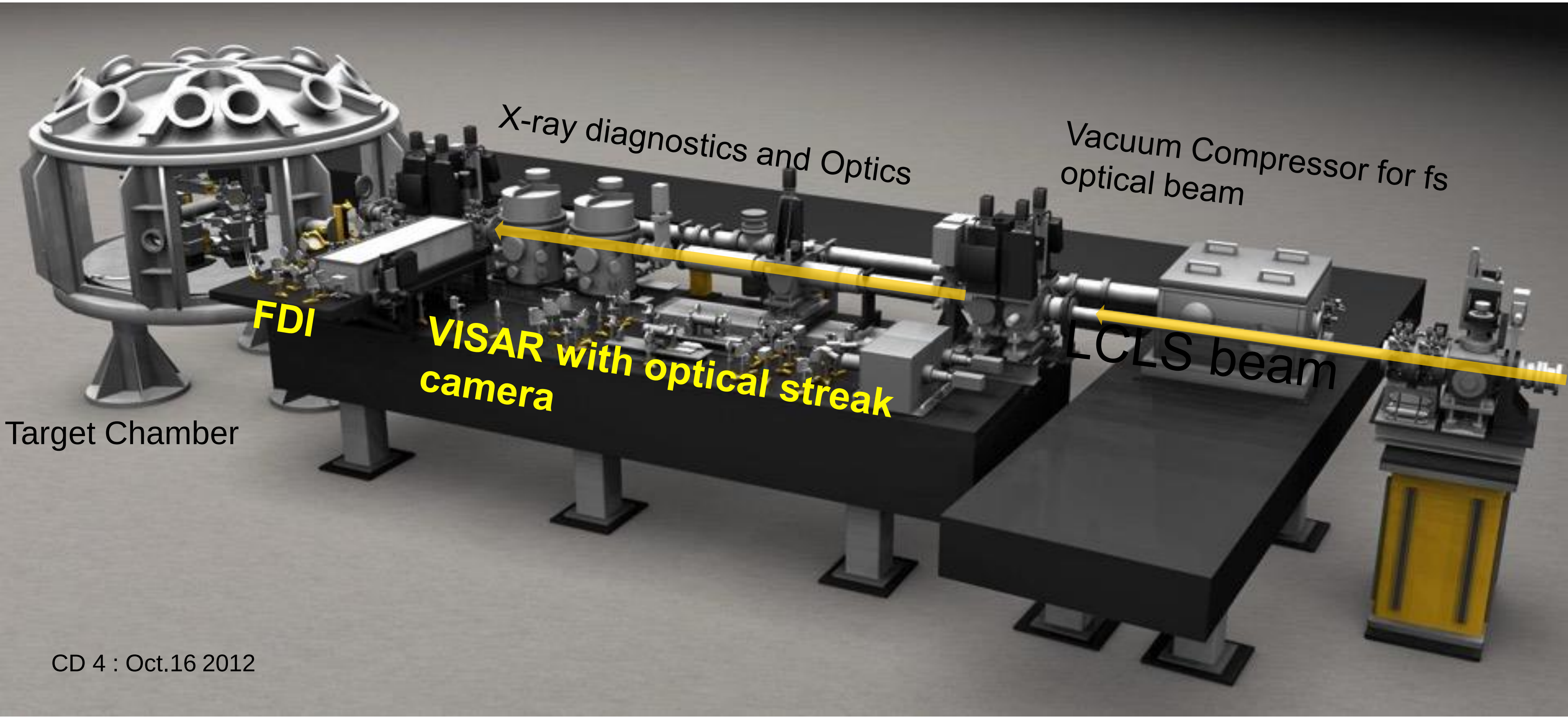




Science Program

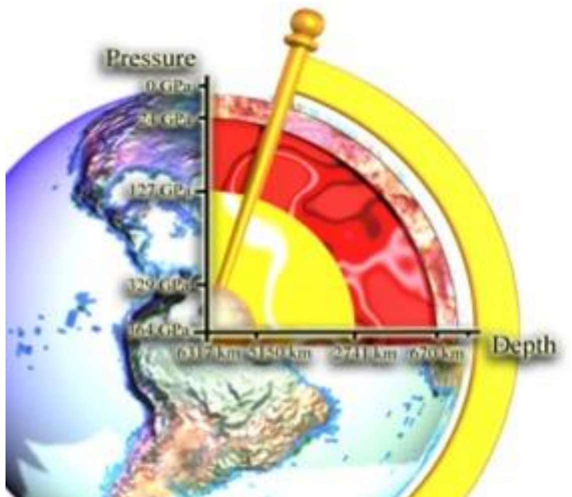
- High Pressure
- Shock phenomena
- Warm Dense Matter
- High Energy Density Matter

