X-Ray Free-Electron Lasers: An Introduction

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U.S. DEPARTMENT OF ENERGY

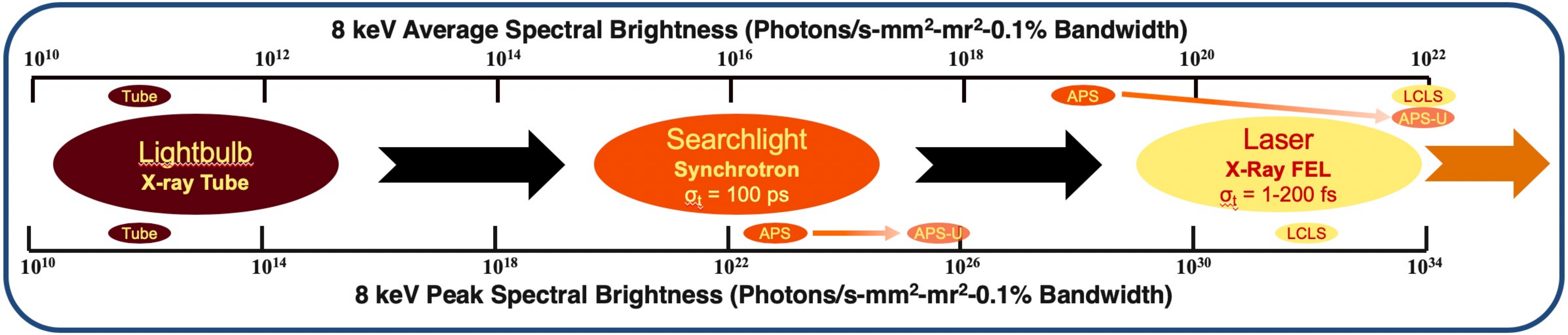
Stanford University

SLAC NATIONAL ACCELERATOR LABORATORY

X-ray Free Electron Lasers

- FLASH (Germany) - 2005, LCLS (US) - 2009, FERMI (Italy), SACLA (Japan), PAL (Korea), SwissFEL (Switzerland), European XFEL (Germany), SHINE (China)
- FLASH and FERMI are soft/XUV, all others have hard x-ray capabilities

Evolution of X-Ray Sources



Typical XFEL Performance – LCLS

- 3 mJ/pulse (2×10^{12} 10 keV photons)
- <100 femtosecond long pulses
- 120 pulses/second
- Full transverse coherence (it is a laser)
- Stochastic energy spectrum with 0.1% width

Light source advances enable:

- X-ray measurements of ultrafast behavior
- Coherent scattering studies of atomic structure and dynamics

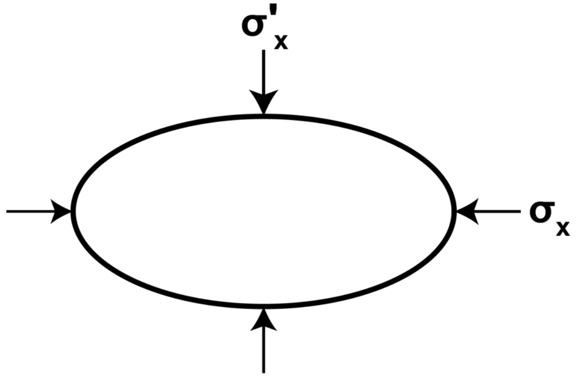
These allow development of new analysis techniques and deeper insight into fundamental processes.

Key Properties of Photon Beams

Flux	Typically expressed as the number of photons per second. But at FEL facilities it is usually expressed as by mJ/pulse.
Spectral Brightness	$$B = \frac{N_{photons}}{4\pi^2 \Sigma_x \Sigma'_x \Sigma_y \Sigma'_y \frac{dE}{E}}$$ Photons/(sec-mm^2-mrad^2-0.1%BW) is typically cited.
Peak Brightness	Critical for ultrafast measurements. FELs can generate pulses of attosecond duration with significant intensity.
Pulse Bandwidth	Critical for spectroscopy and, to a lesser extent, scattering. FEL's can create transform limited pulses. In that case, there is a strict relationship between pulse length and bandwidth. $$\hbar = 0.658\ meV\text{–}ps$$
Polarization	Storage rings and FELs typically have a horizontal polarization vector which generally requires scattering in the vertical plane. The LCLS-II hard x-ray undulator has a vertical polarization vector. Circular polarization is possible and important for magnetic measurements.
Number of Modes	The number of modes is important for coherent scattering measurements. Storage rings typically have large numbers, FEL's a few. The goal with lasers is often to have all the photons in a single mode.
Pulses per Second	Storage rings can produce well over a million pulses/second. Room temperature FELs typically are 60-120 pulses/second. Superconducting FELs can produce up to a million pulses/second.

Phase Space Ellipse

(One for each dimension)

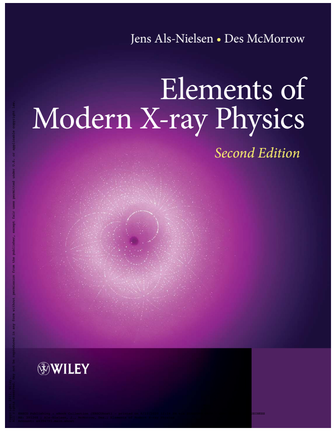


$$\Sigma = \sqrt{\sigma^2_{electrons} + \sigma^2_{x-rays}}$$

$$\Sigma' = \sqrt{\sigma'^2_{electrons} + \sigma'^2_{x-rays}}$$

Creating Hard X-Ray Beams at the Diffraction Limit

Why: At the diffraction limit, the x-rays are almost completely transversely coherent.
Coherent x-ray scattering techniques can yield unique structural information.

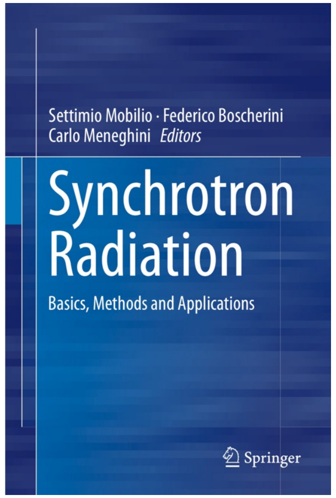


Look at the ESRF-EBS

- Horizontal emittance of 110 pm-rad yields a diffraction limited wavelength of ≈13.8Å.
- Vertical emittance of 5 pm-rad yields a diffraction limited wavelength of ≈0.6Å.

$$\epsilon = 2\pi\sigma_x{\sigma_x}' = \frac{\lambda}{4\pi} = \frac{0.1\ nm}{4\pi} = 8\ pm\text{-}rad$$

Even the best of the current generation of storage ring sources don't reach the full diffraction limit for typical hard x-ray experiments.



https://www.esrf.eu/home/UsersAndScience/Accelerators/ebs---extremely-brilliant-source/ebs-parameters.html

Scaling of Electron Emittance

The emittance is an equilibrium property in a storage ring driven by quantum fluctuations (the emission of x-ray photons). For a storage ring, the emittance scales like:

$$\mathcal{E}_x \propto E^2\theta^3$$

Where:

E = Electron Energy

θ = Angular deviation per period

Nuclear Instruments and Methods in Physics Research A264 (1988) 497–501 497
North-Holland, Amsterdam

HIGH ENERGY ELECTRON ACCELERATOR BASED SYNCHROTRON RADIATION SOURCES

P.H. FUOSS

AT&T Bell Laboratories, Crawfords Corner Road, Holmdel, NJ 07733, USA

Received 5 May 1986 and in revised form 28 July 1987

This paper discusses the possibility of using electron linear accelerators as picosecond synchrotron radiation sources. Calculations presented show that the Stanford Linear Collider could exceed the spectral brilliance of existing storage rings (although at a much lower total flux) while producing 3 ps long pulses at a repetition rate of 180 pulses per second. Higher performance sources might be feasible but would require major modifications of existing linear accelerators or the development of new facilities.

Status in 1987	Emittance	Electrons per pulse	Pulse Length	Electrons per picosecond
Advanced Light Source	17 nm-rad	5×10^{9}	20 ps	2.5×10^{8}
ESRF	11 nm-rad	7×10^{9}	27 ps	2.6×10^{8}
SLAC Linear Collider	0.3 nm-rad	5×10^{10}	3 ps	1.7×10^{10}

A Brief History: Invention of the Free Electron Laser

SLAC

John Madey at Stanford University first proposed a free-electron laser (FEL) 50 years ago in the Journal of Applied Physics

Early FEL development focused on producing infrared and visible light.

Advances in theory and accelerator technology led to proposals in the early 90's for x-ray FEL's.

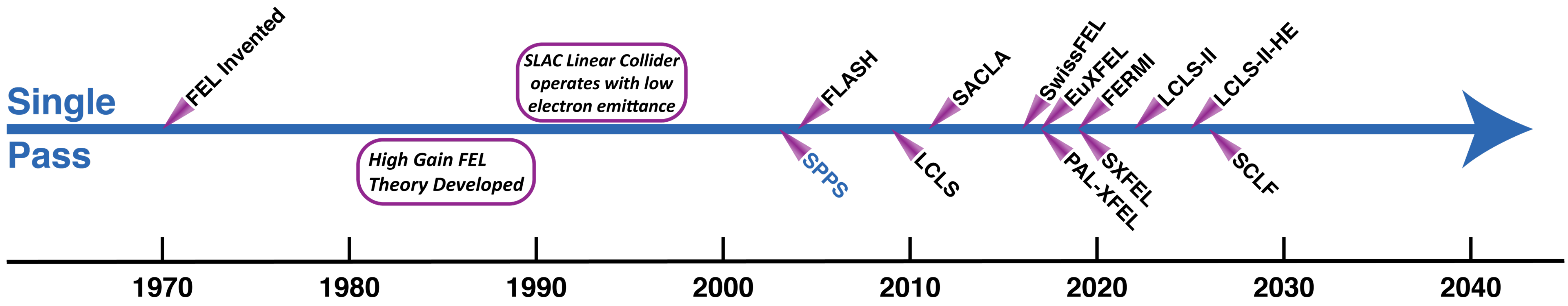
JOURNAL OF APPLIED PHYSICS VOLUME 42, NUMBER 5 APRIL 1971

Stimulated Emission of Bremsstrahlung in a Periodic Magnetic Field

John M. J. Madey
Physics Department, Stanford University, Stanford, California 94305

(Received 20 February 1970; in final form 21 August 1970)

The Weizsäcker–Williams method is used to calculate the gain due to the induced emission of radiation into a single electromagnetic mode parallel to the motion of a relativistic electron through a periodic transverse dc magnetic field. Finite gain is available from the far-infrared through the visible region raising the possibility of continuously tunable amplifiers and oscillators at these frequencies with the further possibility of partially coherent radiation sources in the ultraviolet and x-ray regions to beyond 10 keV. Several numerical examples are considered.



A Brief History: Invention of the Free Electron Laser

SLAC

Particle Accelerators
1980 Vol.10 pp.207-216
0031-2460/80/1003-0207$06.50/0

GENERATION OF COHERENT RADIATION BY A RELATIVISTIC ELECTRON BEAM IN AN ONDULATOR*

A. M. KONDRATENKO and E. L. SALDIN
Institute of Nuclear Physics, 630090, Novosibirsk, USSR

(Received January 28, 1980)

A detailed study of the self-modulation of a relativistic electron beam in an ondulator in the single-pass regime is carried out. Beam-parameter conditions are obtained under which the radiative instability in question occurs. The possibility of constructing a source of coherent radiation based on this principle is discussed. The radiation specifications of such a source are analyzed. Control the mass of longitudinal motion with the help of an additional longitudinal magnetic field introduced in the ondulator is discussed. Numerical examples are given for sources of submillimeter and infrared-range radiation.

Volume 50, number 6 OPTICS COMMUNICATIONS 15 July 1984

COLLECTIVE INSTABILITIES AND HIGH-GAIN REGIME IN A FREE ELECTRON LASER

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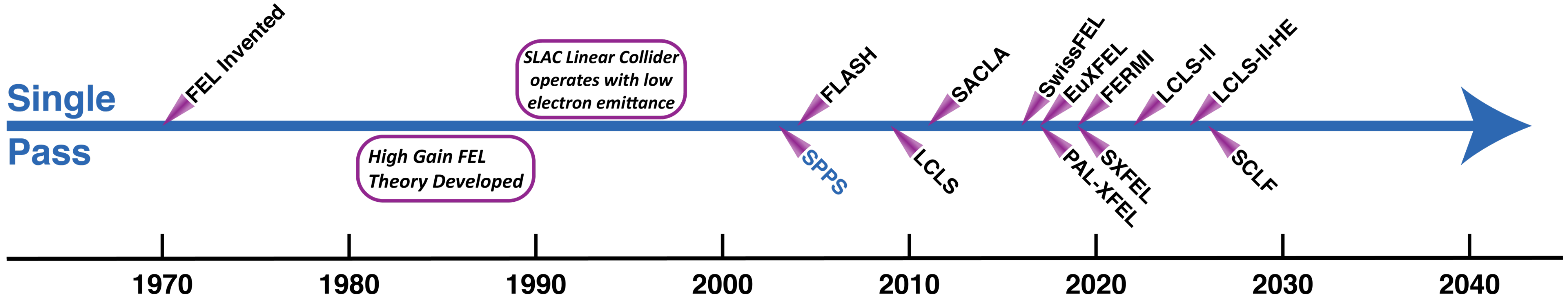
National Synchrotron Light Source, Brookhaven National Laboratory, Upton, NY 11973, USA

and

L.M. NARDUCCI
Physics Department, Drexel University, Philadelphia, PA 19104, USA

Received 5 April 1984

We study the behavior of a free electron laser in the high gain regime, and the conditions for the emergence of a collective instability in the electron beam-undulator-field system. Our equations, in the appropriate limit, yield the traditional small gain formula. In the nonlinear regime, numerical solutions of the coupled equations of motion support the correctness of our proposed empirical estimator for the build-up time of the pulses, and indicate the existence of optimum parameters for the production of high peak-power radiation.



