Ultrafast Science with X-ray FELS

- X-ray laser capabilities
- Survey of new science with X-ray FELS
- Ultrafast science with LCLS

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Imperial College

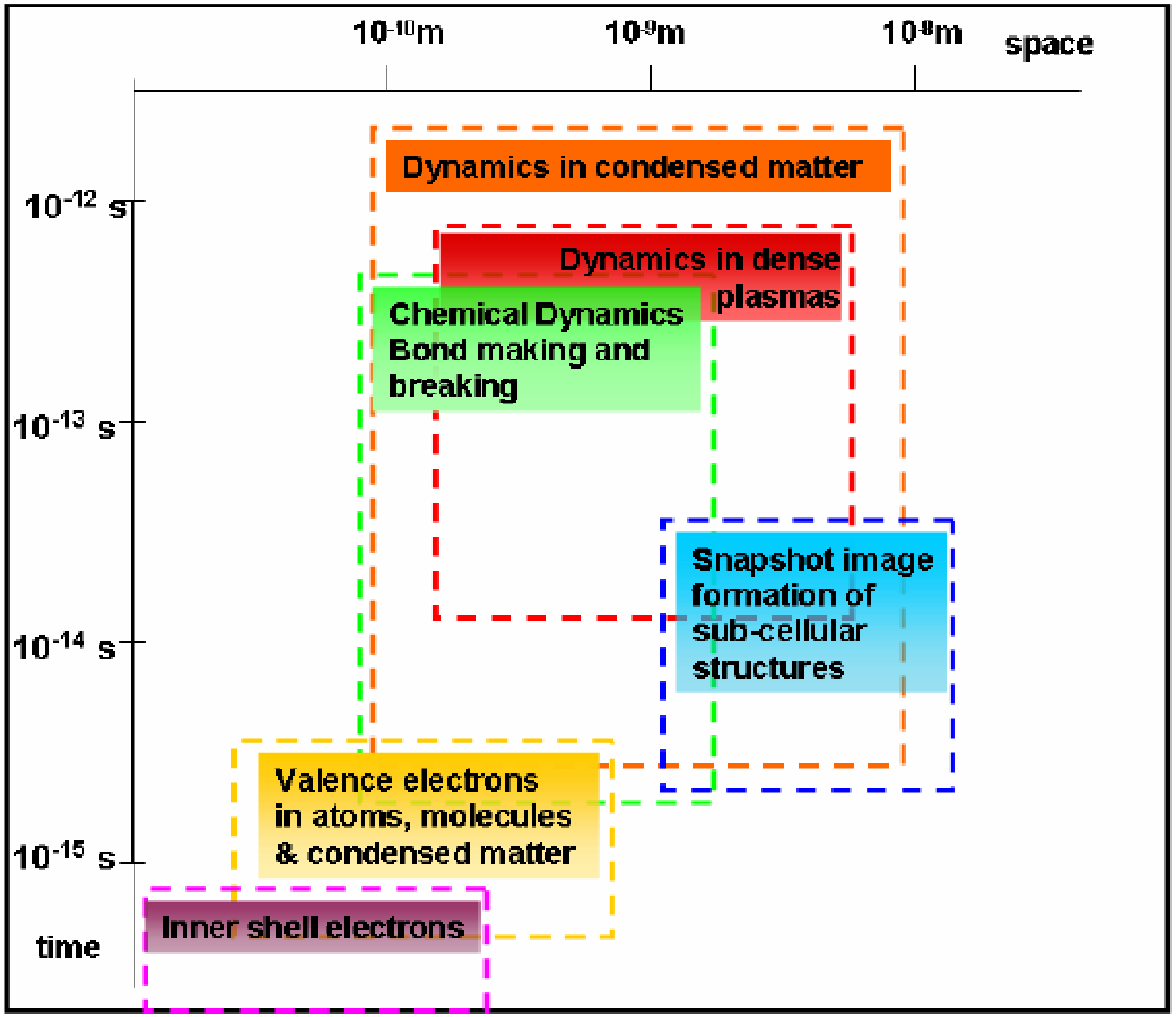
Frontiers In Science for the 21st Century Include

- ***Nanometre scale imaging of arbitrary objects in their native state:*** *Capturing a living cell at nanometre resolution*

- ***Measuring the mechanisms of physical, chemical and biochemical processes at the atomic scale:*** *Making molecular movies*

- ***Controlling electronic processes in matter:*** *Directing attosecond dynamics*

Nanometer Spatial Resolution and Femtosecond Temporal Resolution are Needed to Meet These Challenges



The science calls for:

- **ULTRAFAST**
- **HIGH BRIGHTNESS**
- **HIGH REP-RATE**
- **X-RAY**

light sources

- **X-ray laser capabilities**

- Survey of new science with X-ray FELS

- Ultrafast science with LCLS

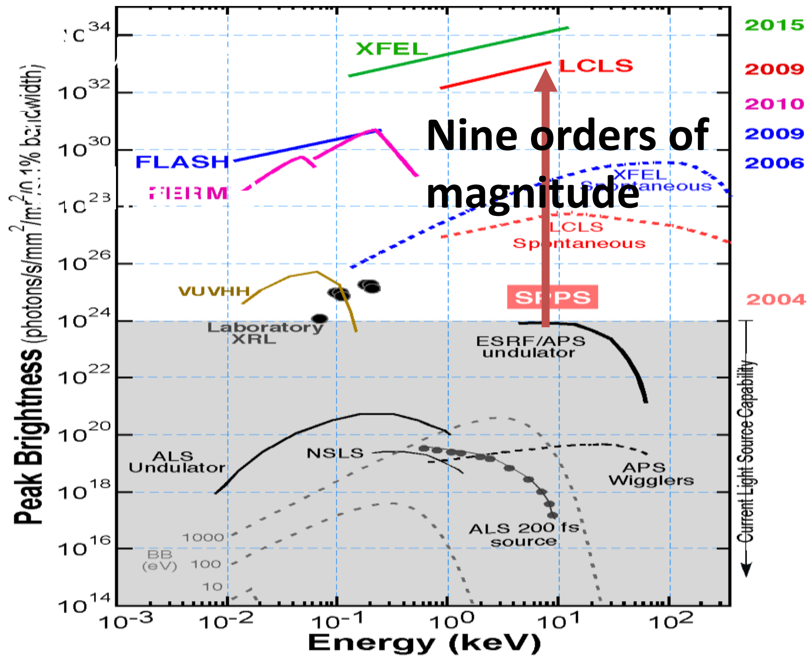
Free Electron Laser Capabilities

FELs v Synchrotron

- 10^9 Brighter

- 10^{-4} Shorter pulse

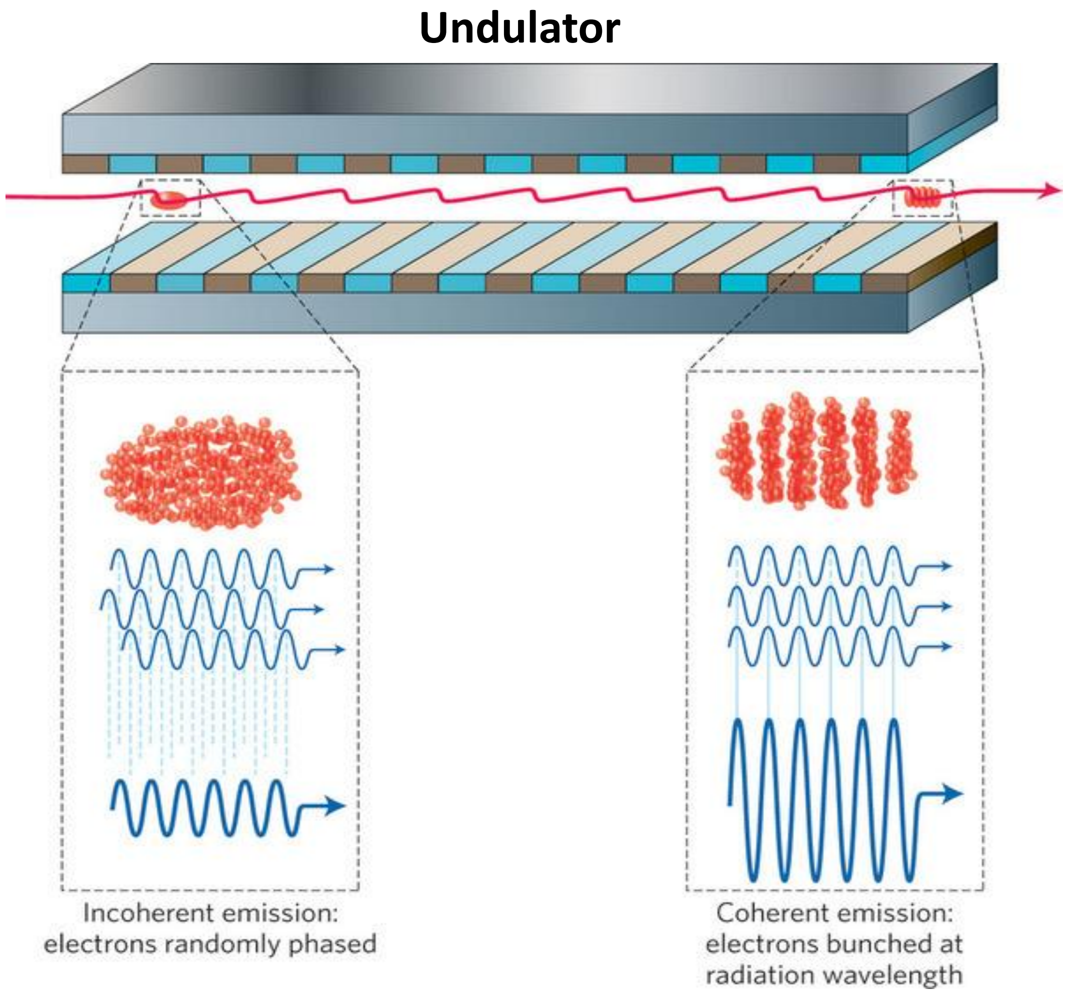
- Coherent



- High temporal resolution with <20fs pulses
- Pulses partially coherent
- Multi-keV photons for structural methods (e.g. XAS, IXS, X-ray diffraction)
- High peak brightness at wavelengths <0.1nm for single-shot imaging techniques

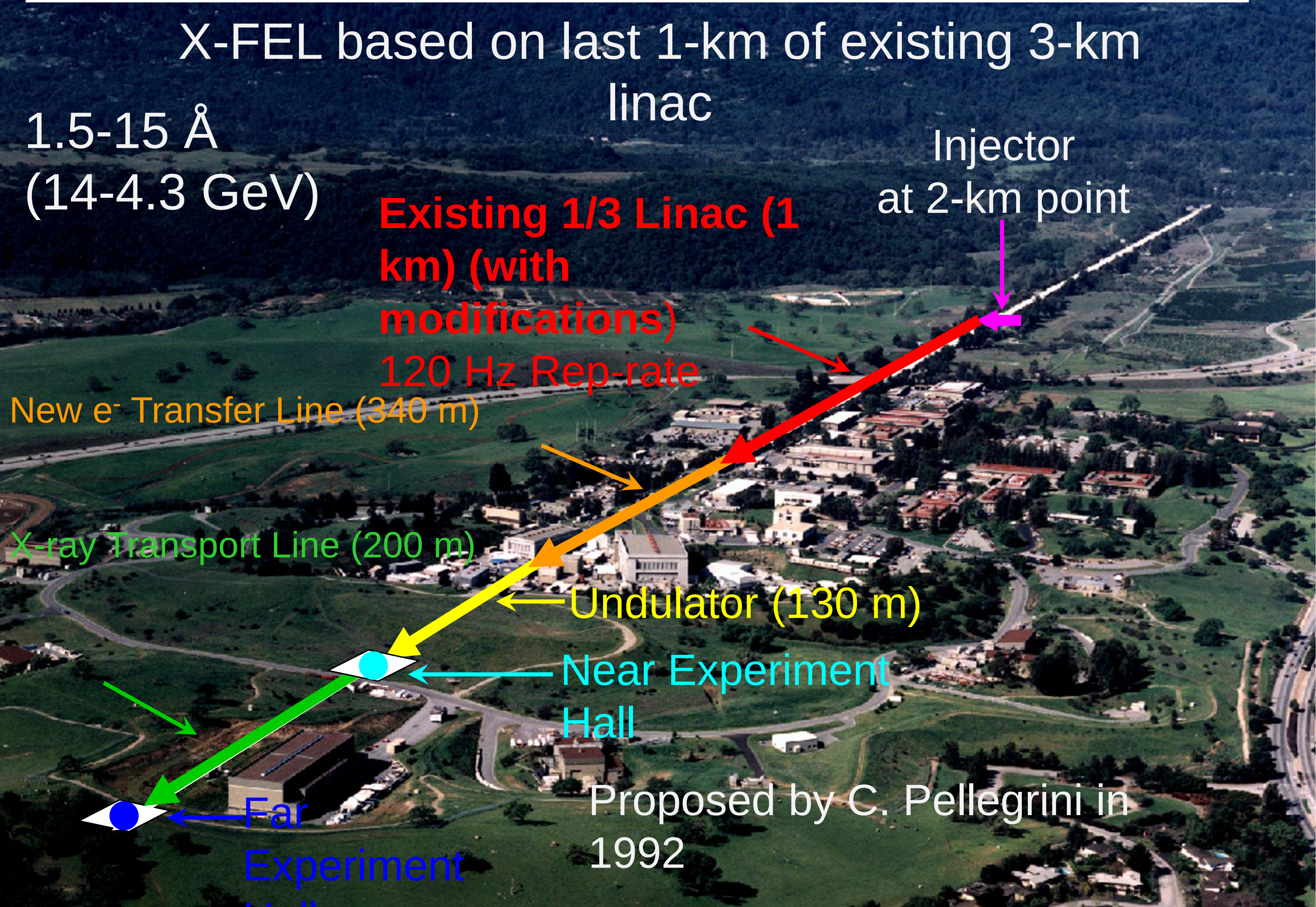
SASE (Self Amplified Spontaneous Emission) Operation for Coherent High Brightness Hard X-rays

Input
Low emittance relativisitic electron bunch



Output
partially coherent, high brightness, short pulse of hard X-rays

Linac Coherent Light Source at SLAC



September 12, 2012

Photon Beam Parameters	**symbol**	**hard x-rays**	**soft x-rays**	**short pulse soft**	**short pulse hard**	**unit**
Fundamental wavelength	λ_r	6.2-1.3	25.8-6.2	25.8-6.2	6.2-1.3	Å
Photon energy	$\hbar\omega$	2000-9600	485*-2000	485*-2000	2000-9600	eV
Final linac e^- energy	γmc^2	6.7-14.7	3.3-6.7	3.3-6.7	6.7-14.7	GeV
FEL 3-D gain length	L_G	3.3	1.5	~1.5	~3.3	m
Photons per pulse	N_γ	2	20	0.5	0.2	10^{12}
Peak brightness	B_{pk}	20	0.3	?	?	10^{32} §
Average brightness (120 Hz)	$\langle B \rangle$	160	8	?	?	10^{20} §
Photon bandwidth (fwhm)	$\Delta\omega/\omega$	~0.2-0.5	~0.2-1.0	?	?	%
Bunch charge	Q	0.15	0.25	0.02	0.02	nC
Init. bunch length (rms)	σ_{z0}	0.65	0.65	0.23	0.23	mm
Final bunch length (rms)	σ_{zf}	7	20	~1	~1	μm
Final pulse duration (fwhm)	$\Delta\tau_f$	50-250	70-400	<10	<10	fs
Final peak current	I_{pk}	3.0	1.0	~3	~3	kA

LCLS Parameters - under development

Hard X-ray self seeding is under development (with Argonne). Hardware is installed. Testing is ongoing.