MEC Instrument optics and diagnostics

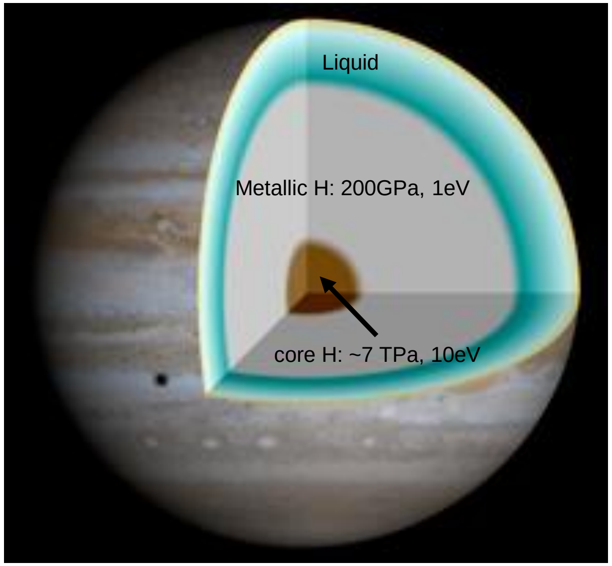


Photon energy: 2keV - 10keV fundamental (~10^{12} photons)
up to 24keV in third harmonic (10^{10} photons)
Pulse length : 60fs - 30fs (<10fs with penalty in photons)
bandwidth : 0.3% in SASE

Matter in Extreme conditions



A.M. Dziewonski and D. L. Anderson
Physics of the Earth and Planetary Interiors 25, 297 (1981).