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Eur. Phys. J. H
DOI: 10.1140/epjh/e2012-20064-5

THE EUROPEAN PHYSICAL JOURNAL H

The history of X-ray free-electron lasers

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Introduction to Free Electron Lasers

Andy Wolski

The Cockcroft Institute, and the University of Liverpool, UK

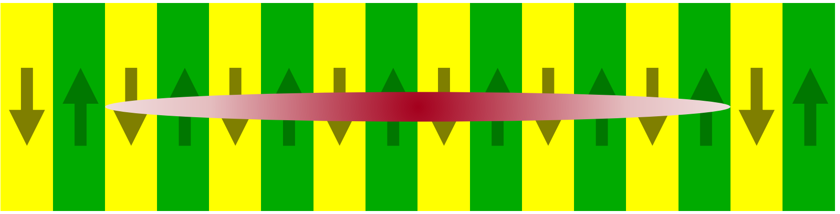
CAS: Introduction to Accelerator Physics Prague, Czech Republic September 2014

Free-Electron Lasers

https://indico.cern.ch/event/983080/contributions/4140483/attachments/2201441/3723528/Lecture_FELs.pdf

Electrons in an Undulator

FEL theory takes into consideration the dynamics of the electrons due to the co-propagating electric field as well as that of the undulator B field



$$B_y = B_0 \sin(k_u z)$$

$$k_u = \frac{2\pi}{\lambda_u}$$

Transverse

$$\ddot{x}(z) = \frac{d^2x}{dz^2} = -\frac{eB_0}{\gamma m_e c}\sin(k_u z)$$

$$\dot{x}(z) = \frac{eB_0}{\gamma m_e c}\frac{\cos(k_u z)}{k_u} = \frac{K}{\gamma}\cos(k_u z)$$

$$x(z) = \frac{K}{\gamma k_u}\sin(k_u z)$$

Electrons in an Undulator

Longitudinal velocity

$$\bar{v_z} \approx c\left(1 - \frac{1}{2\gamma^2}\left(1 + \frac{K^2}{2}\right)\right)$$

$$x(t) = \frac{K}{\gamma k_u}\sin(\omega_u t)$$

$$z(t) = \bar{v_z} t - \frac{K^2}{8\gamma^2 k_u}\sin(2\omega_u t)$$

$$(\omega_u = c k_u)$$

Putting this electron in a constant electric field:

$$E_x(z,t) = E_0 \cos(k_r z - \omega_r t + \psi_0)$$

ψ_0 is an initial phase offset and $\omega_r = c k_r$

Electrons in an Undulator – low gain regime

Electron energy change within the co-propagating electric field

$$\frac{dW}{dt} = -ev_x(t)E_x(t) = -e\frac{cK}{\gamma}\cos(k_u z)\, E_0 \cos(k_r z\ - \omega_r t + \psi_0)$$

$$-\frac{ecKE_0}{2\gamma}[\cos((k_r + k_u)z - \omega_r t + \psi_0) + \cos((k_r - k_u)z\ - \omega_r t + \psi_0)]$$

$$\frac{dW}{dt} = -\frac{ecKE_0}{2\gamma}[\cos(\psi(t)) + \cos(\chi(t))]$$

We want the electrons to give up energy to the electric field

Electrons in an Undulator – low gain regime

Much math and change of reference frame to find the electron energy gain/loss as a function of its position in the undulator

$$\frac{d\psi}{dt} = 2k_u c\eta$$

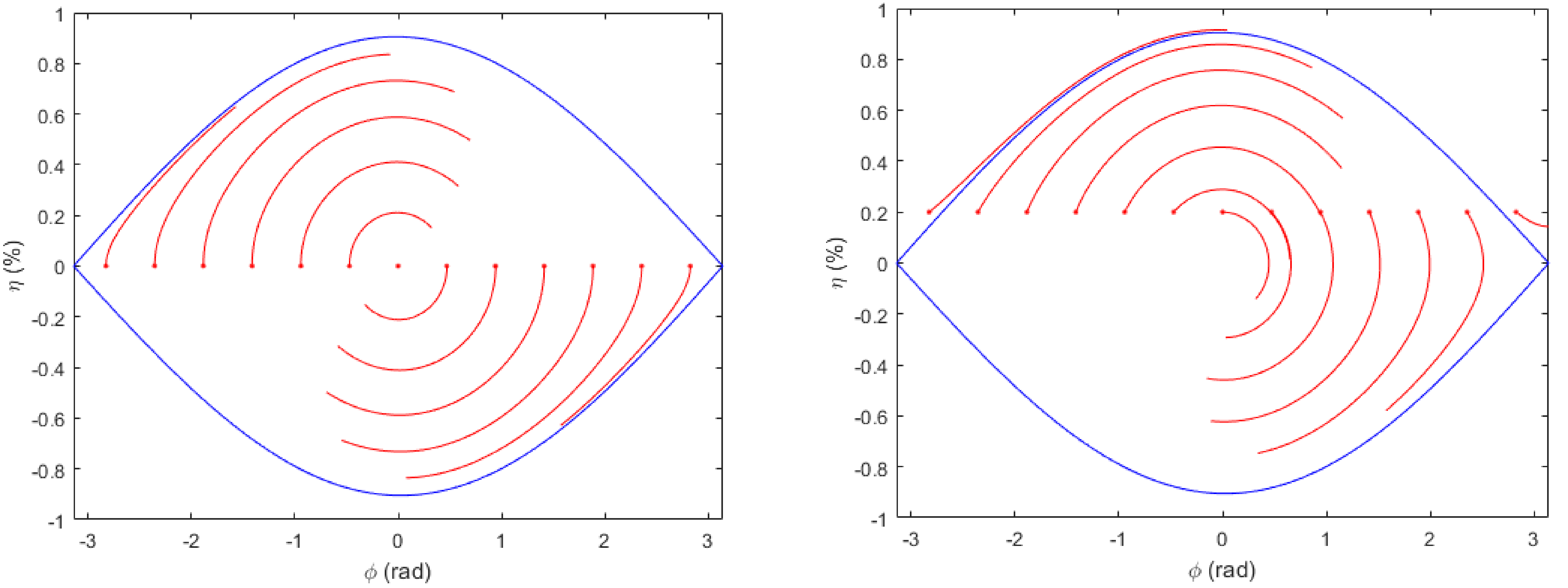
$$\frac{d\eta}{dt} = -\frac{eKE_0}{2\gamma_r^2 m_e c}\cos(\psi(t))$$

η relative energy deviation of the electron

Pendulum Equations

Electrons in an Undulator – low gain regime

If the electrons are tuned to the resonant undulator frequency with a homogenous phase distribution, equal numbers of electrons gain and lose energy. Detuning the electron energy breaks the symmetry and net energy can be transferred from the electrons to the field

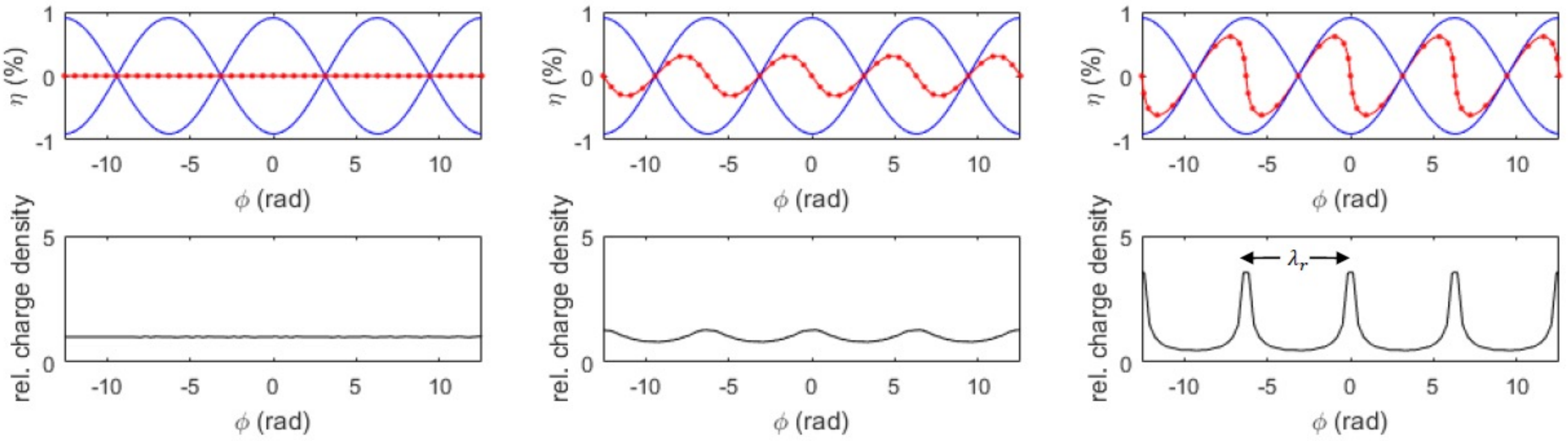


High Gain FELs

High Gain Theory considers:

- Growth of the co-propagating electric field along the undulator
- Microbunching of the electron bunch due to electron energy modulation at the resonant wavelength

Much more complicated math

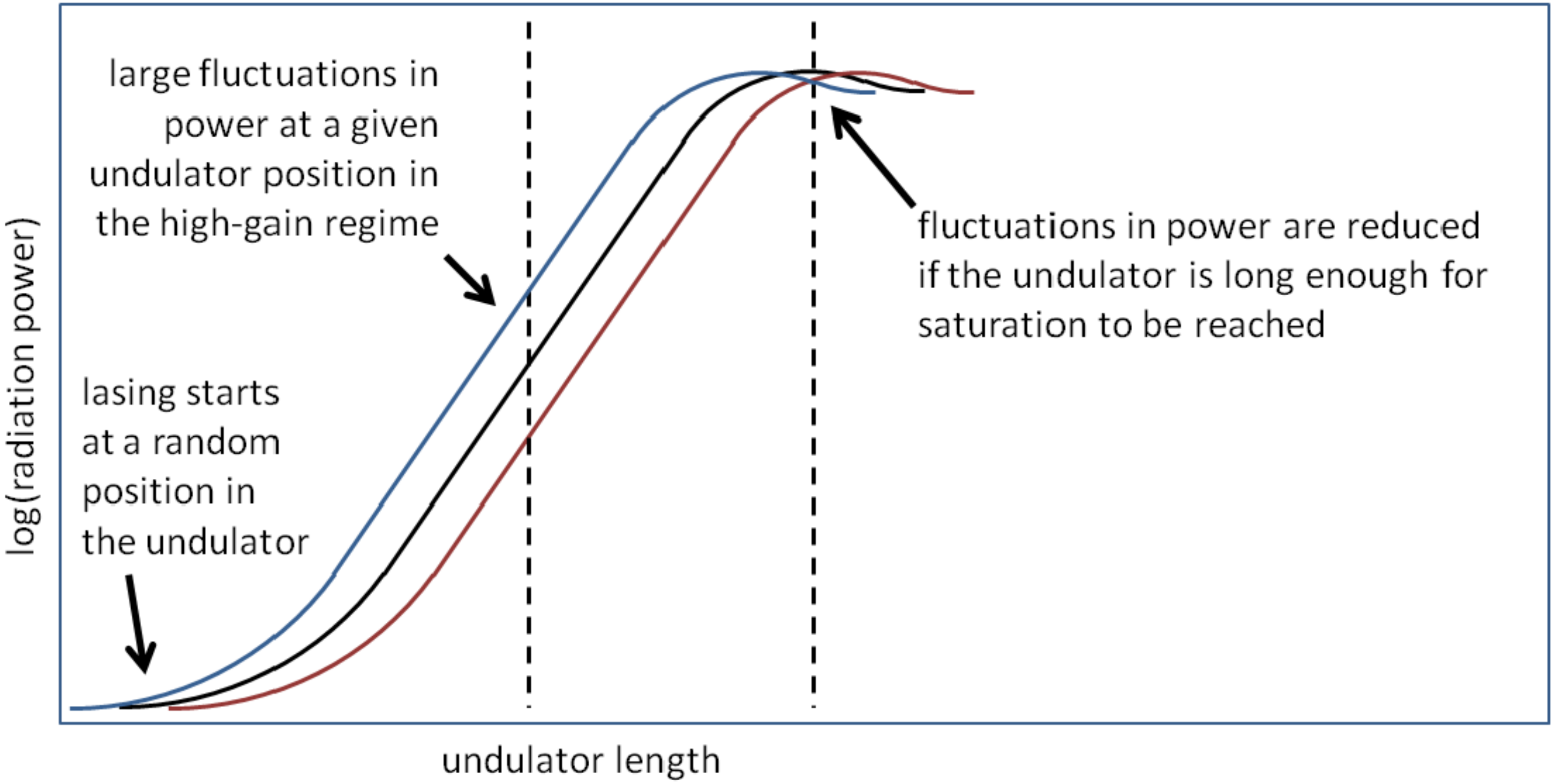


High Gain FELs

Some parameters and terminology

- Gain Length
- FEL (Pierce) Parameter
- Saturation

The process of microbunching, exponential gain and saturation to create photon bunches is referred to as Self-Amplified Spontaneous Emission (SASE)