Simultaneous delivery of X-rays to two hard X-ray hutches is under development.

Production of longer wavelength X-rays is under development.

Thz radiation is being tested.

Two color double pulse using slotted foil is under development.

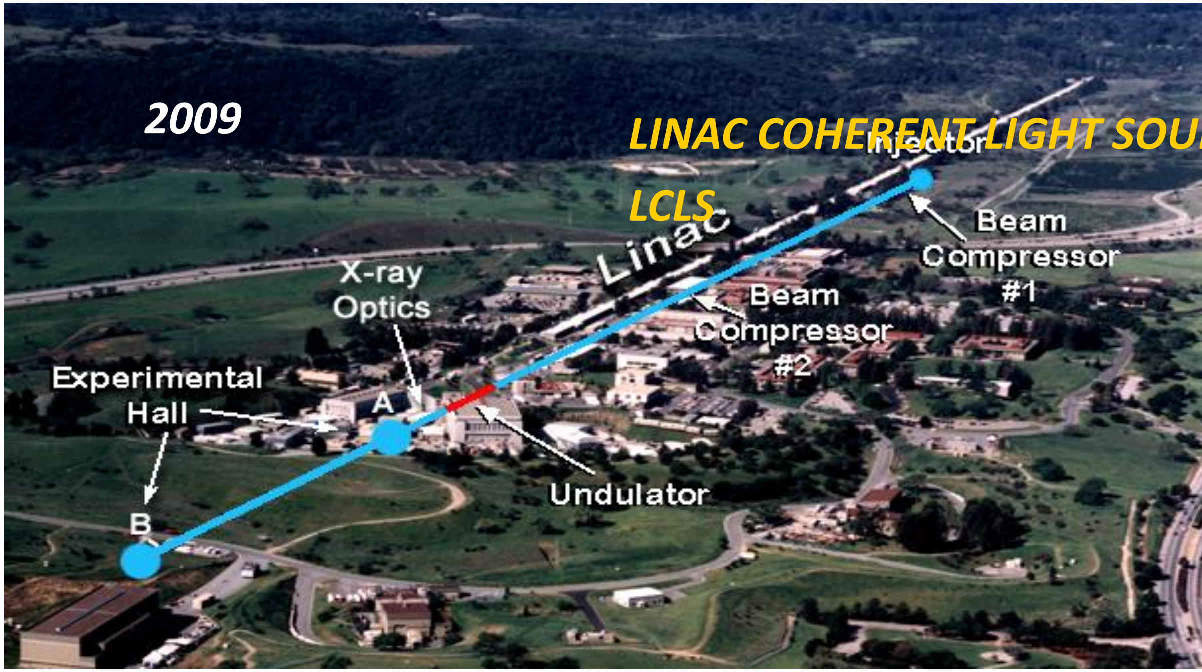
Multi-bunch is under development.

Double pulse: a double slotted foil to produce pulse pairs 20-100fs separation is now available.

Shorter pulse length using BC2 slots is now available.

Hard X-ray projects

X-ray SASE Free Electron Lasers



XFEL in Hamburg: A High Rep Rate SASE Machine
~ 10,000 shots per second

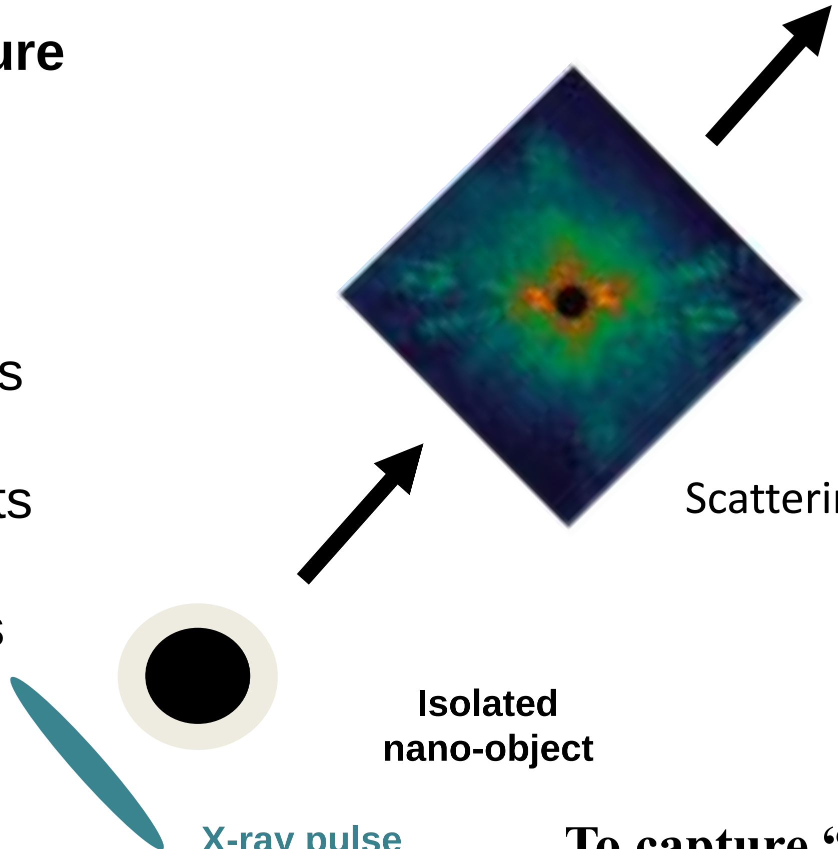
- X-ray laser capabilities
- **Survey of new science with X-ray FELS**
- Ultrafast science with LCLS

IMAGING NANOSCALE STRUCTURES

Imaging of Isolated Objects by Coherent Diffraction Imaging

Instantaneous capture of:
Shape
Atomic Structure
Magnetic structure
Electronic properties

in Nanoscale Objects
AND
Biological Systems



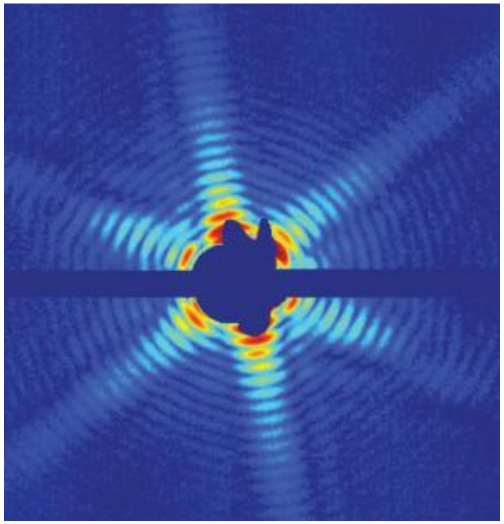
To capture "soft" systems like biomaterials need to use "Diffract and Destroy"