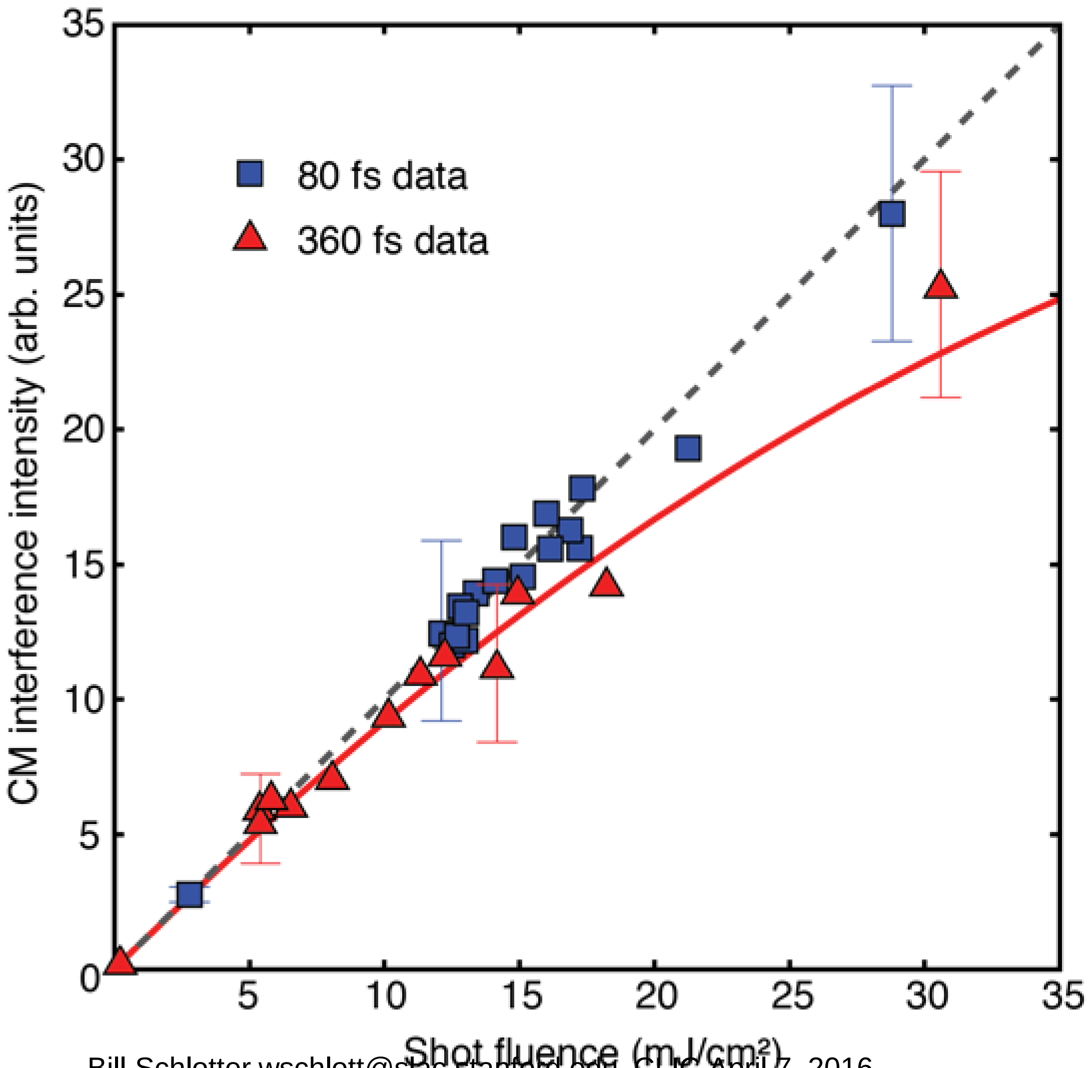


- Matter in extreme conditions is extremely interesting state
  - Solid or near solid density: Pressure typically tens GPa – a few of TPa
  - Heated to 1,000 K < 1,000,000 K
  - Inside the Earth, structure of large planet, planetary impact phenomena…
  - High Energy Density Physics, Warm Dense Matter,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