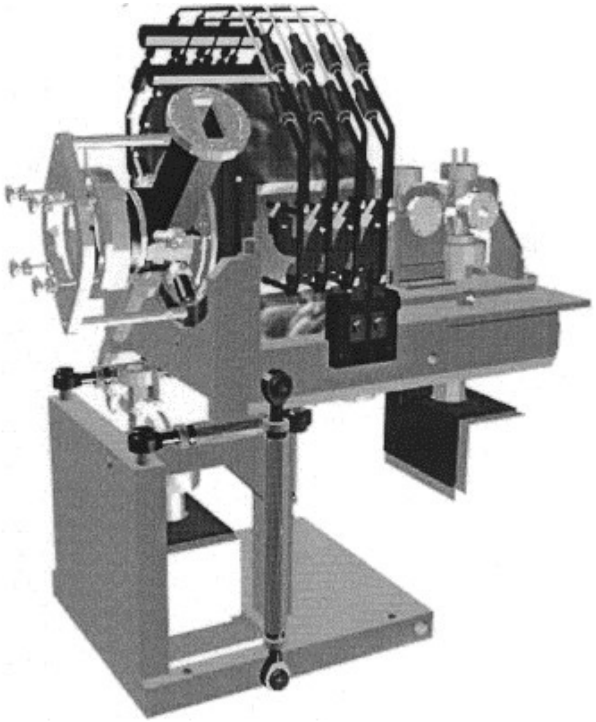
Technical Challenges for an FEL

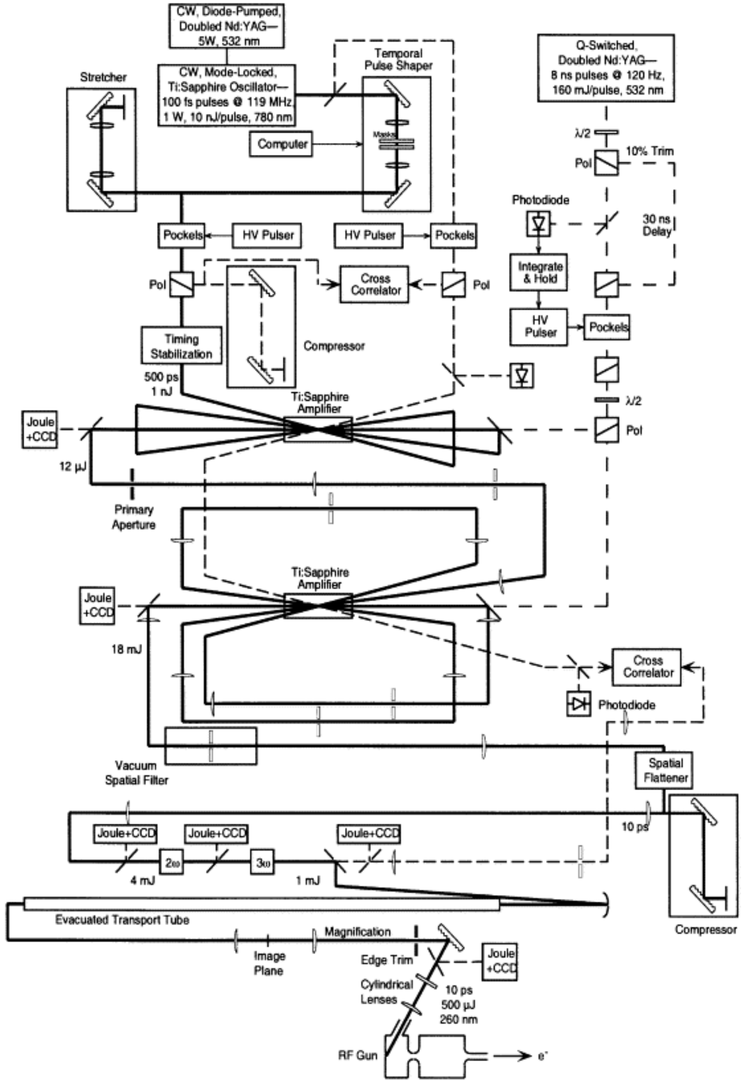
SLAC

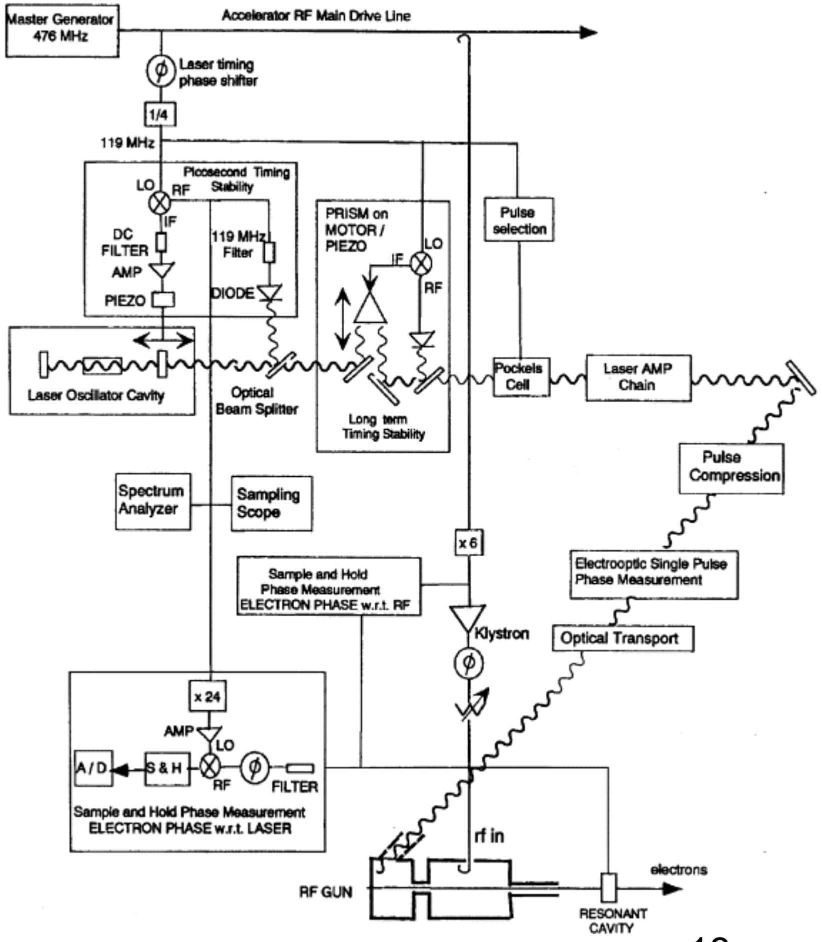
- A very high electron density is required to drive the SASE process.
  - This requires an electron gun with a very low electron emittance.
  - Periodic bunch compression is required to produce the extremely short electron pulses are needed.
- High electron density pulses have many instabilities that need to be controlled. Laser heaters can be used to destroy correlations.
- The magnetic properties of the undulator need tight tolerances to keep the photon and electron beams overlapped.
- Optics have to be able to handle high instantaneous photon power.
- Long undulators, FELs require up to 20 gain lengths to reach saturation
- The femtosecond long pulse is triggered two miles from the experiment. Precise timing synchronization is challenging.

Photoinjector

- the photoinjector was the largest portion of the LCLS R&D budget



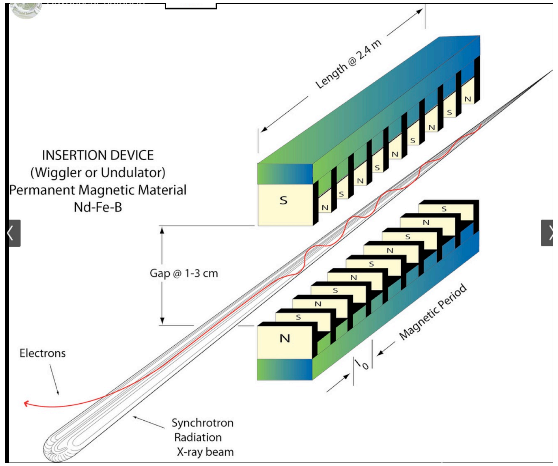




Undulators

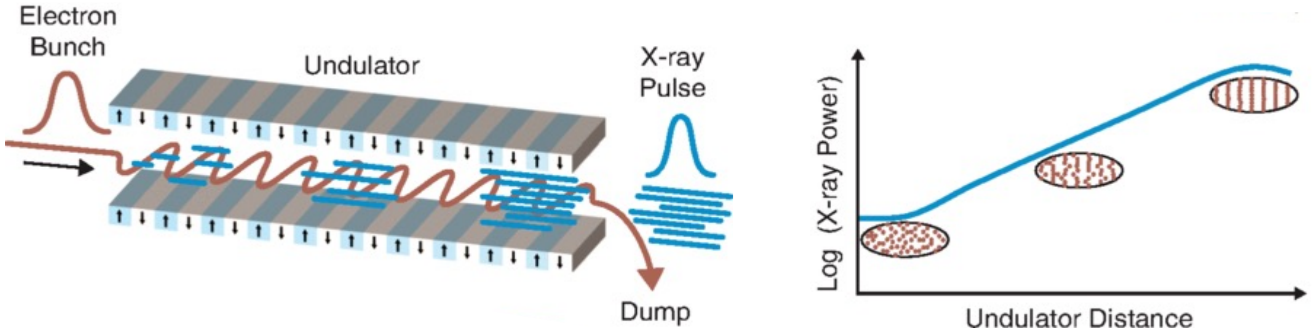
Synchrotrons

Typ. 1 to 5 meter long



Free Electron Lasers

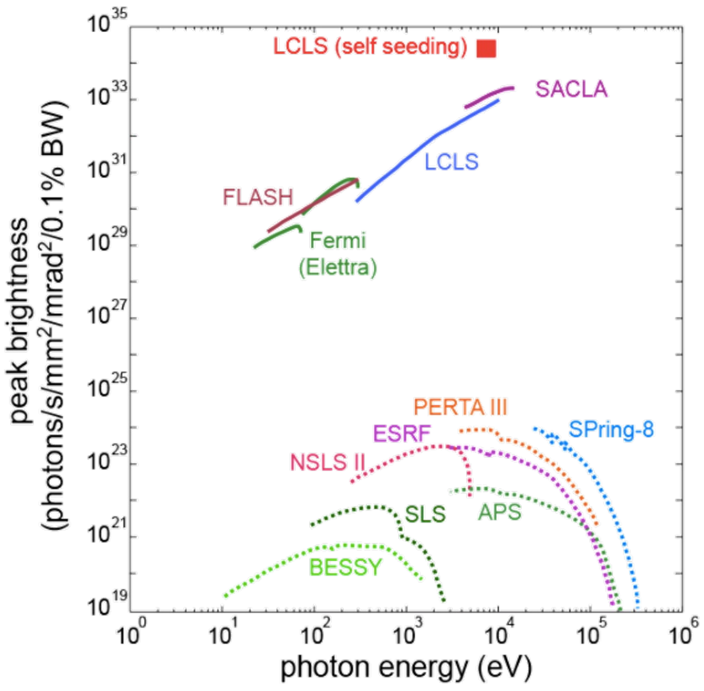
VERY long : typ. >100 meters
Small e-beam emittance



When to use an FEL?

High Peak Brightness

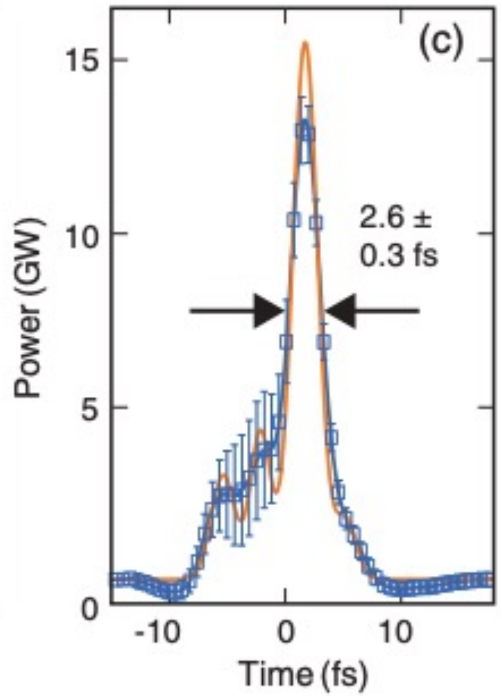
- Radiation sensitive samples
  - Diffract and Destroy
- Non-linear phenomena



Nature Photonics **6**, 693 – 698 (2012)

Short Pulses

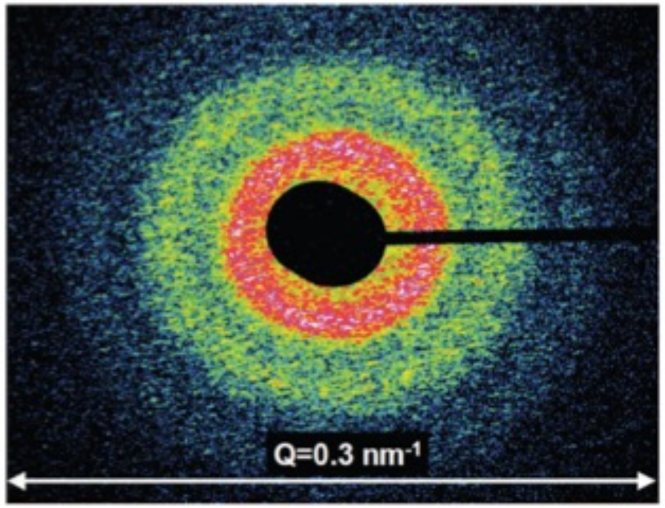
- Time-resolved dynamics
  - Fs to ns dynamics
- typical pulse is 30fs



Rev. Mod. Phys. **88**, 015007 (2016)

Coherence

- Fully coherent laser source
- Coherent techniques (XPCS, CDI)



PRL **108**, 024801 (2012)
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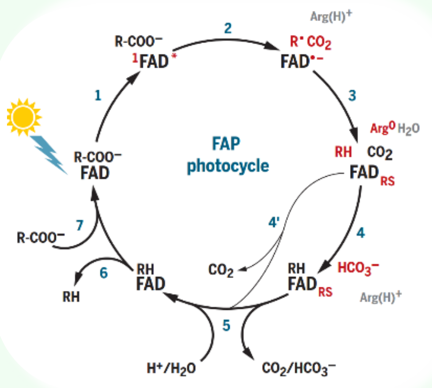
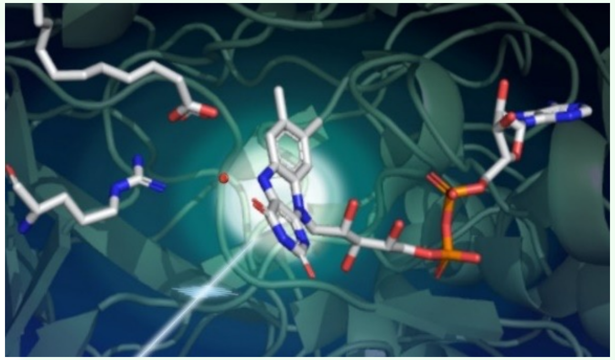
LCLS Structural Biology

Photo-enzyme: Fatty Acids to Hydrocarbons





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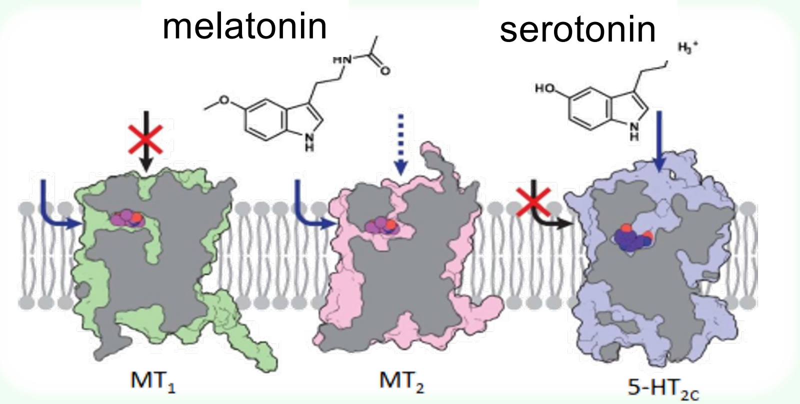
Structure of Human Melatonin Receptors



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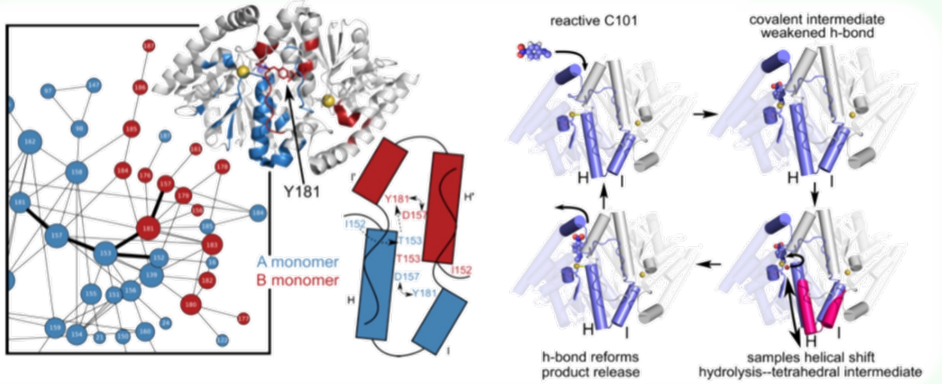
Conformational Dynamics – Enzyme Catalysis



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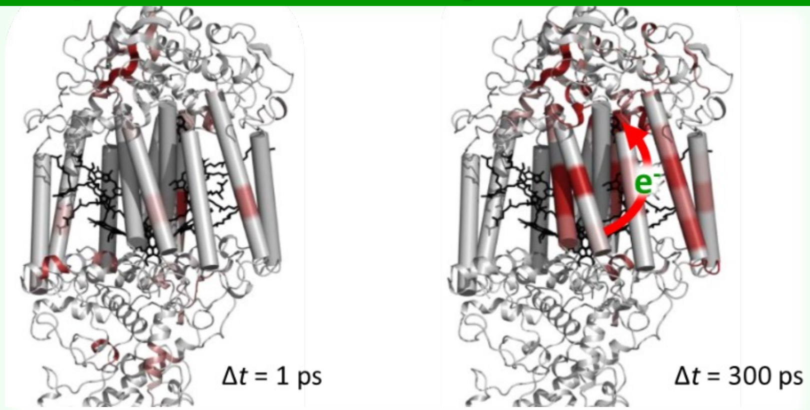
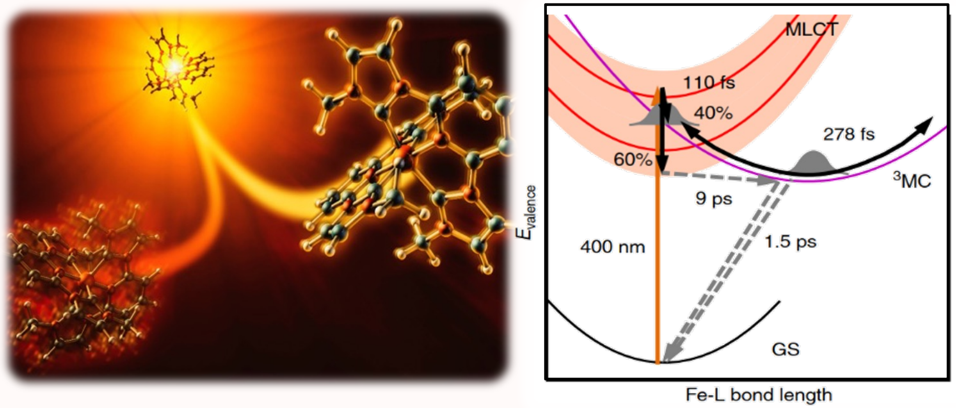
Light Response of Photosynthetic Protein