Recent Results from LCLS

LETTER

doi:10.1038/nature09748

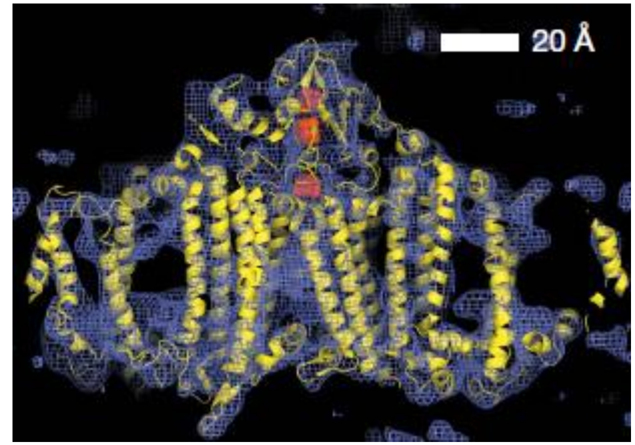
Single mimivirus particles intercepted and imaged with an X-ray laser



LETTER

doi:10.1038/nature09750

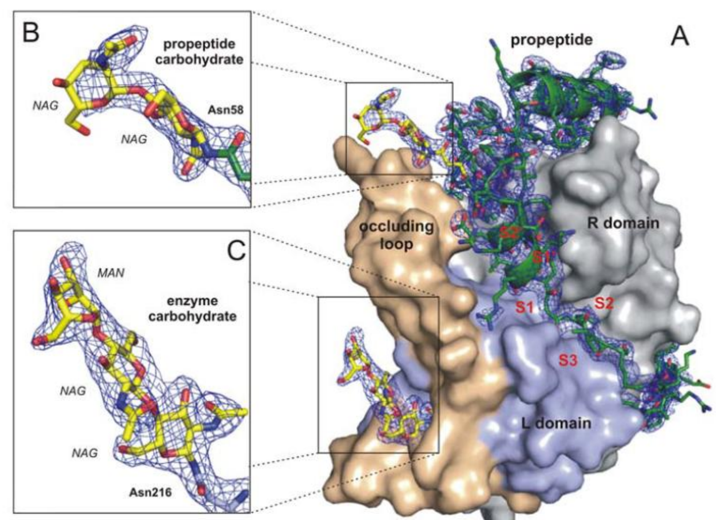
Femtosecond X-ray protein nanocrystallography



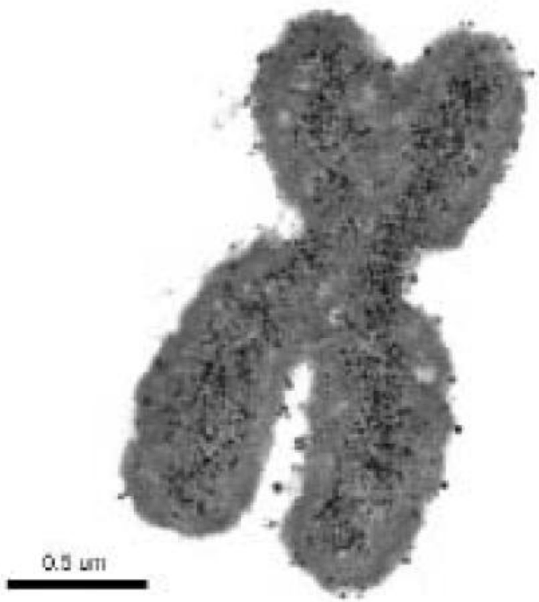
Sciencexpress Reports

Natively Inhibited *Trypanosoma brucei* Cathepsin B Structure Determined by Using an X-ray Laser

developed during the last century, without knowledge of the biochemical pathways. These treatments are limited in their efficacy and safety, and drug resistance is increasing (*2–4*). Thus new compounds that selectively inhibit vital pathways of the parasite without adverse affects to the host are

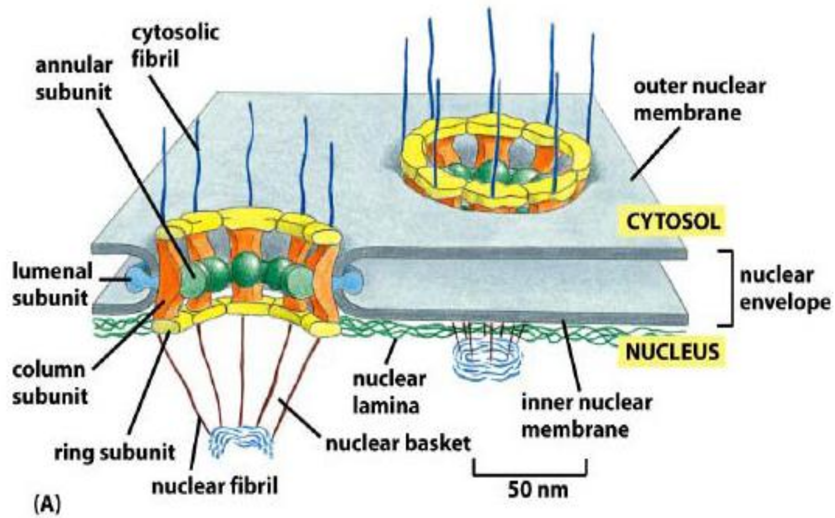


Key Problems That Could Be Resolved Include:



Imaging intact condensed chromosomes

The functioning of the nuclear pore complex



Breakthroughs will impact drug design and medicine

CAPTURING FLUCTUATING AND RAPIDLY EVOLVING SYSTEMS

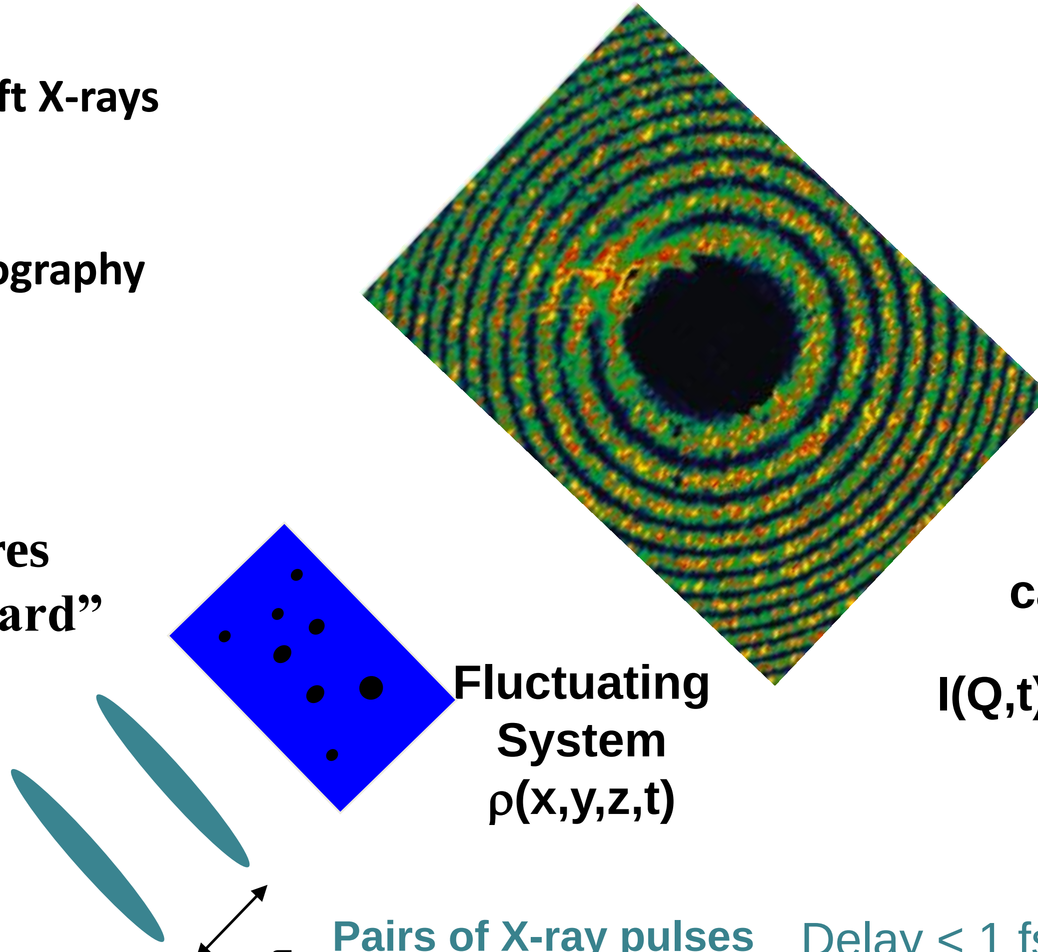
Spontaneous dynamics in condensed matter: Correlation Spectroscopy