LCLS Instrument
Backup
SXR,CXI

Avoiding demagnetization during the x-ray pulse

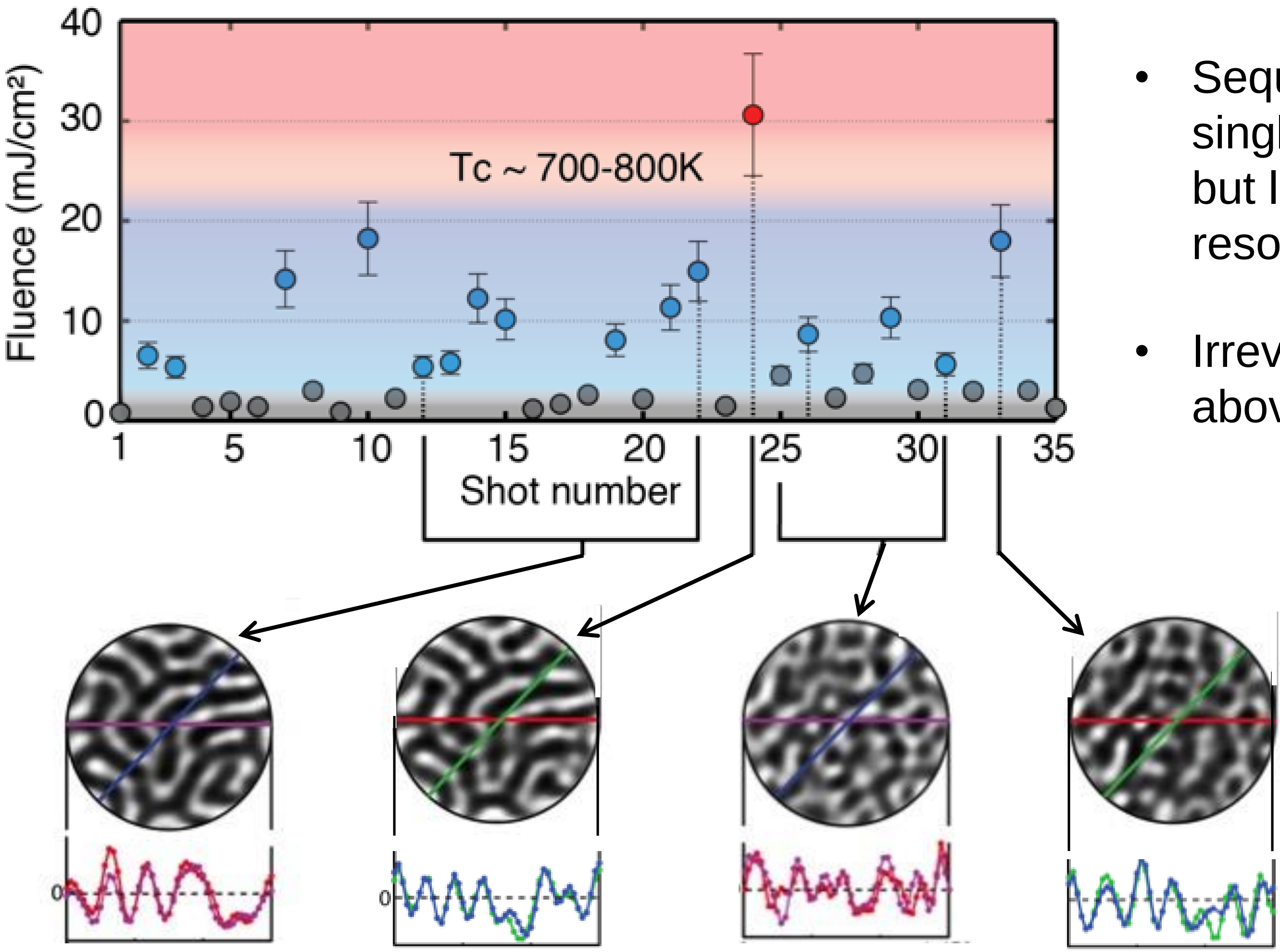
SLAC



Illumination with 20mJ/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

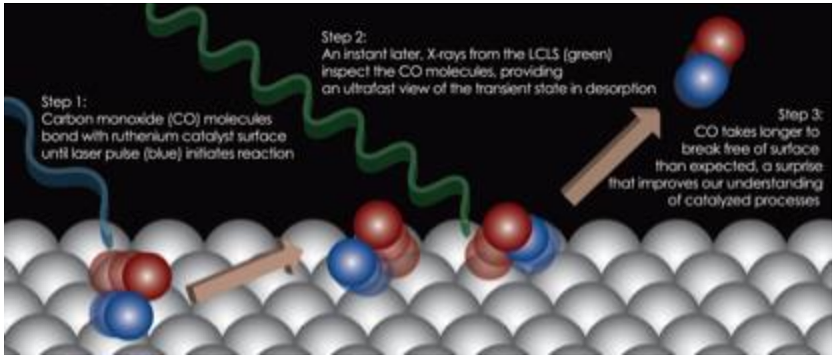
After effects of heating: damage thresholds



- Sequential imaging on a single sample possible but limited to 50nm resolution
- Irreversible damage above ~30mJ/cm^2

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

SLAC



Experiment:

- An ultrafast laser pulse heats the metal surface and initiates the process of converting CO to CO_2.
- Snapshots of the electronic states of oxygen are captured in x-ray spectra.

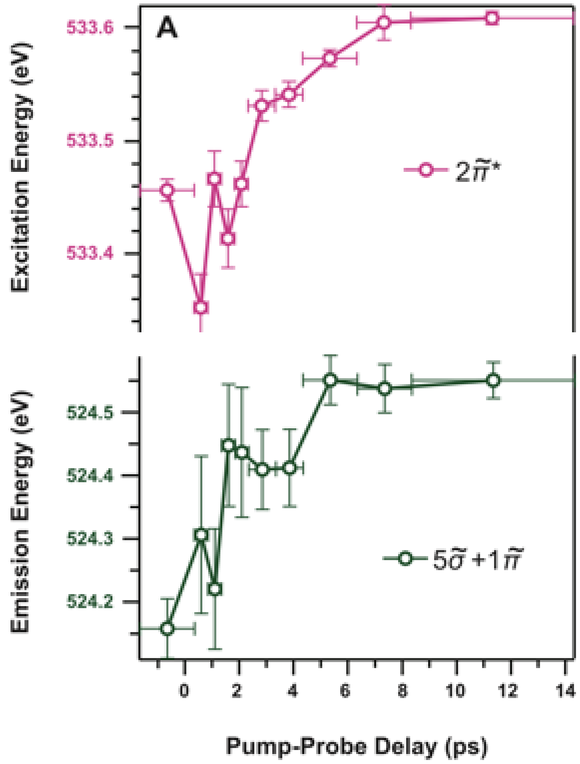
Nilsson Group, Surface Science End Station
M. Dell'Angela, *et al.*, Science **339** 6125 (2013)
M. Beye, *et al.*, Phys. Rev. Lett. **110** 186101 (2013)