R. Dods, *et al.*, *Nature*, 589, 310 (2021)

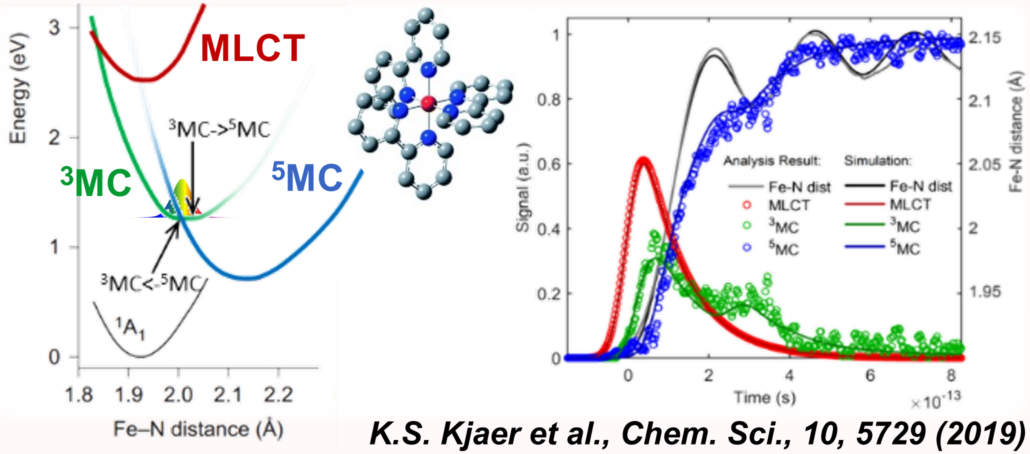
LCLS Chemistry

Photosensitizer Charge Relaxation Pathways



K. Kunnus, K.J. Gaffney, et al., Nature Comm. 11, 634 (2020)

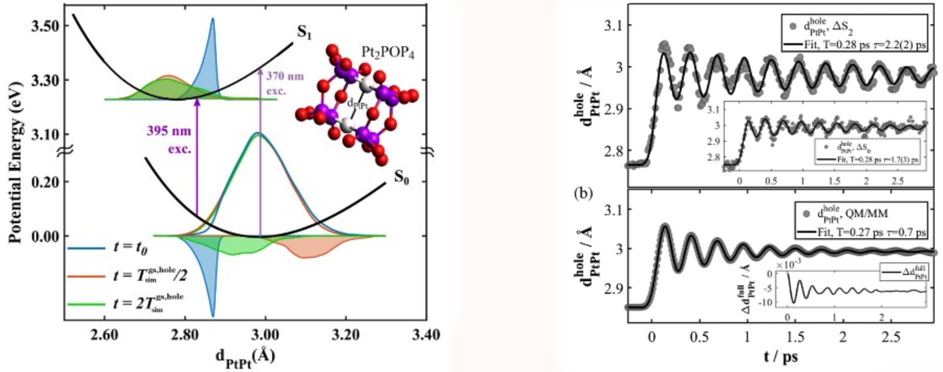
Electronic Excited-state Conical Intersections



K.S. Kjaer et al., Chem. Sci., 10, 5729 (2019)

Molecular Ground-state Structural Dynamics

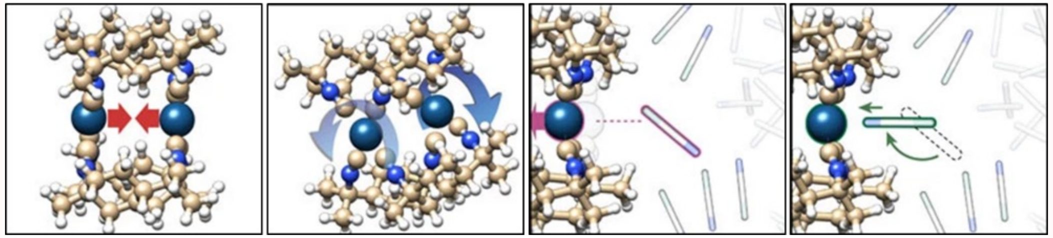
$[Pt_2(POP)_4]^{2+}$



K. Haldrup, et al., Phys. Rev. Lett. 122, 063001 (2019).

Solvation Dynamics of a Model Photocatalyst

$[Ir_2(dimen)_4]^{2+}$



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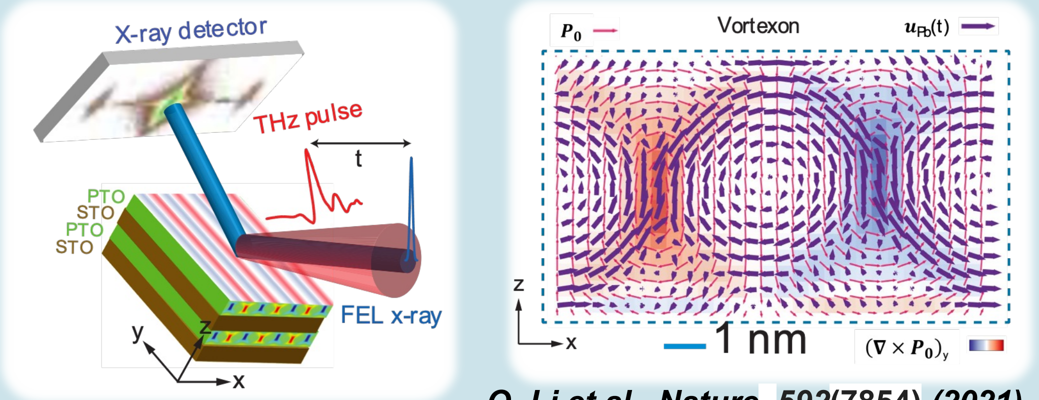
LCLS Materials Science

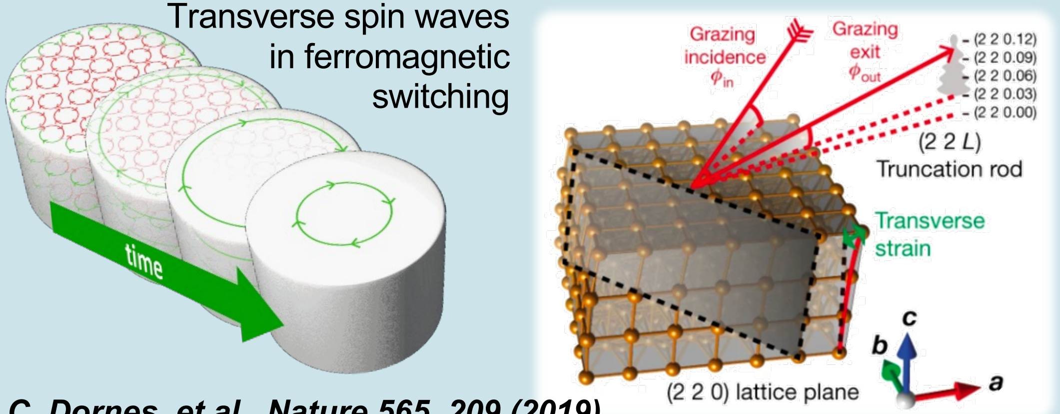
Ultrafast Collective Dynamics of Polar Vortices



Q. Li et al., Nature, 592(7854) (2021)

Ultrafast Einstein - de Haas Effect

Transverse spin waves in ferromagnetic switching



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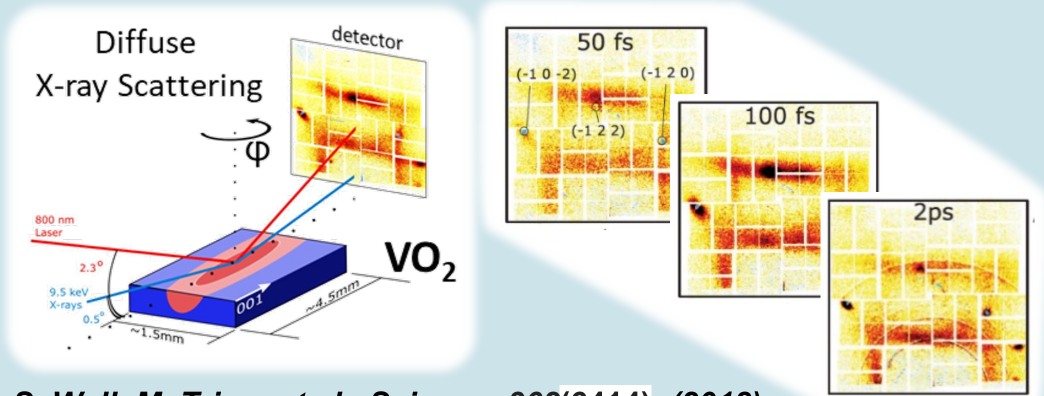
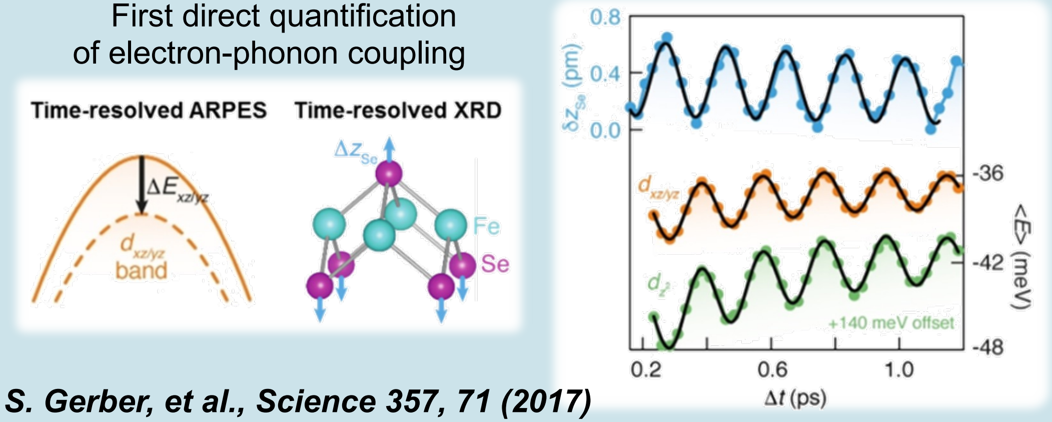
Ultrafast Disorder in Insulator-Metal Transition



S. Wall, M. Trigo. et al., Science, 362(6414) (2018)

e-ph Coupling in FeSe Superconductor

First direct quantification of electron-phonon coupling

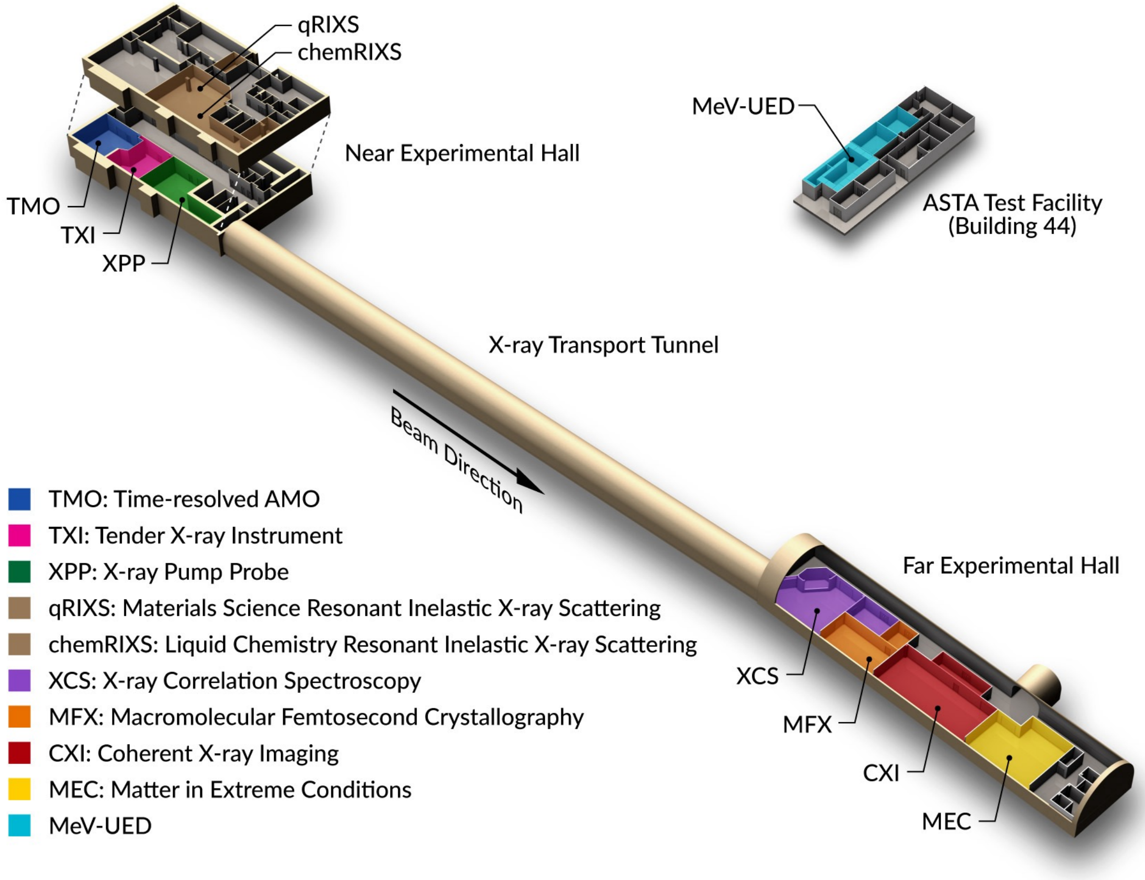


S. Gerber, et al., Science 357, 71 (2017)

LCLS instruments

LCLS – 8 X-ray instruments

– 2 soft x-ray hutches
– 1 Tender X-ray instrument (2keV-7keV)
– 5 hard X-ray instrument
– 1 ultrafast electron source



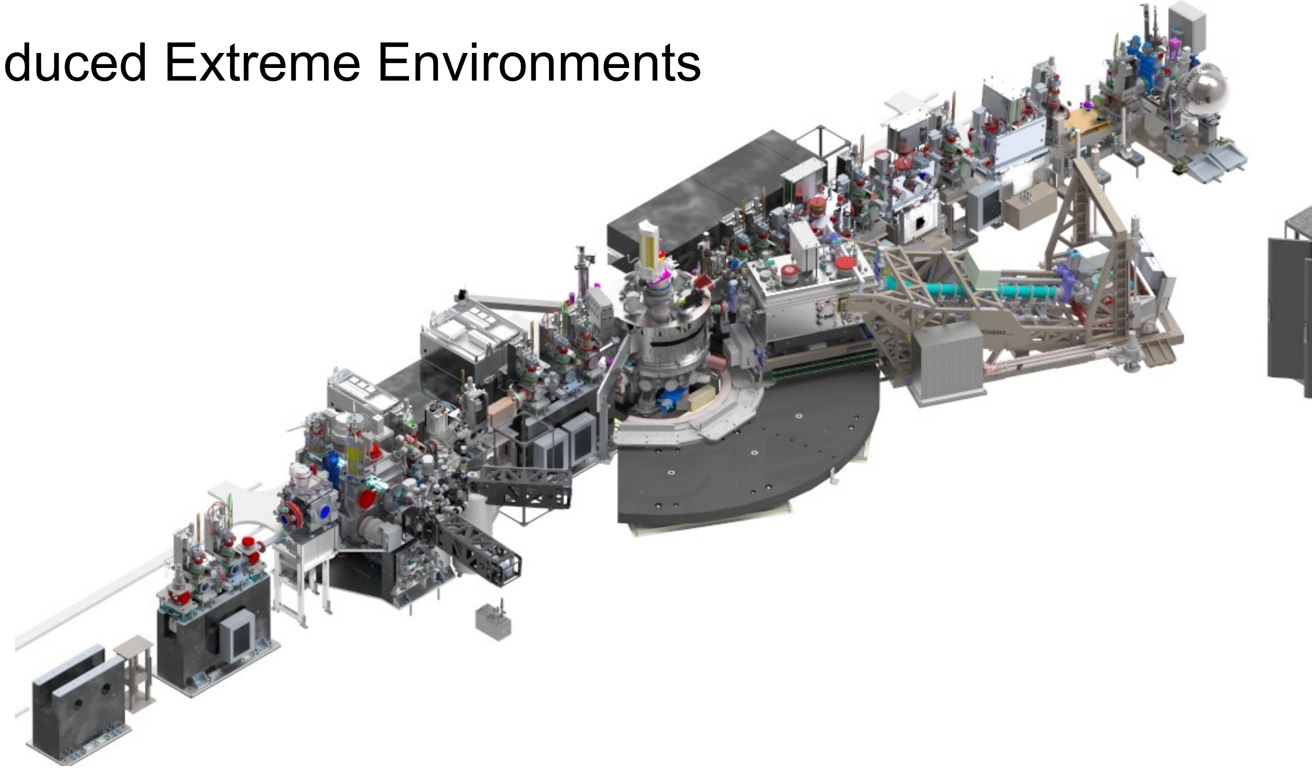
Because it is a linear source, often only one experiment runs at a time!