Ultra-fast Bright Soft X-rays Enable:

Time Resolved Holography

Ultra-fast XPCS

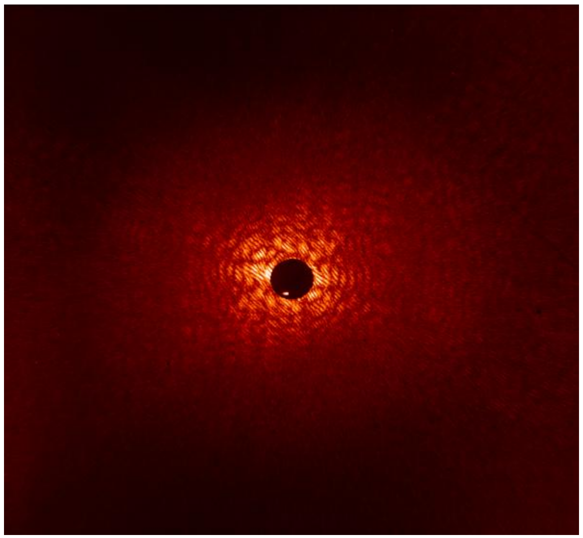
Multiple exposures only work for "hard" samples



Pairs of X-ray pulses Delay < 1 fs - 100 ns

300 eV - >5 keV

Key Problems That Can Be Tackled Include:

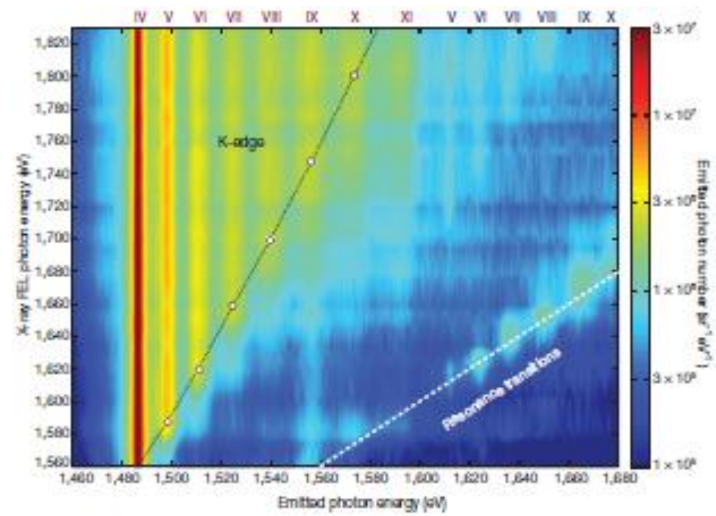


Imaging complex quasi-particles including Cooper pairs

LETTER

doi:10.1038/nature10746

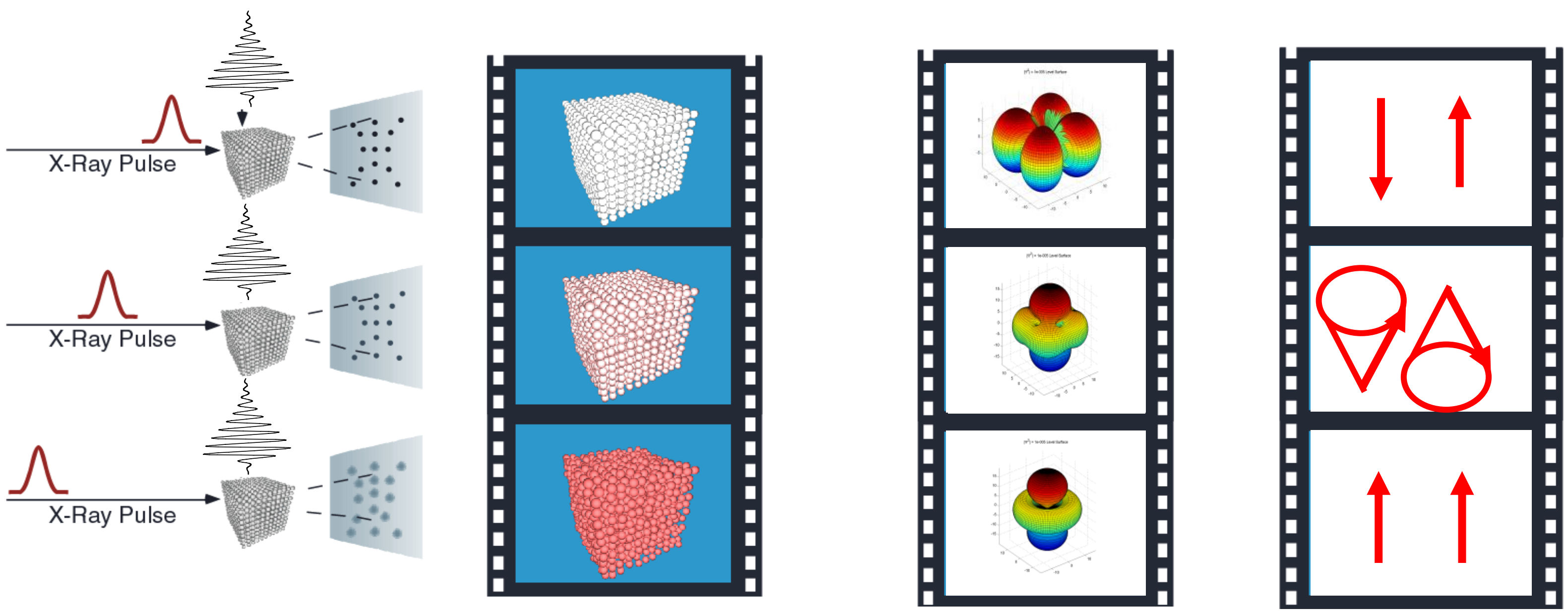
Creation and diagnosis of a solid-density plasma with an X-ray free-electron laser



Could lead to breakthroughs in areas as diverse as high Tc superconductors and fusion energy

STRUCTURAL DYNAMICS UNDERLYING PHYSICAL AND CHEMICAL CHANGES

New Pump-Probe Measurements of Structural Dynamics:
UV-THz short pulse pump to trigger change
Soft X-ray to probe
Dynamics studied by varying pump-probe delay