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

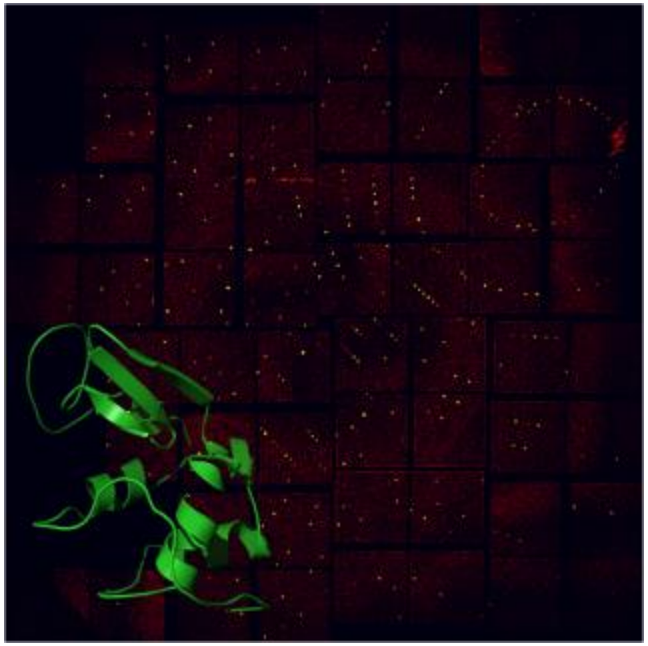


X-ray absorption spectral peak plateaus before reaching 534.2eV which confirms that CO is not completely desorbed.

X-ray emission spectrum peak energy increases with time toward the gas phase spectra. This is constant with bond weakening between CO and the metal substrate

CXI Primary Science Areas

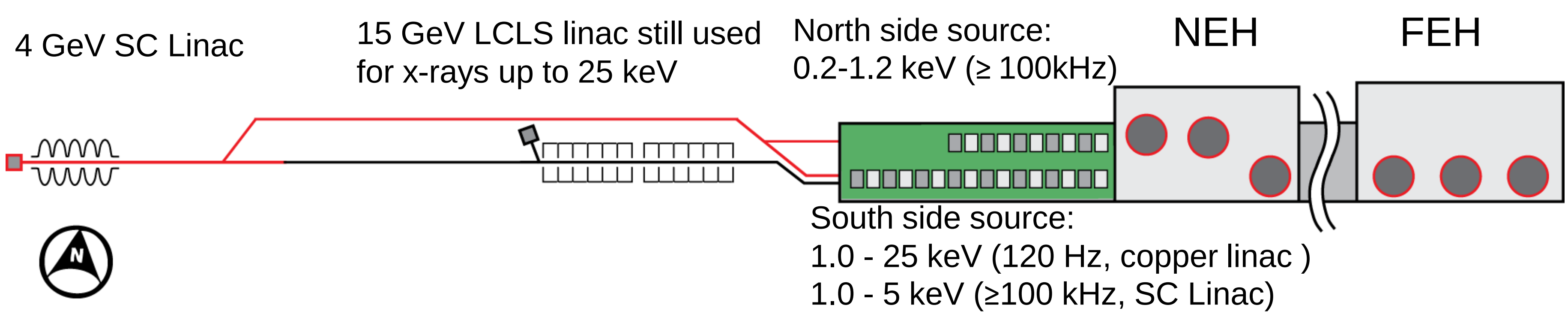
- Structural Biology
  - Serial Femtosecond Crystallography
  - Laser induced Dynamics
  - Coherent Diffractive Imaging
  - Protein Crystal Screening Program
- Nanoparticle Studies and Imaging
  - Clusters
  - Aerosols
- High Field Hard X-ray Physics
  - 100 nm focus is unique capability
    - **Produces 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

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)