LCLS soft x-ray instruments

SLAC

Time-resolved AMO (TMO)

- Quantum Systems in strong fields – laser induced Extreme Environments
- Molecular reaction microscope



ChemRIXS

- Photochemistry - photocatalysis

qRIXS

- Quantum materials – strongly correlated systems

LCLS hard x-ray instruments

X-ray Pump Probe (XPP)

- Materials science, hard condensed matter

X-ray Correlation Spectroscopy (XCS)

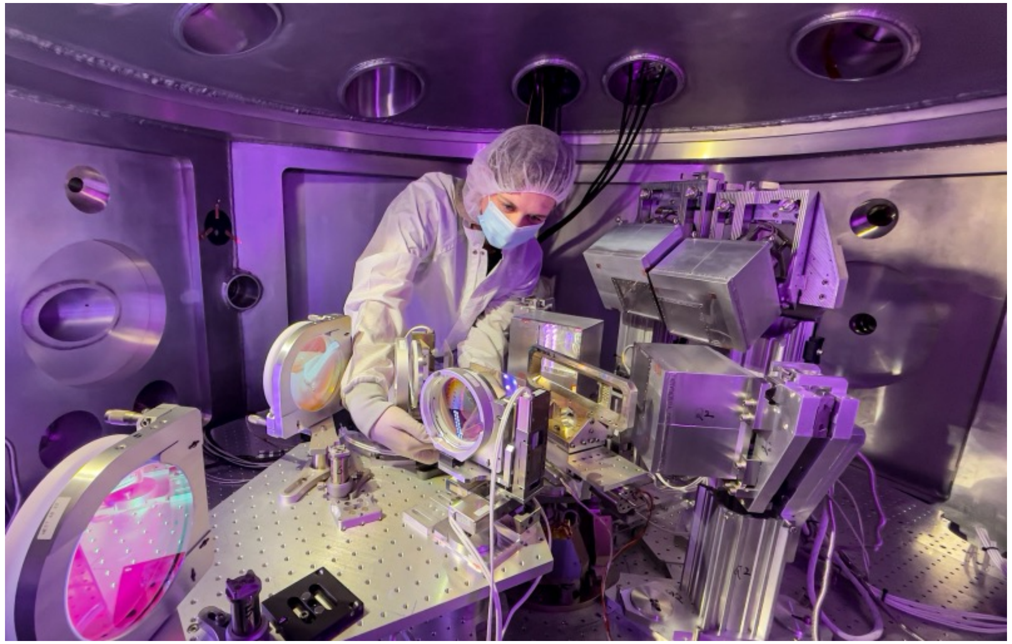
- X-ray correlation spectroscopy, soft condensed matter, solution phase chemistry

Macromolecular Femtosecond Crystallography (MFX)

- Biology at ambient conditions

Coherent X-ray Imaging (CXI)

- In-vacuum forward scattering instrument – Vacuum biology, gas phase photochemistry, non-linear x-ray science

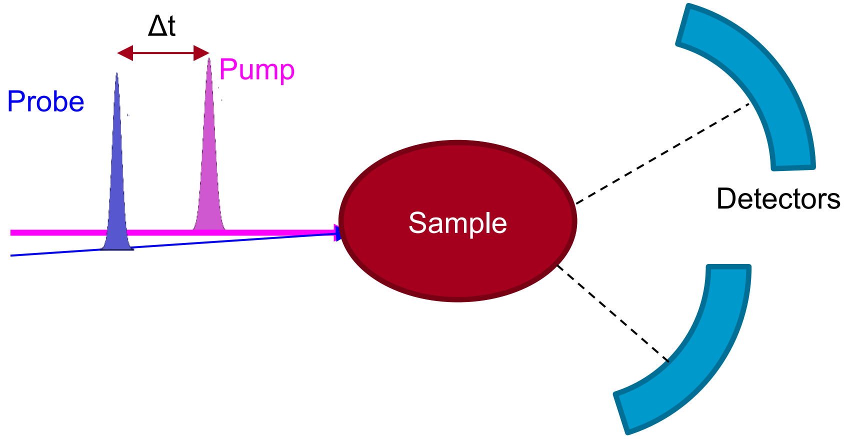


Matter in Extreme Conditions (MEC)

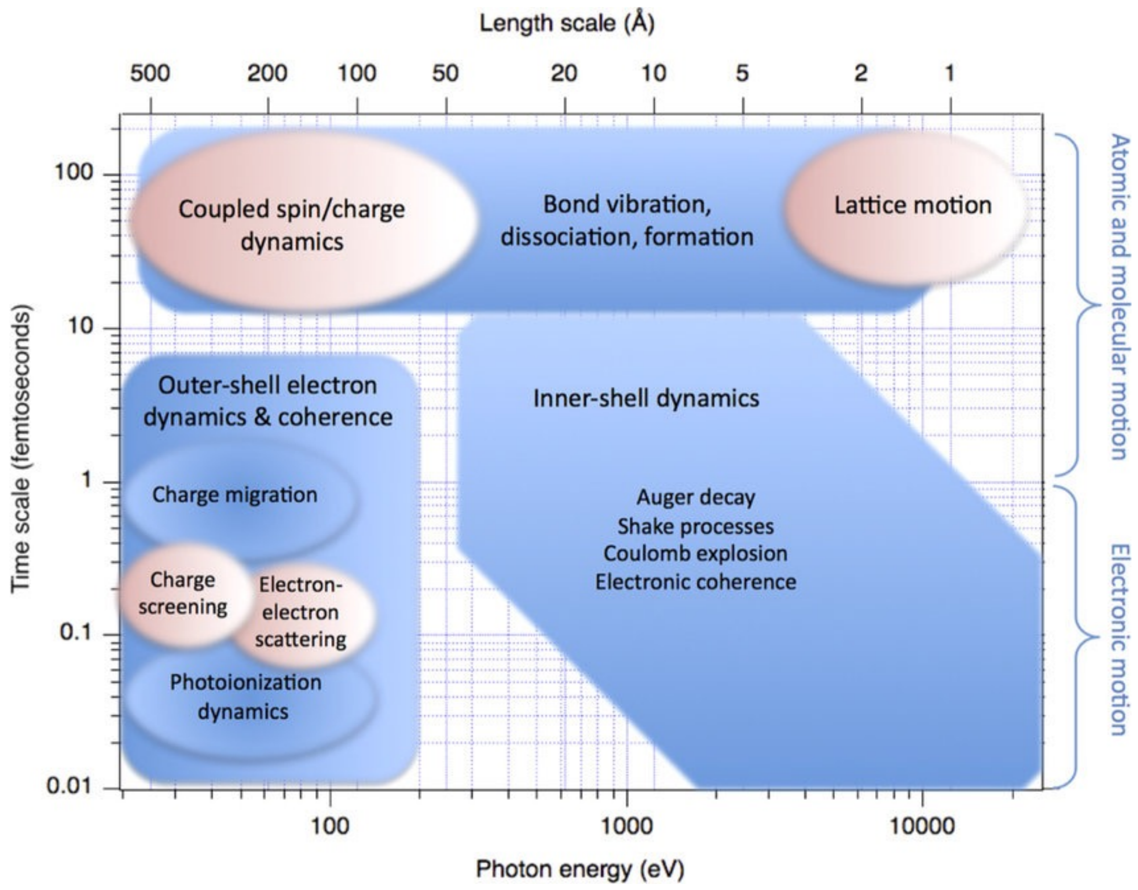
- Warm dense matter, high pressure, shock physics, imaging, fusion

Pump - Probe

- Well over half of LCLS experiments are laser pump – x-ray probe
- Timescales for which FELs are very suited fs-ns



Pump-Probe : evolution of relative signal with X-ray probe at different time delays Δt after excitation (probe)

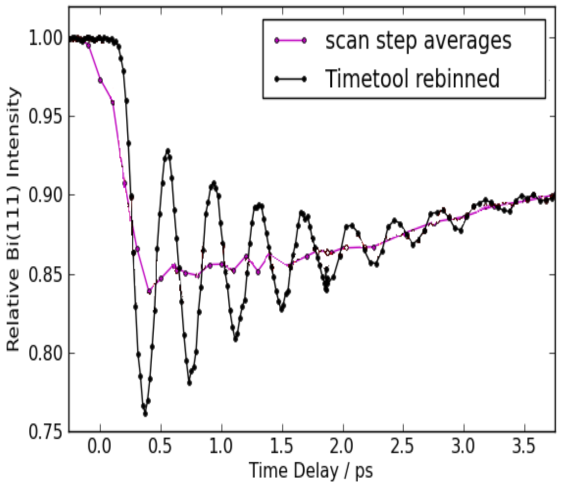


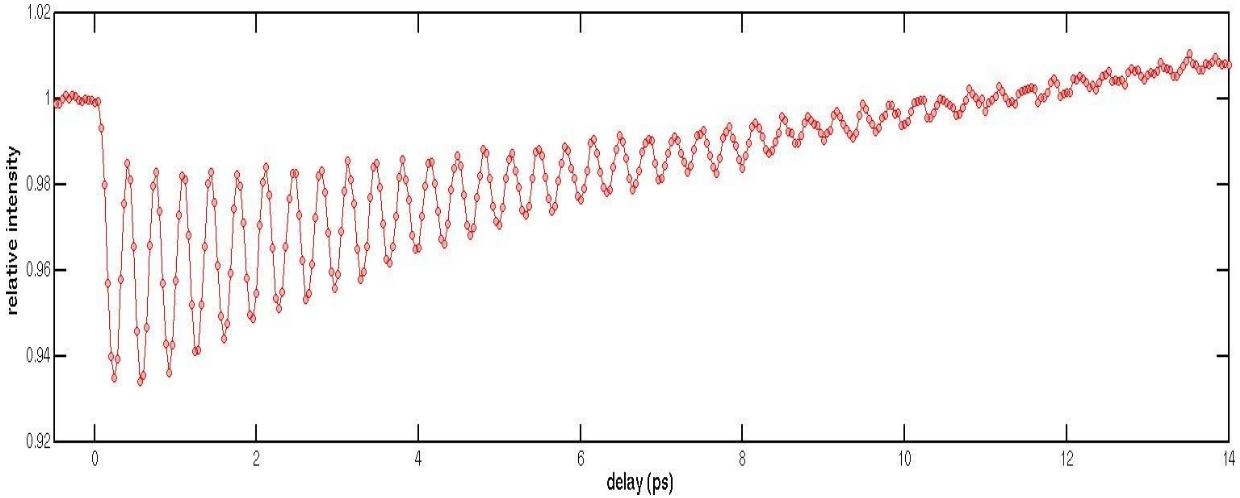
Lasers provide a precise t0

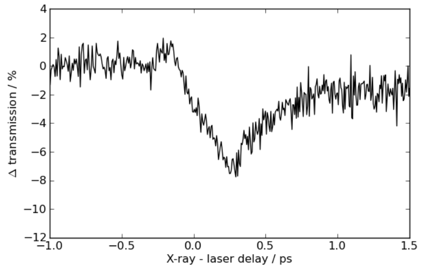
Young, Linda, et al. "Roadmap of ultrafast x-ray atomic and molecular physics." *Journal of Physics B: Atomic, Molecular and Optical Physics* 51.3 (2018): 032003.

Pump - Probe

Jitter in both the laser pump and x-ray probe signal causes ultrafast signal to be washed out. A timing diagnostic (timetool, arrival time monitor) is used to precisely measure (~20fs) the actual Δt between pump and probe





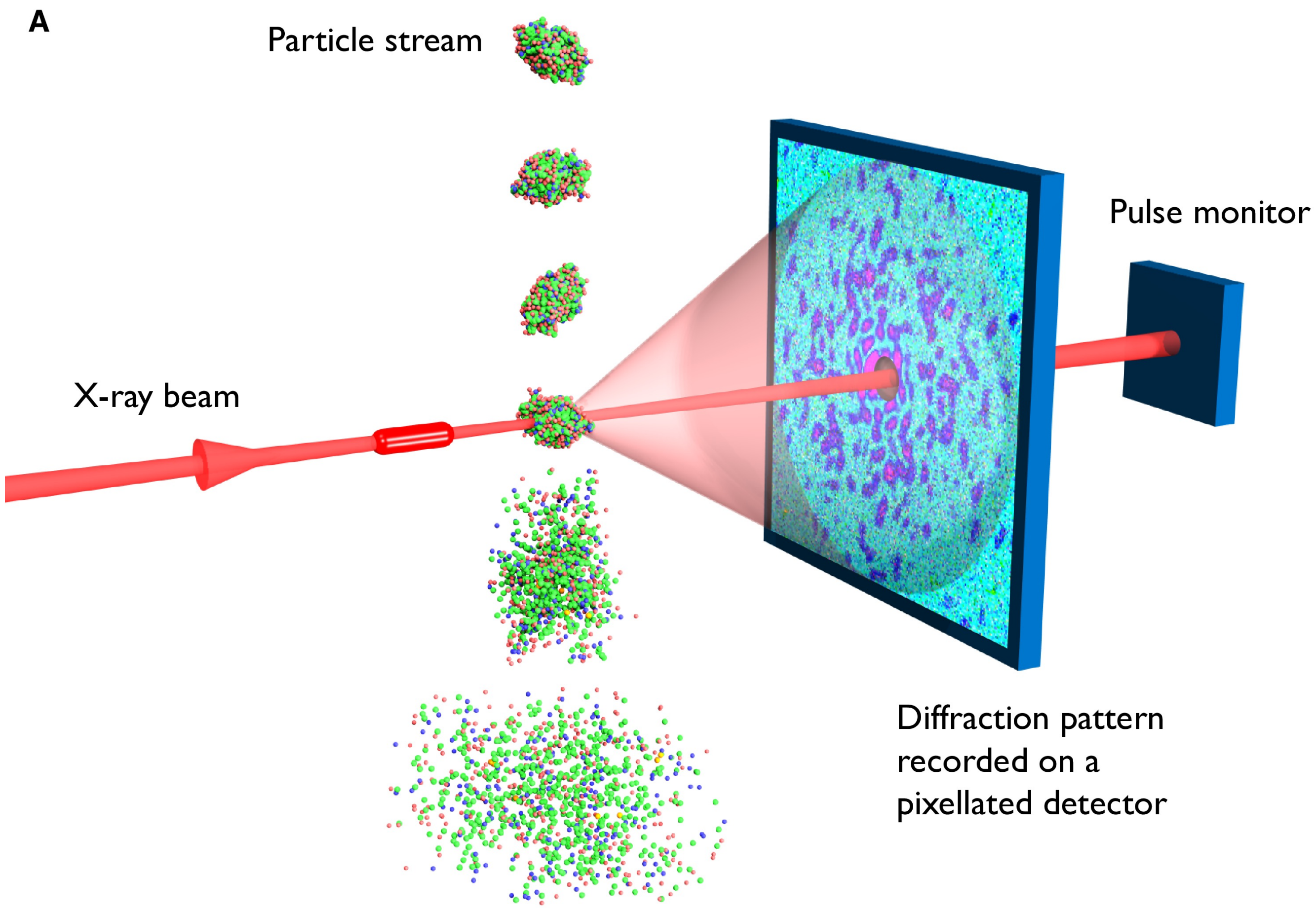


Courtesy XPP (Zhu et al.)