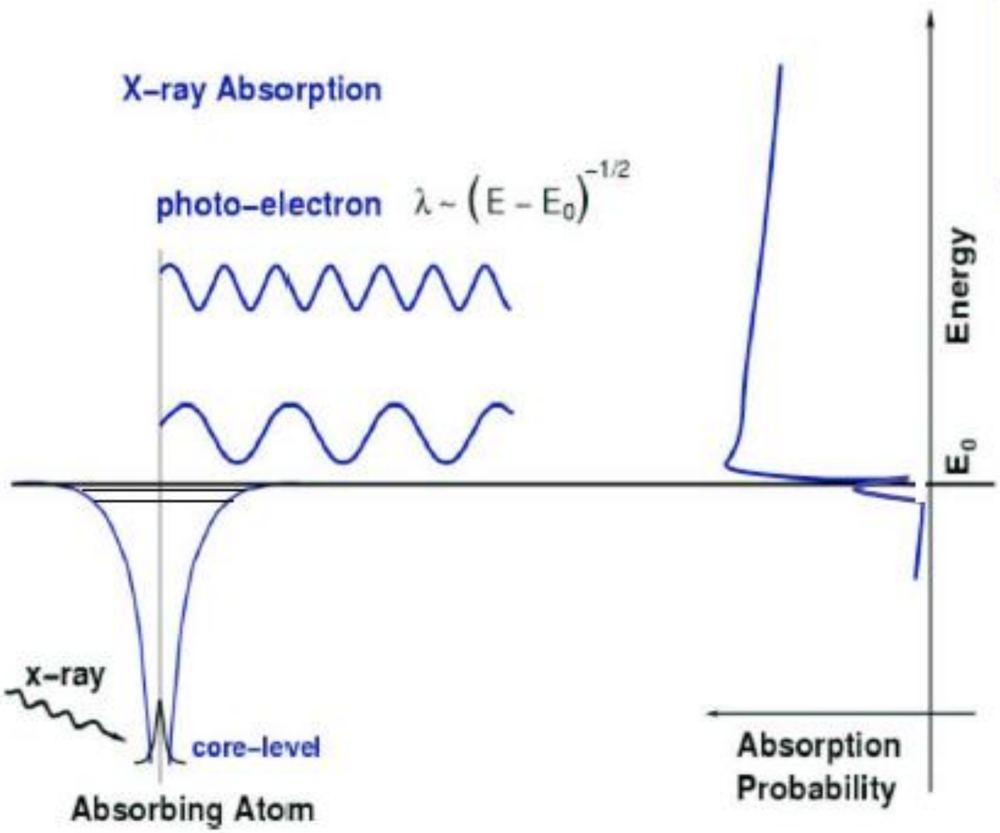


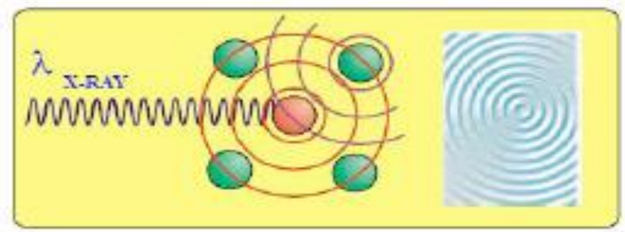
Ultrafast X-rays probe changes in atomic, electronic and magnetic structure following electronic or lattice excitation.

Incisive structural probes such as X-ray absorption may be key to this science

- *UV/IR/THz pump (including optimally shaped control pulses)*
- *Ultrafast X-ray probes e.g. XAS, XPS,XES to give instantaneous structure during chemical reactions and condensed matter changes*

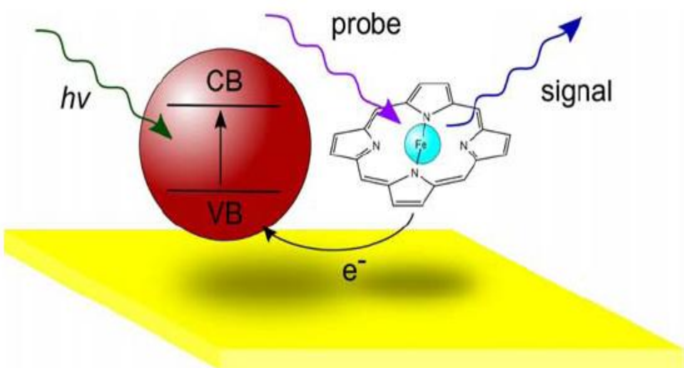
X-ray probing of molecular dynamics





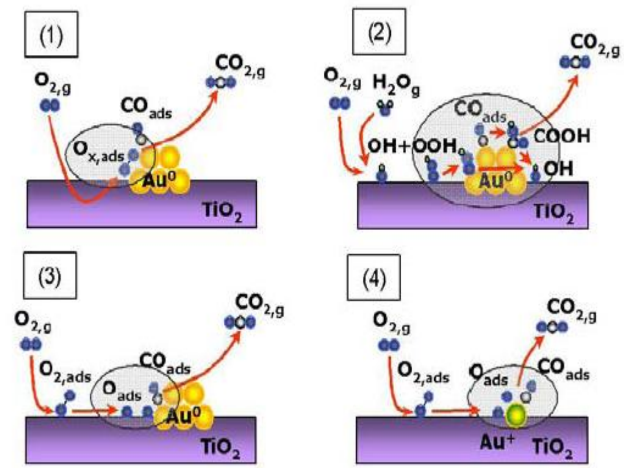
- Core electrons are highly localised
- de Broglie wavelength of electrons is on the atomic scale
- Several modalities eg. XPS, XAS (NEXAFS, XANES), XES, RIXS, Auger etc
- Sensitive to nuclear configuration and local charge state
- Sensitive to environment (solvation, surfaces etc)
- Applicable to all phases of matter in one form or the other

Key Problems That Can Be Tackled Include:



Photosynthesis

More Efficient Catalysis



THE JOURNAL OF PHYSICAL CHEMISTRY A

Article

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Femtosecond X-ray Absorption Spectroscopy at a Hard X-ray Free Electron Laser: Application to Spin Crossover Dynamics

These breakthroughs will impact energy supply, environmental sustainability and life sciences

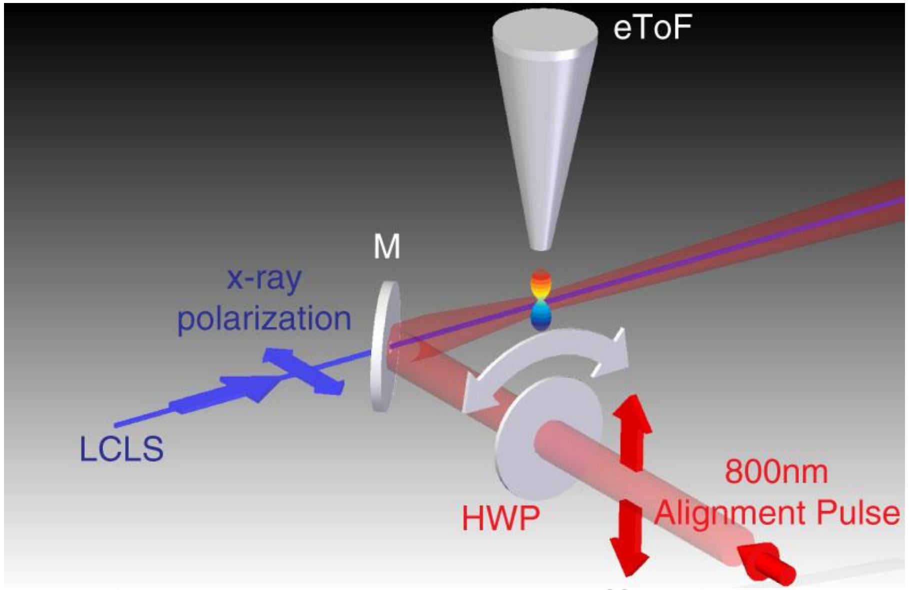
- X-ray laser capabilities
- Survey of new science with X-ray FELS
- **Ultrafast science with LCLS**