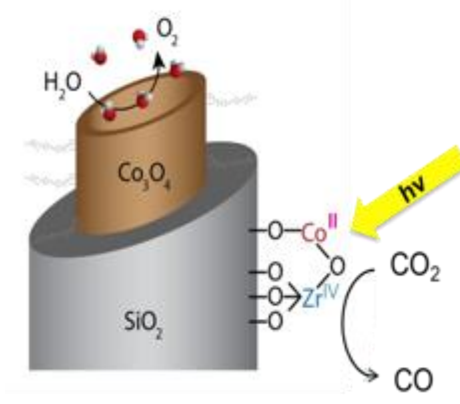


Development of Science Drivers
LCLS-II Science Opportunities Workshops

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**

Predictive understanding of catalysis



LCLS-II Science Opportunity

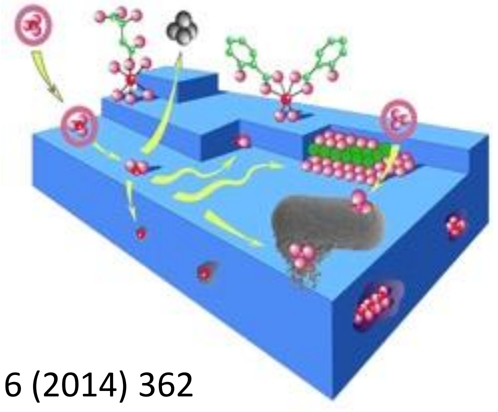
- Understand the fundamental processes that occur on metal surfaces during catalytic reaction conditions in order to design new, efficient, and selective catalysts
- Provide a robust structure-function relationships for materials in electronic excited states
- Understanding and predicting photon driven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



Heinz Frei et al. Nature Chem. 6 (2014) 362

Chemistry: Charge migration and redistribution

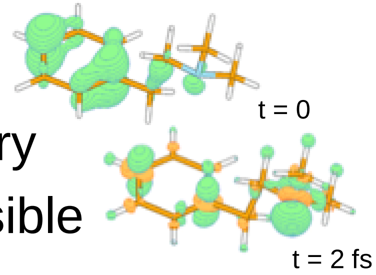
Follow molecular transformations & bond formation

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

LCLS-II Science Opportunity

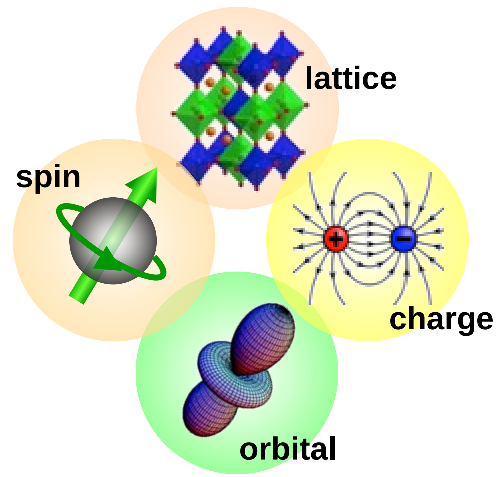
- Magnetic, lattice, and charge degrees of freedom are strongly intertwined makes it difficult to understand the mechanism of HTSC.

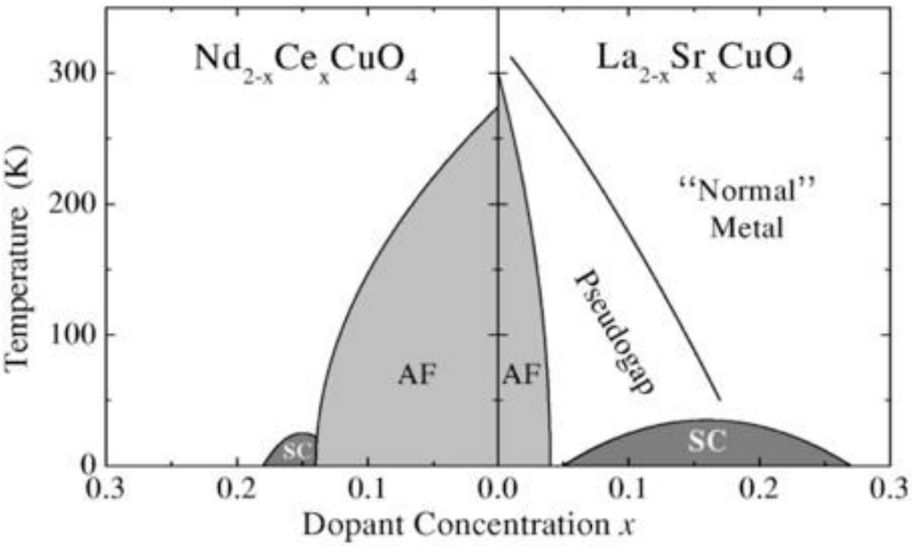
Significance & Impact

- 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.