Different processes can be excited by different laser wavelengths – UV (bond dissociation), visible (biological processes), IR (heating), THz (lattice motion), etc

Diffract and Destroy, Serial experiments

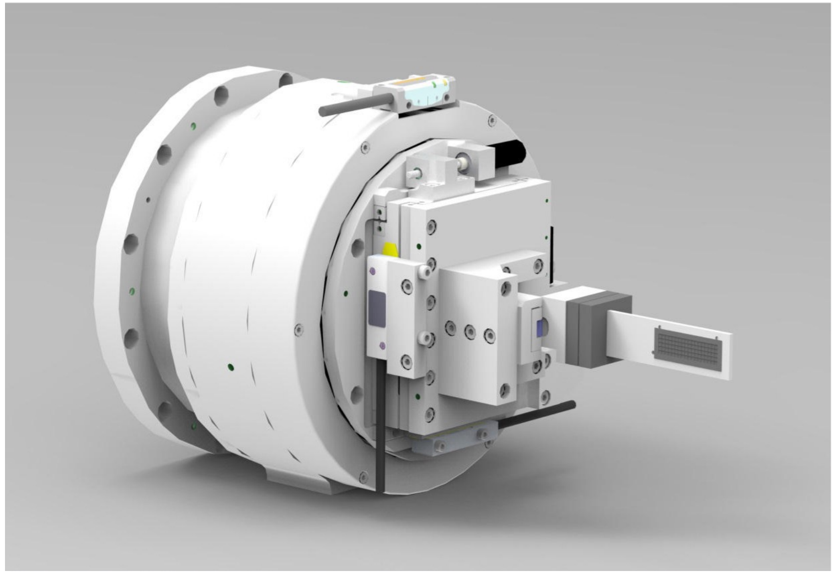
- Full flux FEL beams can destroy most samples
- The short pulse duration of a single FEL pulse means that the diffracted data is acquired before the sample is destroyed "diffract and destroy"
- FEL data is radiation damage free
- Counterintuitively, the more radiation damage sensitive a sample, the better suited it is for the FEL
- Need lots of sample – serial data

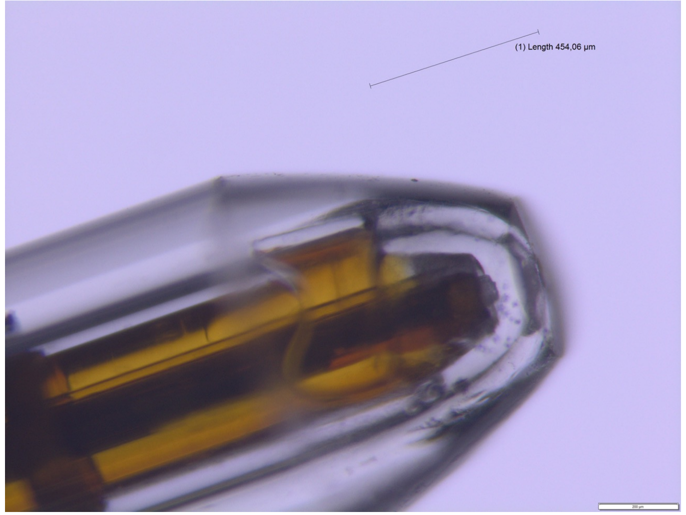


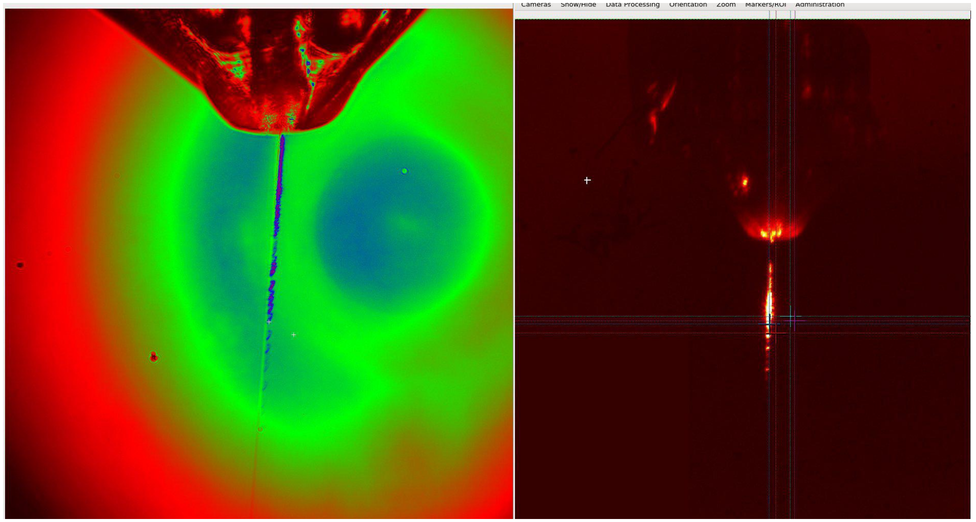
Sample delivery

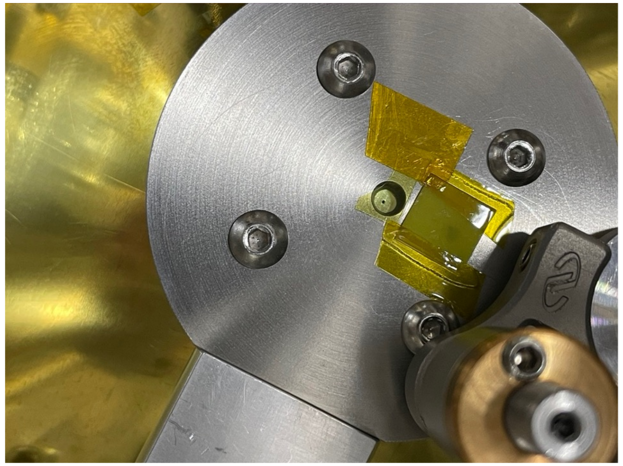
Different types of sample delivery for gases, liquids and solids to replenish the sample with each FEL pulse

- Liquid jets
- Gas cells
- Fast scanning fixed target stages









Detectors

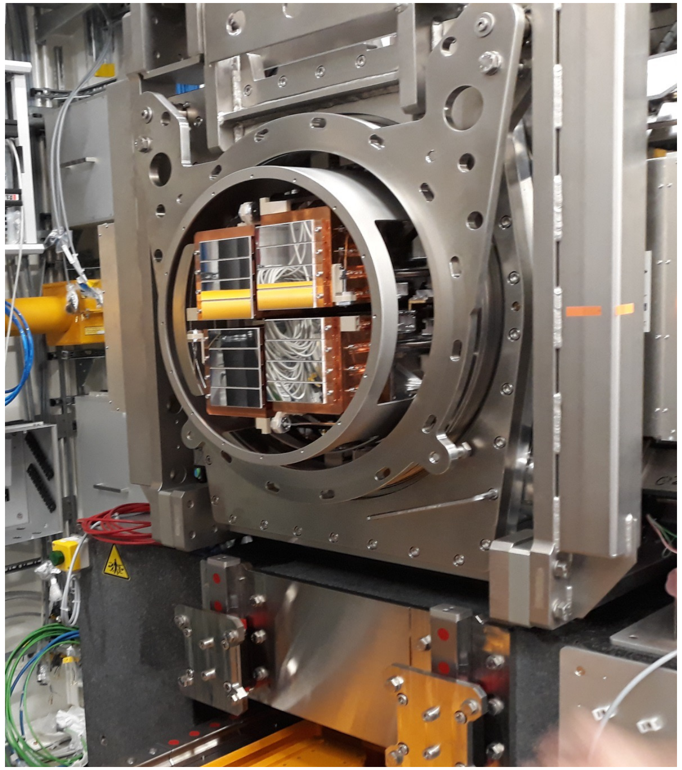
Almost every FEL has detectors that are optimized for their facility. This is totally unlike the case for storage ring experiments.

Also, because of the nature of FELs, one cannot in general either:

- Use signal averaging on the detector
- Do single photon analysis

Since the detectors are all developed locally, all have different software, and all have different idiosyncrasies.

Most likely your experiment will fail if you don’t pay careful attention to the detector.



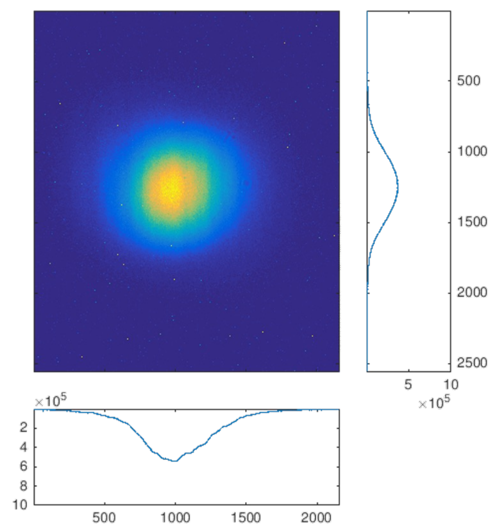
If you are coming to LCLS, ask for help. We have detector experts standing by.

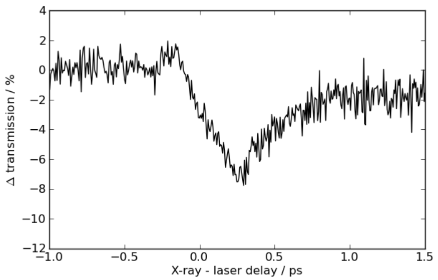
Data Analysis: Normalizing, Filtering, Binning

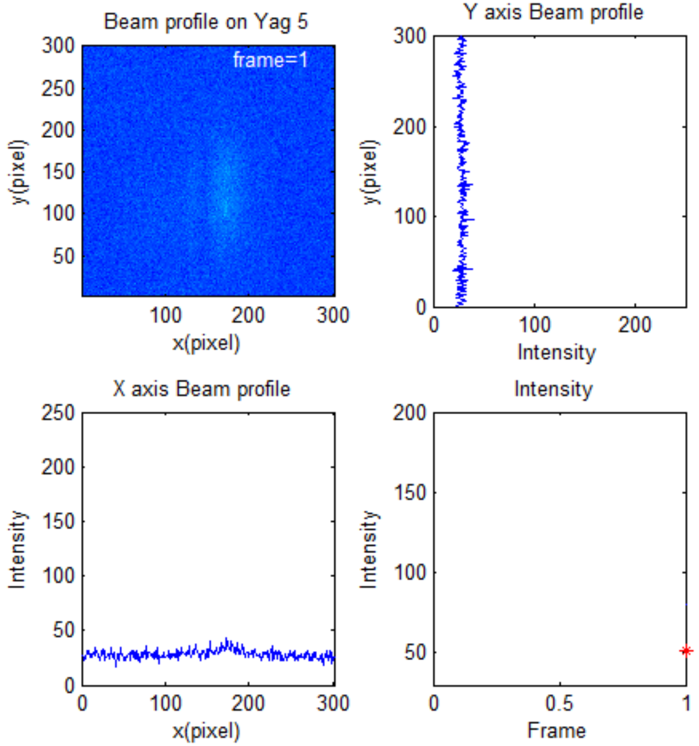
- Each X-ray Pulse is UNIQUE
- Each X-ray pulse fluctuates in many way

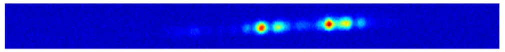
- It is critical to characterize every pulse with precision to the extent possible
- Diagnostics are critical

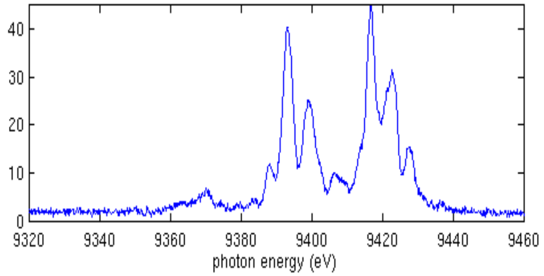
- Filtering
- Normalizing
- Binning
- Averaging



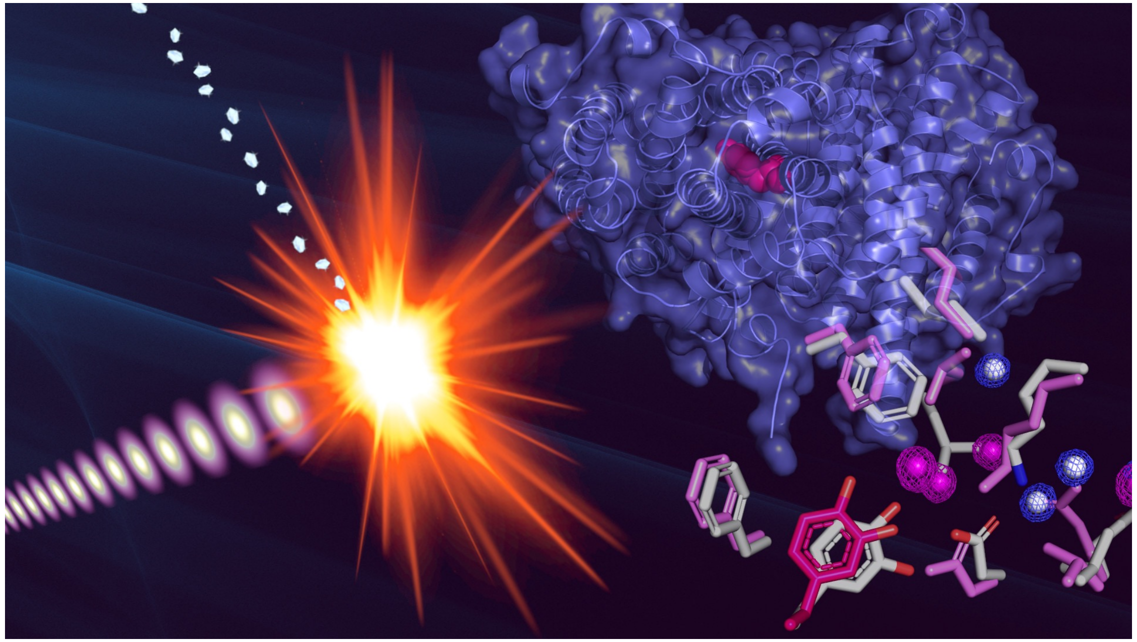








Radical enzyme system initiating DNA synthesis



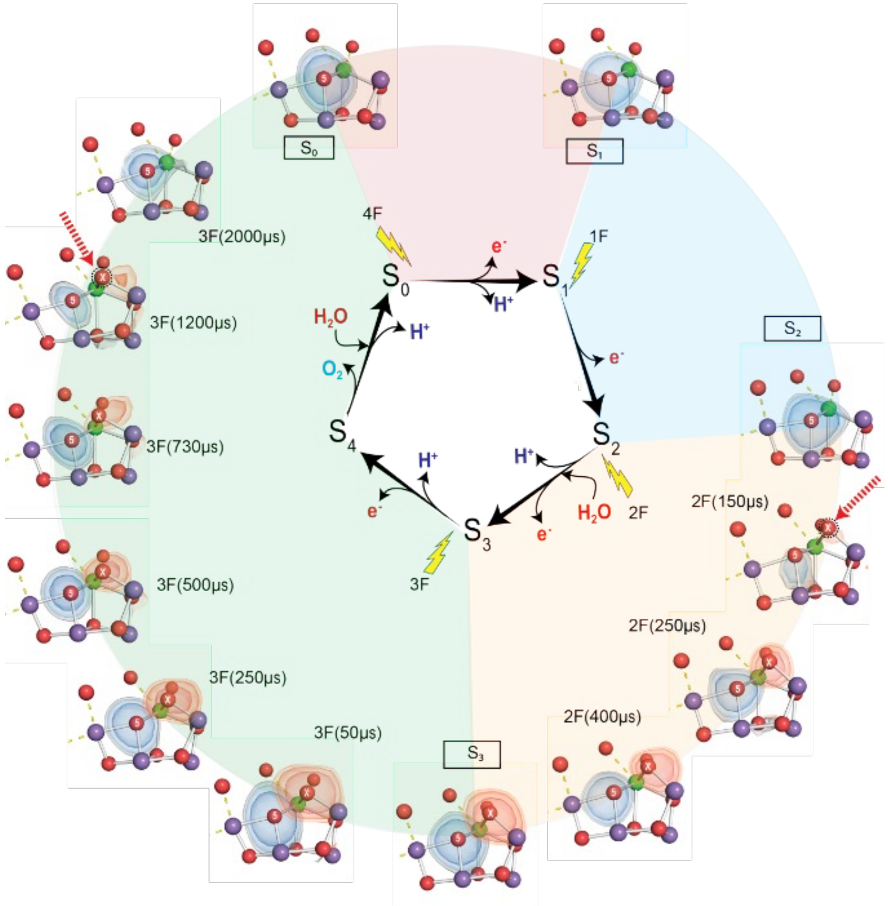
H. Lebrette et al. Science 382,109-113 (2023).
DOI:10.1126/science.adh8160.