With “low bunch charge” operation intense few-fs X-ray pulses can be generated

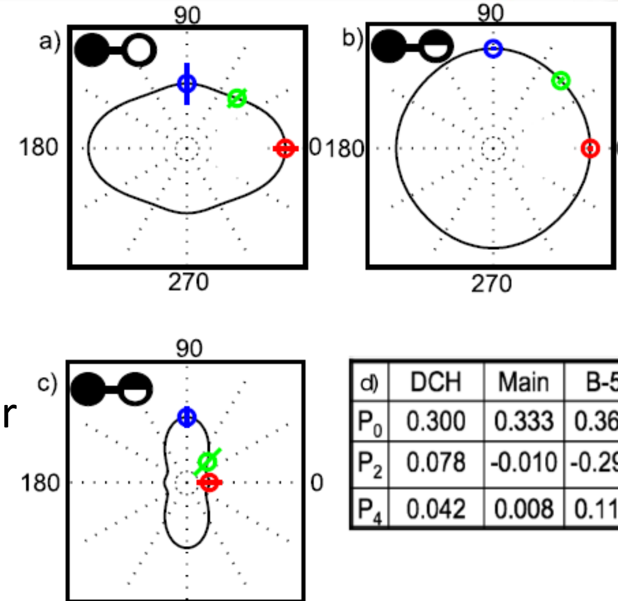
TABLE I. Measured (@ 20-pC and 250-pC) and design (@ 1-nC) LCLS parameters.

Parameter[a]	20 pC	250 pC	1 nC	Unit
UV laser energy on cathode	1.5	20	250	μJ
UV spot diameter on cathode	0.6	1.2	2	mm
UV pulse duration (fwhm)	4.0	6.5	10	ps
Injector bunch length (rms)	1.3	2.5	2.8	ps
Initial peak current	5	30	100	A
Injector slice emittance	0.14	0.6	1.0	μm
Injector projected emittance	0.20	0.7	1.2	μm
Final bunch length (rms)	~3	~30	80	fs
Final peak current	~3	~3	3.4	kA
Final projected emittance	0.4	1.0	1.5	μm
FEL pulse duration (fwhm)[b]	~2	~60	230	fs
FEL peak power[b]	~400	~20	~10	GW

Ding et al PRL, 102 254801 (2009)

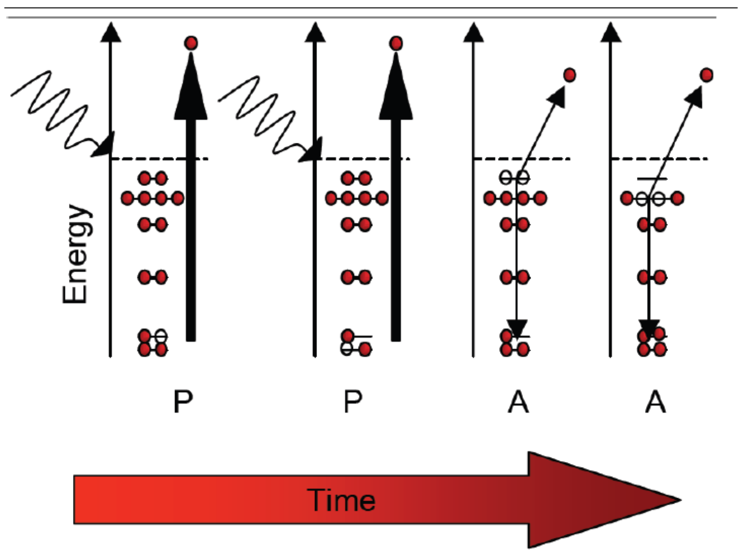


Short intense X-ray pulses enable single (SCH) and double core hole (DCH) formation in molecules. Impulsive alignment allowed us to measure the angular distribution of the Auger electrons from these states for the first time (Cryan et al, PRL, 105, 083004)



d)	DCH	Main	B-5
P_0	0.300	0.333	0.369
P_2	0.078	-0.010	-0.293
P_4	0.042	0.008	0.115

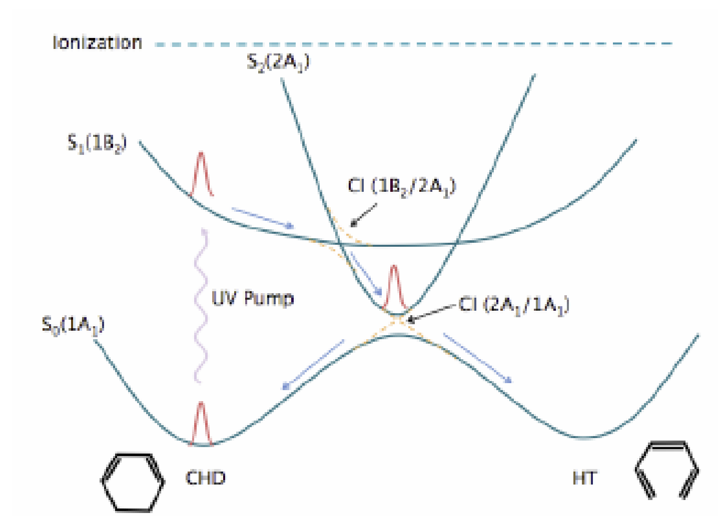
The high intensity FEL X-rays lead to new probes of chemical dynamics



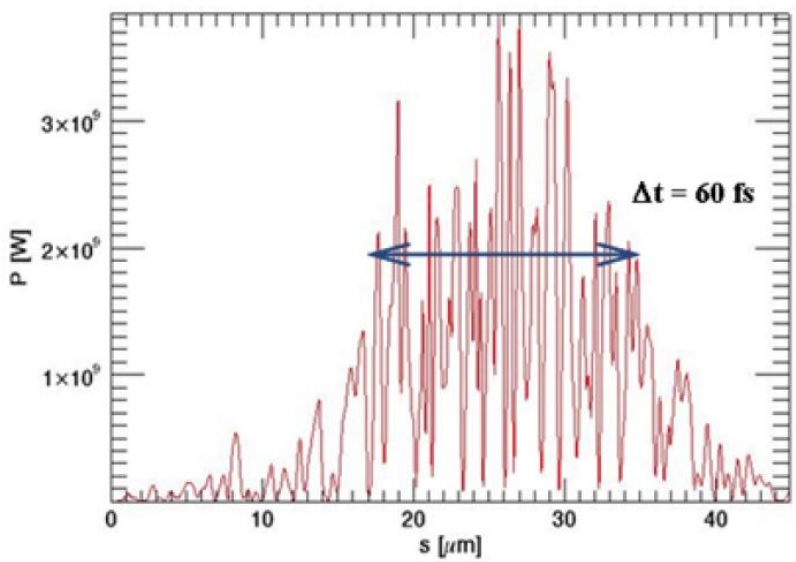
Bright X-rays lead to new time resolved probing techniques for Chemistry:
e.g. Double core holes created in molecules by an intense X-ray pulse could lead to highly sensitive analytical methods
c.f. L. S. Cederbaum et al *On double vacancies in the core* J. Chem. Phys. 85 (1986) 6513
Fang et al ***PRL* 105,** 083005 (2010)
Cryan et al ***PRL* 105,** 083004 (2010)
Berrah et al ***PNAS,* 108,** 16912 (2011)