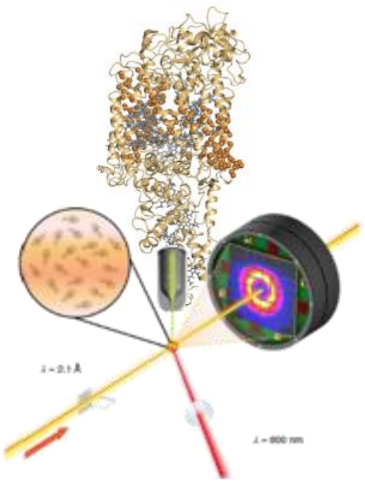


Wei-Sheng Lee, SLAC

Life Sciences & Matter in Extreme Conditions at LCLS-II

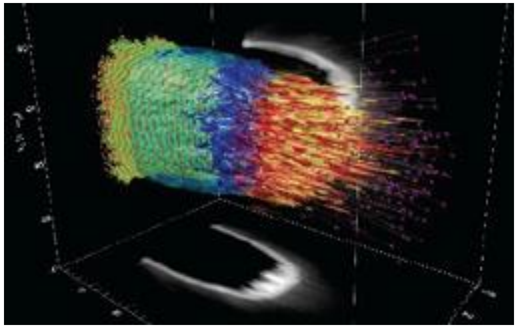
Life Science

- 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

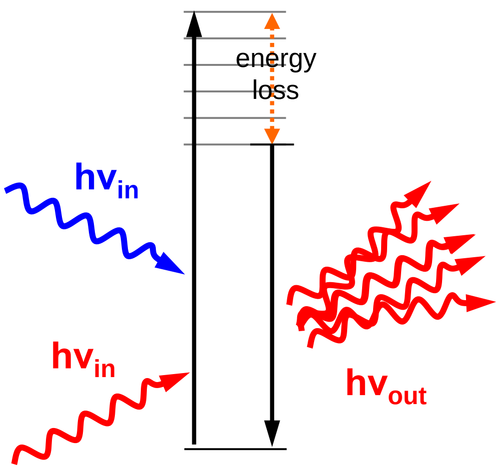
SLAC

future

X-ray Lasers

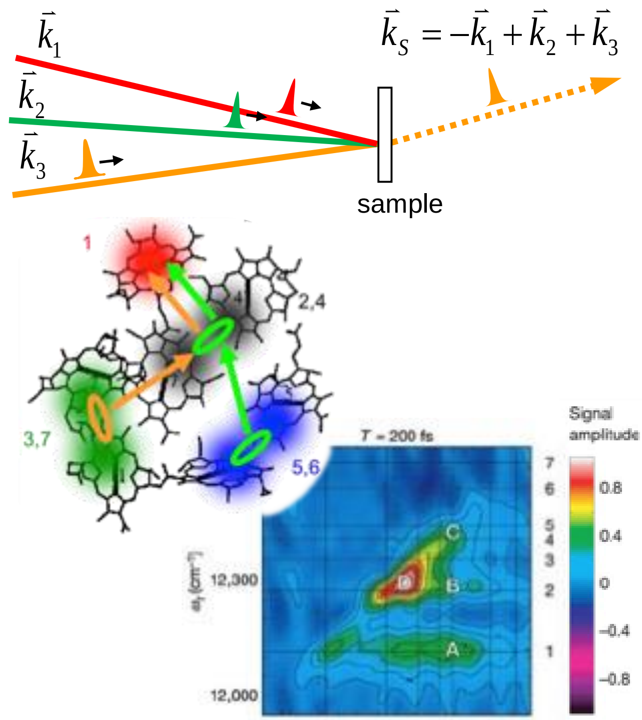
today

Time-resolved X-ray Raman, stimulated emission



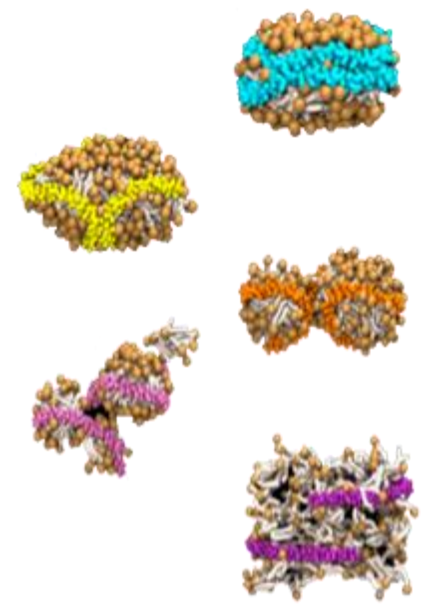
X-ray emission spectrum

Multi-dimensional nonlinear spectroscopy