The research team observed the atomic structure of a radical enzyme involved in ribonucleotide reduction, an essential step in DNA synthesis.

The ultrafast pulses from the LCLS outrun the effects of x-ray radiation damage, making it possible to image intact radicals inside of an enzyme for the first time.

- Small enzyme crystals were investigated at the LCLS X-ray free electron laser and synchrotrons (Swiss Light Source and SOLEIL)
- The radical-lost state (captured at the synchrotron) was compared to the active radical state, imaged with the femtosecond pulses coming from LCLS.
- The active radical state structure reveals how the radical is stabilized in the enzyme

Photosynthesis



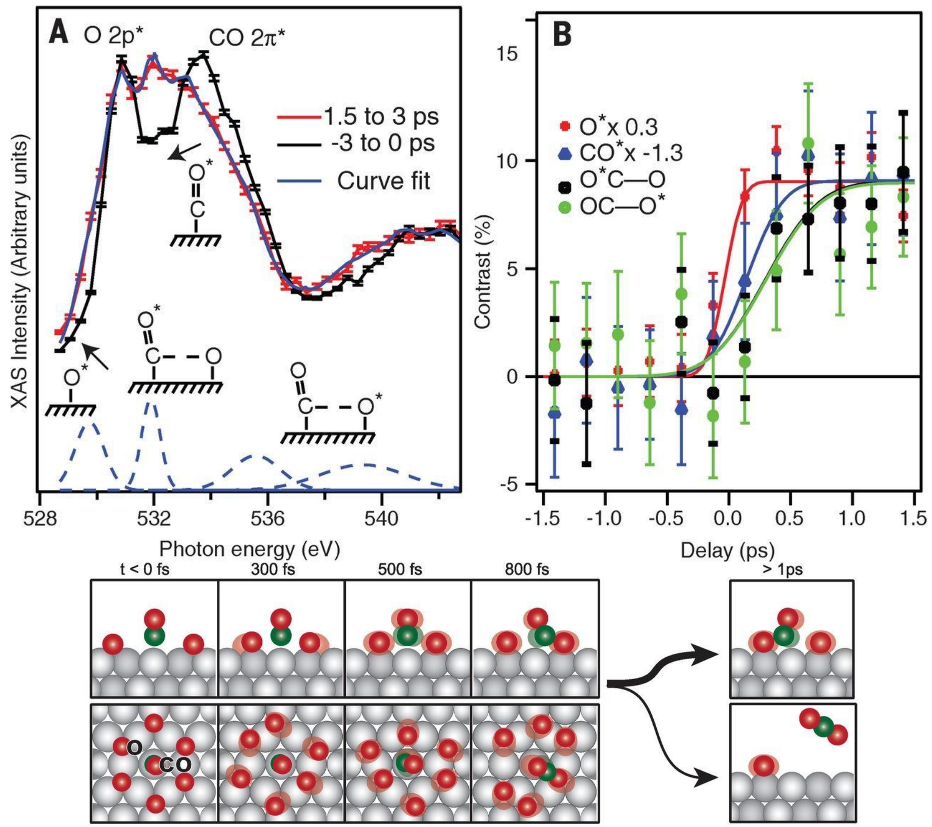
Time-resolved structural changes in the catalytic Mn_4CaO_5 cluster. Bhowmick *et al.* (2023) *Nature.*

Multi-modal experiments (Serial Femtosecond X-ray Crystallography and X-ray Emission Spectroscopy) can capture the atomic motions and electronic state of photosystem reaction intermediates

- LCLS has supported a scientific campaign led by the Yano group (Lawrence Berkeley National Lab) and collaborators to map the photosystem II dynamics along the Kok cycle
- The team captured the insertion of the water substrate (S_2 to S_3), the release of O_2, and the reset of the catalytic Mn_4CaO_5 cluster (S_3 to $[S_4] \rightarrow S_0$)

Transition States in Heterogeneous Catalysis

- Short-lived transition states determine the kinetics of a chemical reaction, and are key to understanding reactivity
- Ultrafast X-ray absorption spectroscopy can probe the electronic structure of species in the transition state region with elemental specificity
- Öström *et al.* probed the catalytic CO oxidation reaction on a ruthenium surface on an ultrafast time scale, following the evolution of the unoccupied valence electronic structure around the adsorbed O and CO after laser excitation
- Applications
    - Capturing short-lived transition states
    - Studying surface chemistry in heterogeneous catalysis



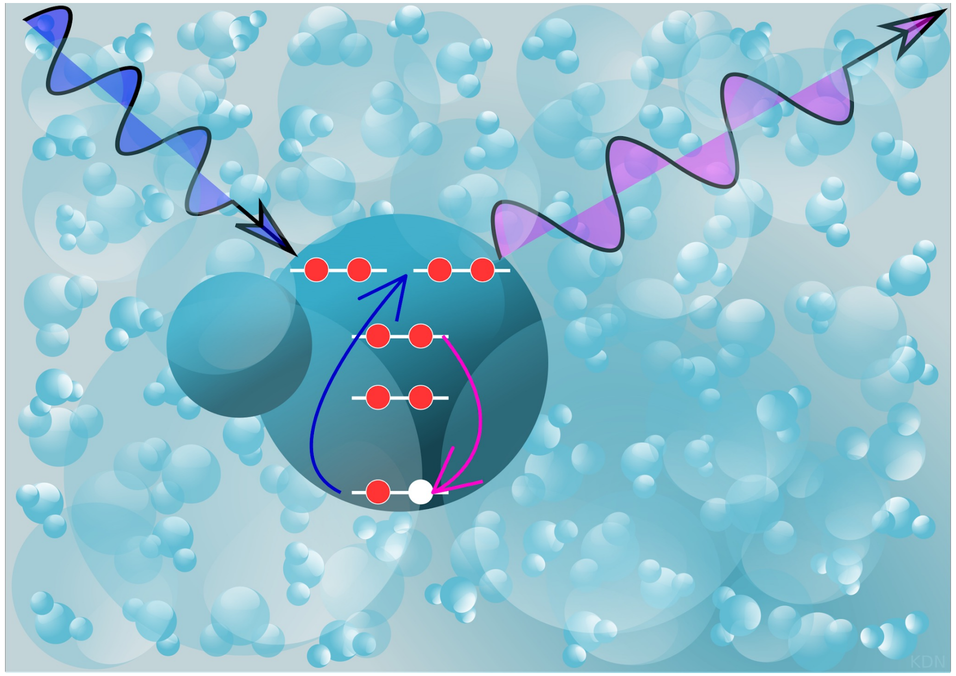
Time-dependent changes in the electronic structure, capturing activation, collision and the formation of a transition state.

Resonant inelastic X-ray scattering at the Soft X-ray Research (SXR) instrument of LCLS

Öström et al. (2015) *Science* 347: 978 – 982.

Free radicals at the shortest timescales

- Free radicals are critical in environmental remediation and nuclear waste processing, but studying them is challenging due to their short lifetime
- Resonant inelastic X-ray scattering can identify local, ultrafast $\pi \rightarrow \sigma$ transitions, which are masked in conventional UV spectroscopy
- Kjellson *et al.* identified the fingerprint of an aggressive oxidizing chemical by revealing the hidden signature of short-lived hydroxyl free radicals in water
- Applications
    - Capturing the evolving electronic structure and reactivity of free radicals in aqueous and heterogeneous environments
    - Investigating the electronic and magnetic properties of materials



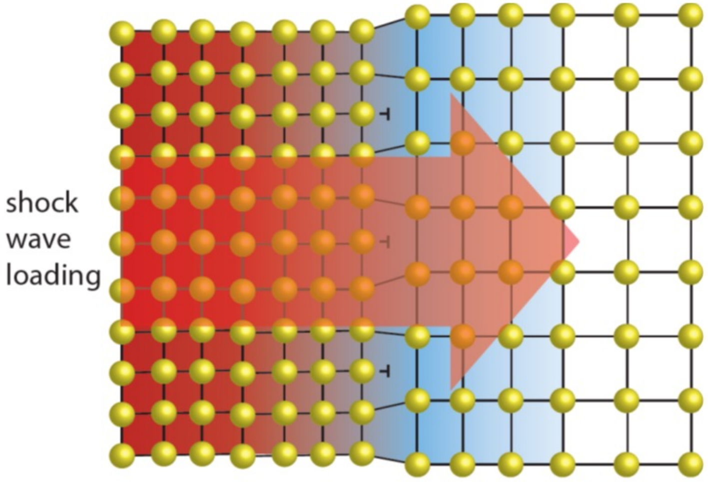
Emission signal of hydroxyl radical, carrying the unique chemical fingerprint.

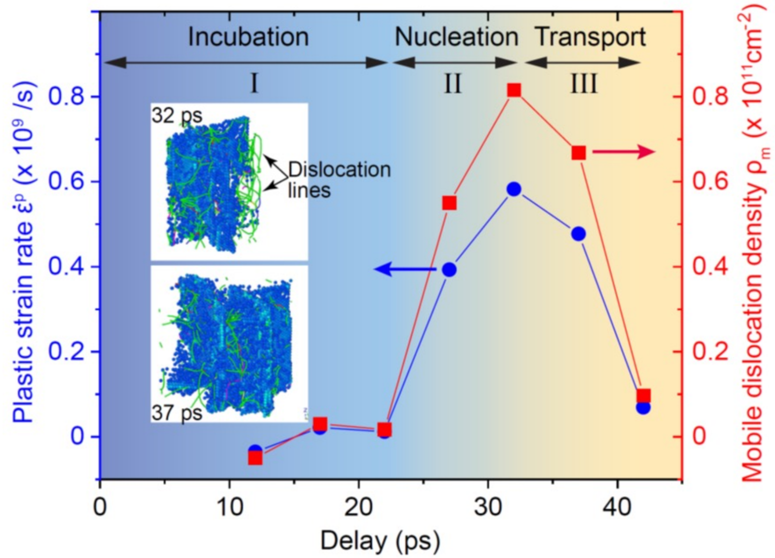
Resonant inelastic X-ray scattering at the Soft X-ray Research (SXR) instrument of LCLS

Kjellsson *et al.* (2020) *Phys Rev Lett* 124: 236001.

Plasticity formation and dislocation effects

- Understanding plasticity is crucial for applications such as high-performance ceramics
- Ultrafast electron diffraction can resolve the lattice dynamics of materials under high strain rates
- Mo *et al.* gained an understanding of the dislocation nucleation and transport processes during plasticity formation in shock-wave compressed aluminum
- Applications
    - Characterizing materials processing and additive manufacturing processes
    - Predicting dynamic material strength and designing stronger materials





Dislocation dynamics in aluminum under shock-wave induced compression.

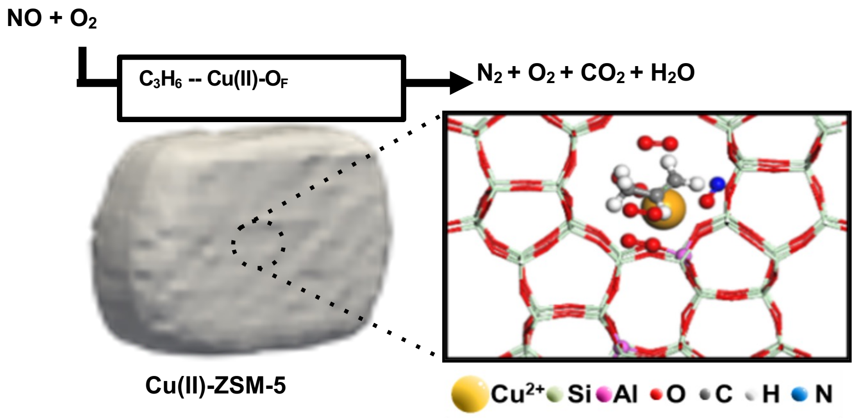
Time-resolved electron diffraction at the MeV-UED instrument

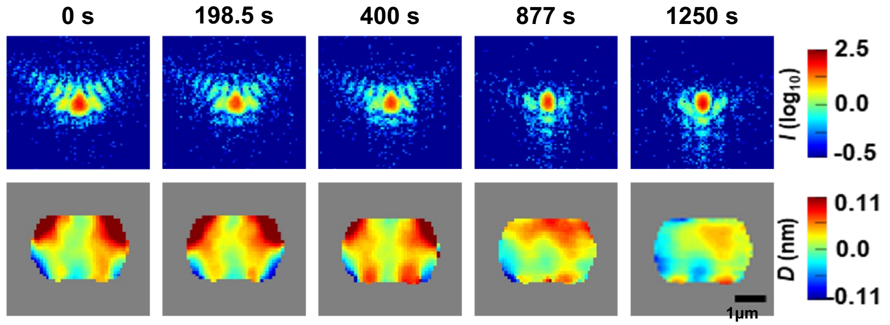
Mo *et al.* (2022) *Nat. Comm.* 13, 1055.

Time-resolved in situ imaging of a catalytic particle

- Structural inhomogeneities in zeolites are known to be important but their evolution is often poorly understood
- Time-resolved coherent X-ray diffraction imaging provides information about the particle shape and the kinetics of atomic displacement
- Kang *et al.* identified an unusual strain distribution during catalytic deoxygenation of NO_x with propene, caused by interactions between the reactants and the active sites

- Applications
  - Designing crystalline nano-catalysts with tunable properties
  - Understanding physical phenomena in additive manufacturing





Dynamic strain maps of operating nano catalysts.

Coherent X-ray Diffraction Imaging (CDI) at the X-ray Correlation Spectroscopy (XCS) instrument of LCLS

Kang *et al.* (2020) *Nat. Comm.* 11, 5901.

LCLS – Linac Coherent Light Source

At the beginning of 2019, almost 10 years after 1st light, LCLS began a major upgrade, the LCLS-II project.

The first stage of that upgrade, the installation of new undulators, was completed in 2021.

The second stage, the superconducting linac, began operations late last year.