Pump-probe

Macromolecular assembly & dynamics

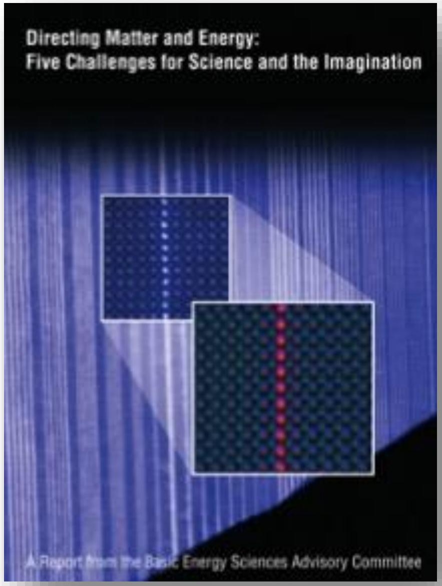


Structure of single molecules

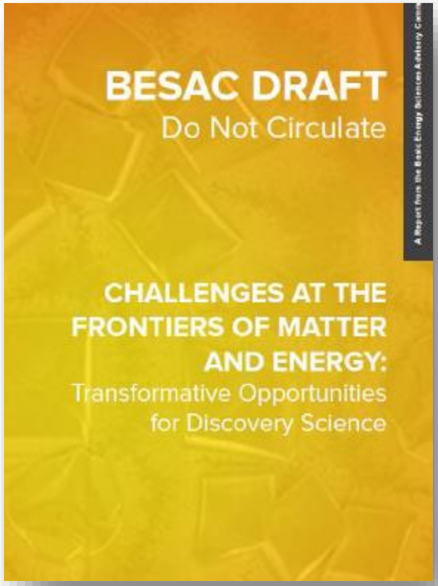
Guiding Scientific Themes

SLAC

Five Grand Challenges for Science and the Imagination (2007)

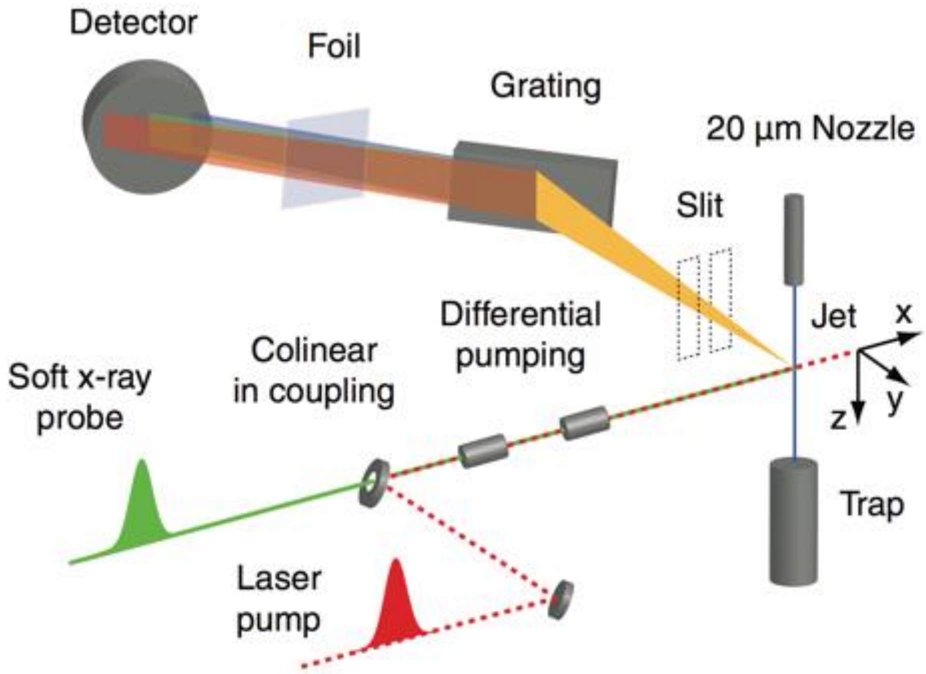


Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science (2015)



RIXS for Chemistry

- RIXS experimental setup for studying liquids



K. Kunnus, *et al.*, Rev. Sci. Inst., **83**, 123109 (2012)