Currently in commissioning and early science for the soft X-ray and Tender instruments: TMO, chemRIXS, qRIXS

TXI still under construction

Phase 1: 2020

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

Phase 2: 2023

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

Phase 3: 2027/8

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

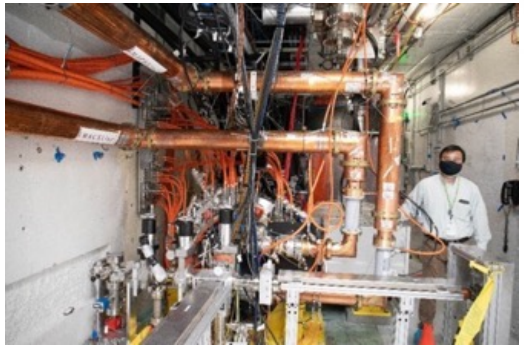
Phase 4: 2030/31

- **MEC Upgrade**
- 1 PW at 10 Hz, plus 1 kJ
- Dedicated experimental cavern

LCLS-II

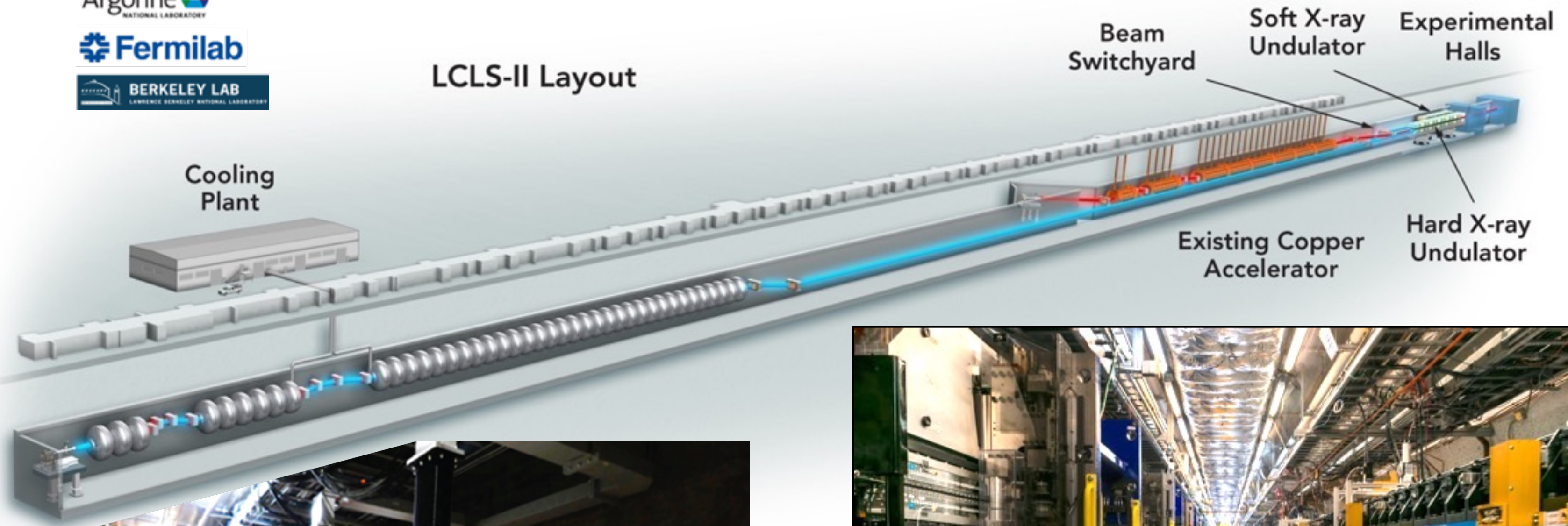
SLAC

Cryoplant commissioning has started



Injector operating

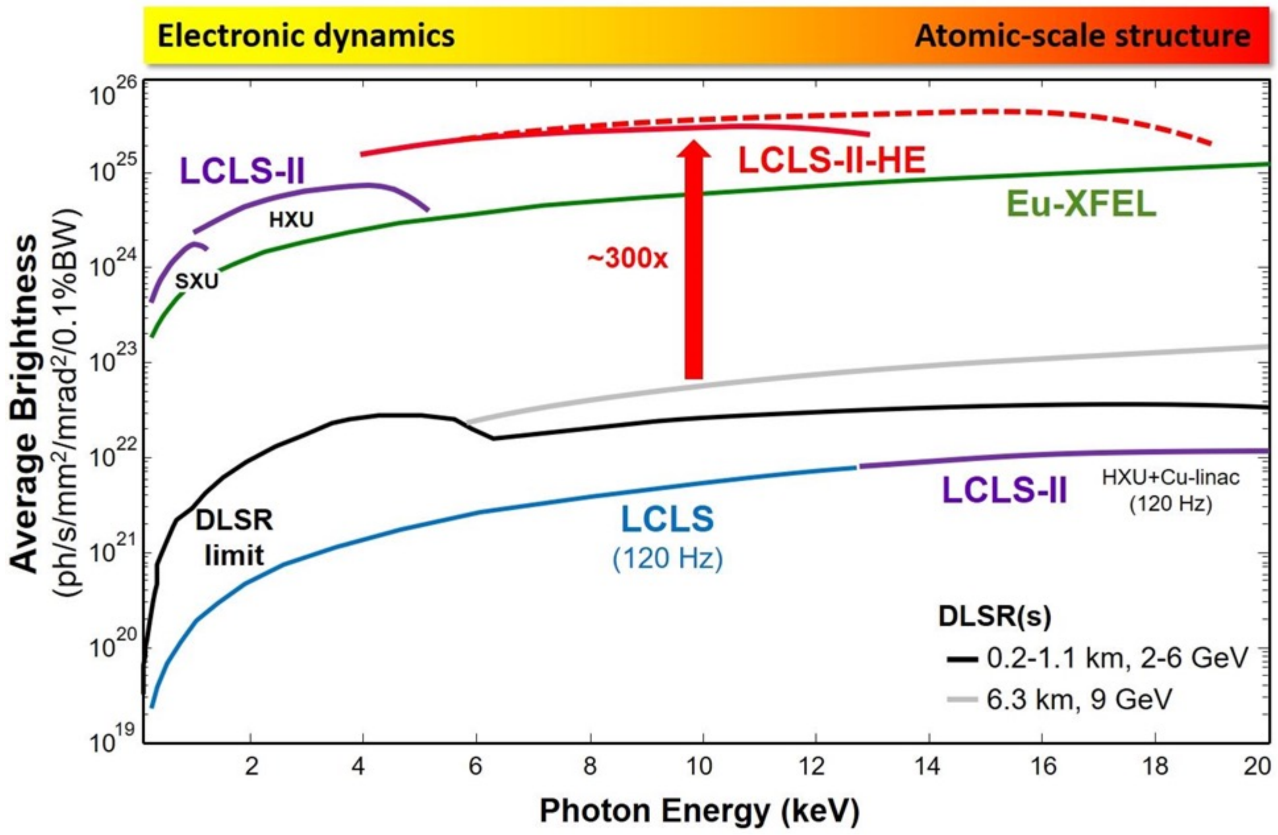
Jefferson Lab
Argonne
Fermilab
BERKELEY LAB



All cryomodules installed and welded

21 soft X-ray undulators
32 hard X-ray undulators
New Front End Enclosure

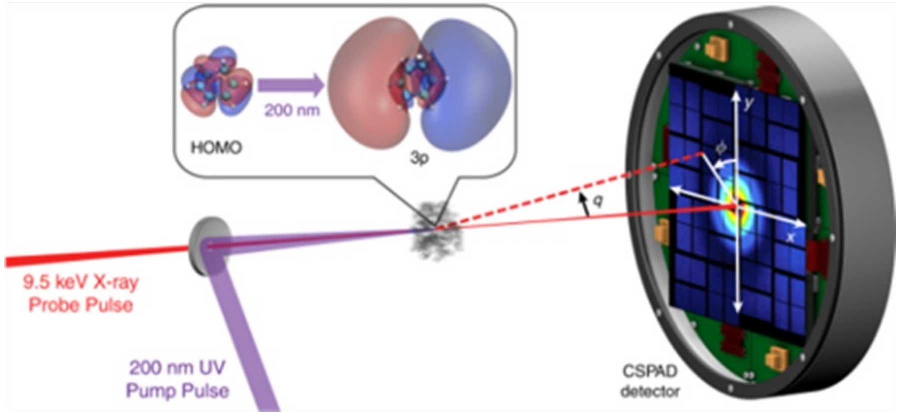
LCLS-II (HE) Science Case

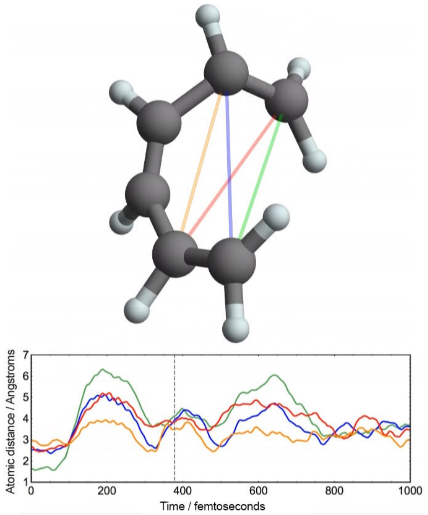


Demonstration to Application
Model Systems to Real World Systems

- Complex
- Varied

LCLS-II (HE) Science Case – molecular photodynamics

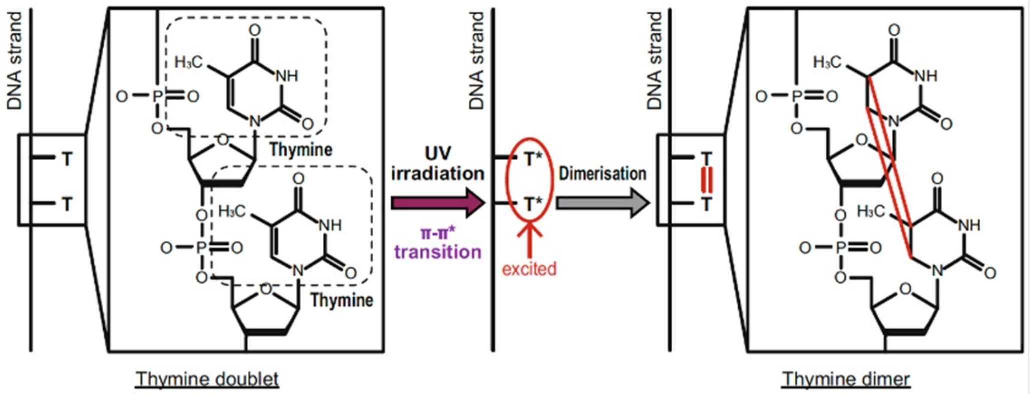




Current limitations:

- Time and spatial resolution
- Sample densities – vapor pressure
- Quantum yield

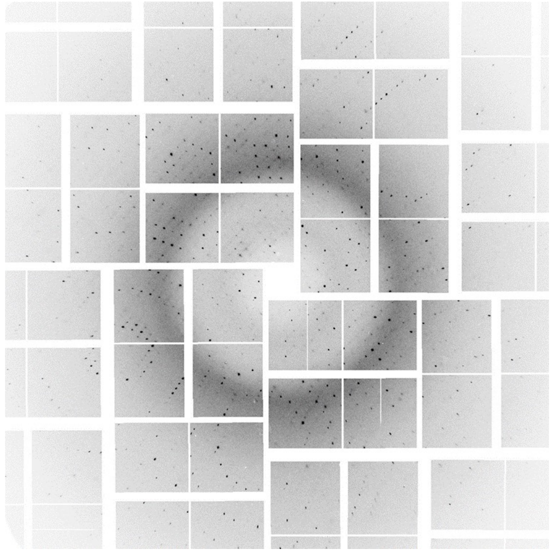
- UV irradiation causes covalent bonds creating cross-links between the thymine bases.
- Can cause DNA to improperly replicate or transcribe, potentially leading to genetic mutations and cancer

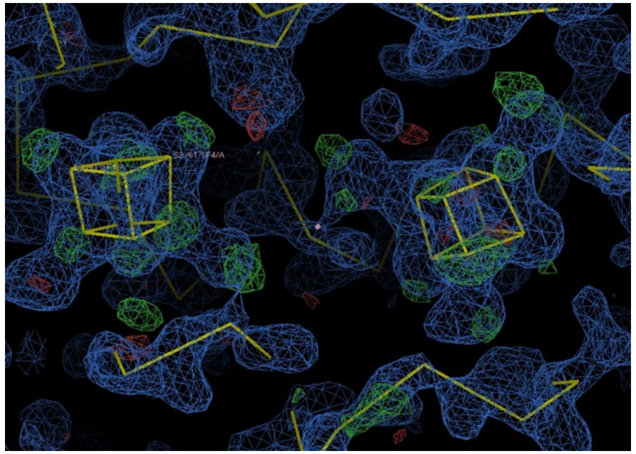


- Too complicated for quantum chemical modeling methods
- Soft X-ray spectroscopy found the lifetime of this state is <100fs but structure elucidation is unknown
- HE would allow for the study of the intermediates states of this low quantum yield, complex reaction

LCLS-II (HE) Science Case – metalloenzymes

Dynamics with SFX
- Photo-initiated processes (pump-probe)
- Mixing

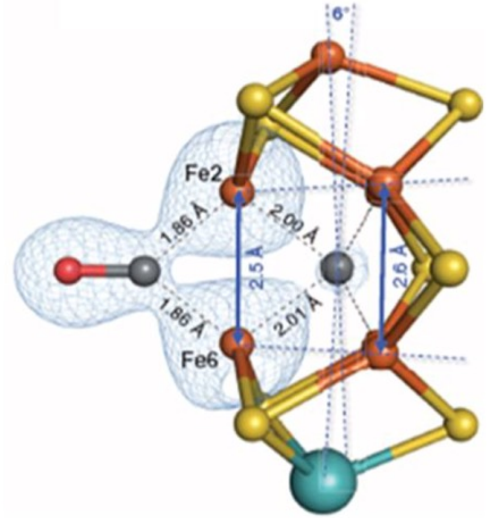




Limitations
- limited time points
- single conformations
- dynamics with large structural differences

Metalloenzymes – biological catalysts with a metal species are particularly susceptible to radiation damage at the metal site which is critical for its function
- Photosynthesis
- Nitrogen fixation

Nitrogenase – converts N2 to ammonia (NH3) which is bioavailable - an energy efficient enzyme in contrast to energy intensive industrial processes which to produce ammonia for fertilizer



LCLS-II-HE will allow for the study of complex systems such as nitrogenase

Opportunities for Early Career Scientists

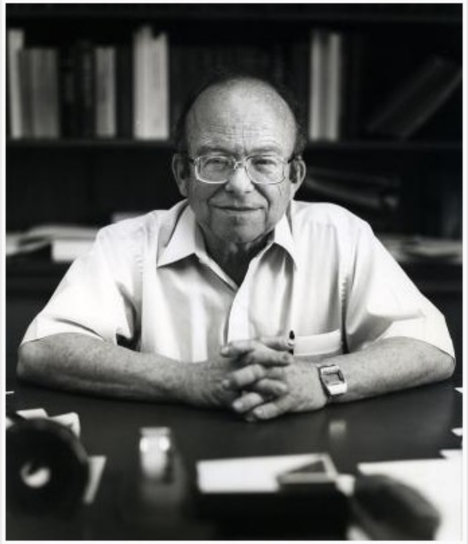
In addition to normal graduate and post-graduate research positions, there are also a few highly competitive prestigious early-career fellowships awarded each year.

Details can be found on the SLAC website:

https://careers.slac.stanford.edu/

NXS Lecture - Mengning Liang:
"Introduction to X-ray Free Electron Lasers"

Panofsky Fellowship Overview



The Panofsky Fellowship honors SLAC National Accelerator Laboratory's founder and first Director, Wolfgang K. H. Panofsky. It is intended to recognize exceptional and promising early career scientists who would most benefit from the unique opportunity to conduct their research at SLAC National Accelerator Laboratory. While the scientific direction of the candidates is expected to have some overlap with existing programs, an emphasis will also be placed on the potential for innovation and growth of new opportunities, aligned with the overall mission and values of the laboratory, as their career develops. The intent is to foster the creativity and high achievement to which W.K.H. Panofsky devoted himself both as a researcher and as a visionary leader in enabling fundamental science research.

The Fellowship celebrates **W.K.H. Panofsky's breadth of activities** and is awarded without regard to a candidate's particular specialty within our programs. The candidate's research plan should encompass one or more areas within the general scope of the **science program at SLAC**:

- Accelerator science & advanced accelerator research
- Applied Energy research
- Biosciences
- Chemical science
- Computer science
- Elementary particle physics
- High energy density matter
- Material and condensed matter science
- Particle astrophysics and cosmology
- X-ray science, including ultrafast science and advanced X-ray instrumentation, at LCLS and SSRL

Applicants are encouraged to contact **OCRO@slac.stanford.edu** to find out the leads of a program to find out more details about the program and the context for developing their proposed research plan as a Panofsky Fellow.