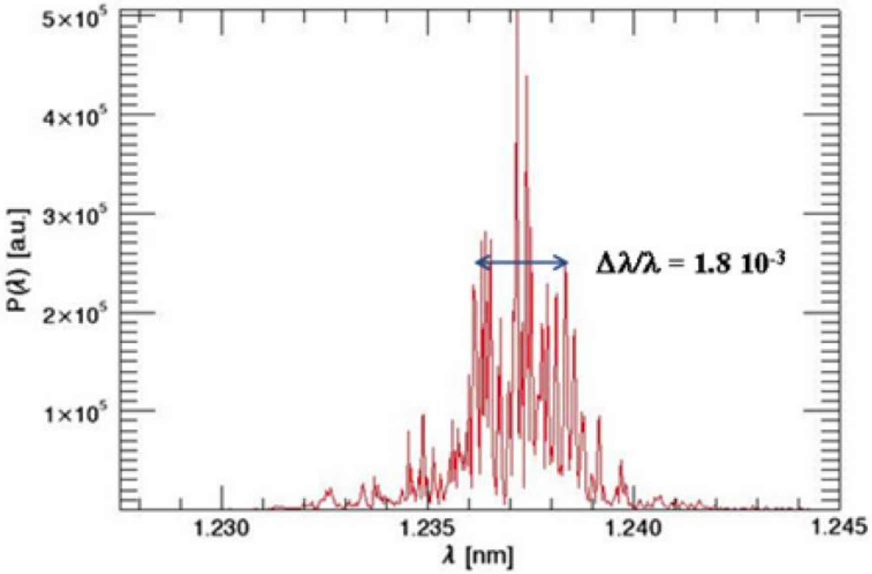
Tracking ring opening triggered by UV pulse using X-ray initiated fragmentation

*Petrovic et al **PRL 108** , 253006 (2012)*



SASE: Wavelength Fluctuation and Temporal Jitter



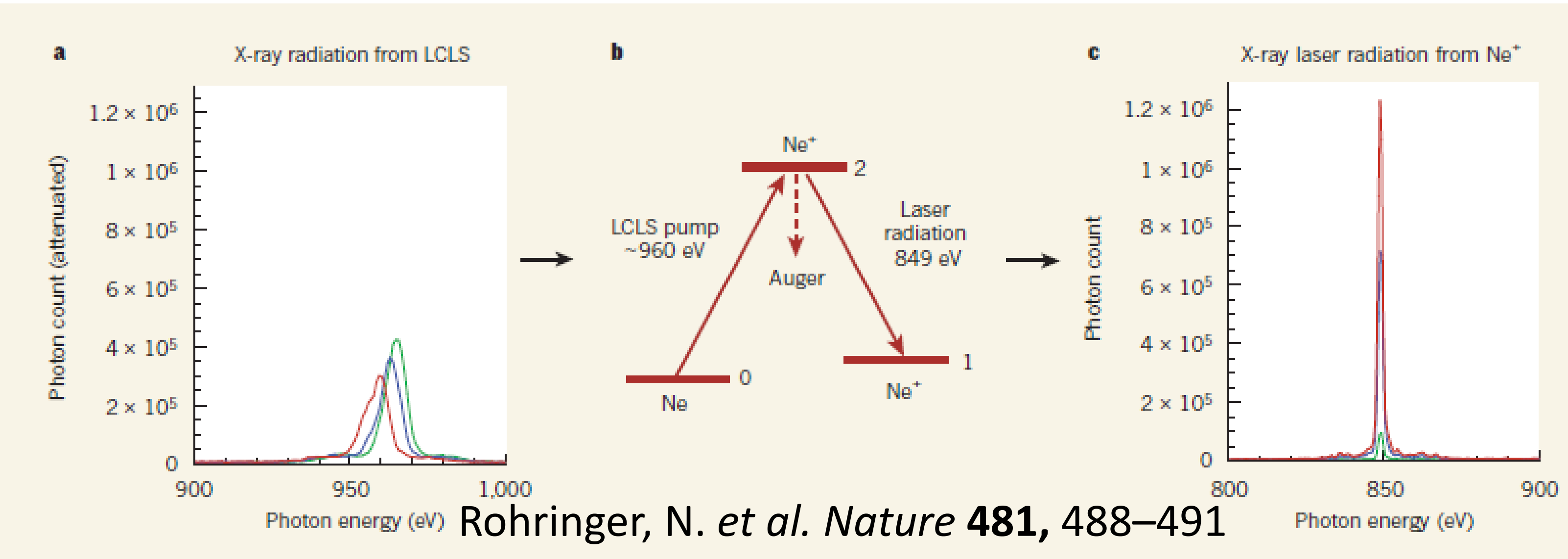


Temporal (+/- 100 fs) jitter inhibits:
- **Synchronisation with external sources**
- **High temporal resolution measurements**
- **Quantitative non-linear interaction studies**

Wavelength fluctuation inhibits:
- **X-ray spectroscopy**
- **Inelastic scattering**
- **Chemically sensitive CDI**

Ultrafast structural dynamic measurements at the femtosecond timescale need to overcome these limitations

Atomic Inversion Laser



Rohringer, N. *et al. Nature* **481,** 488–491 (2012).

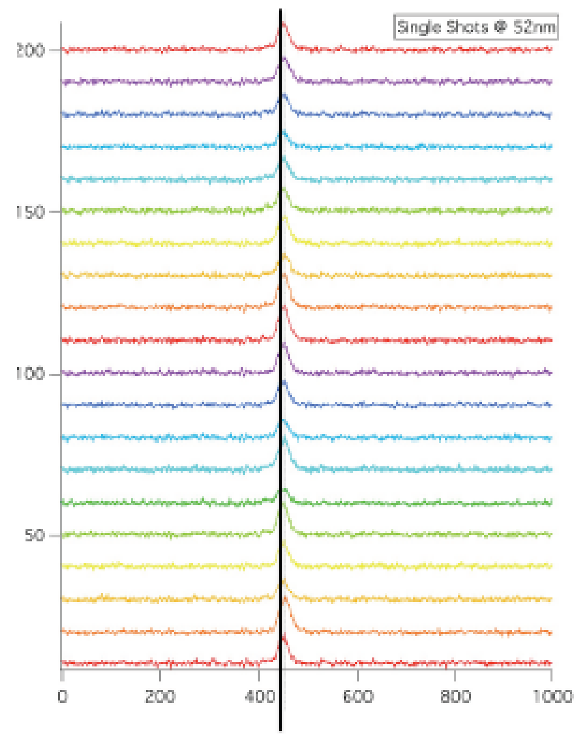
Figure 1 | Atomic X-ray lasing. Rohringer *et al.*[1] have demonstrated X-ray lasing at a photon energy of 849 electronvolts by creating atomic population inversion in a sample of neon gas using the Linac Coherent Light Source (LCLS), which is an ***[OK? to be consistent with main text?]*** X-ray free-electron laser. **a**, The LCLS X-ray radiation has a large spread in photon energy and considerable fluctuation in the average photon energy (about 960 eV) obtained from sequential laser pulses (shown in different colours). Photon count is here measured after transmission through the neon sample and is strongly attenuated. ***[OK?]*** **b**, The LCLS 'pumps' many of the neon atoms from the ground state (state 0) into a higher-energy state of ionized neon (state 2). Most of the ions in this excited state decay through an Auger process, but some will make the radiative transition to a state (state 1) that has a lower energy than state 2. This transition is accompanied by the emission of laser radiation that has a precise average photon energy (849 eV). **c**, The laser radiation has a smaller energy spread than that of the LCLS.

Results in a fixed wavelength but hard to do……..

Injection Seeding

SASE AND SEEDED BANDWIDTH AND SPECTRAL STABILITY

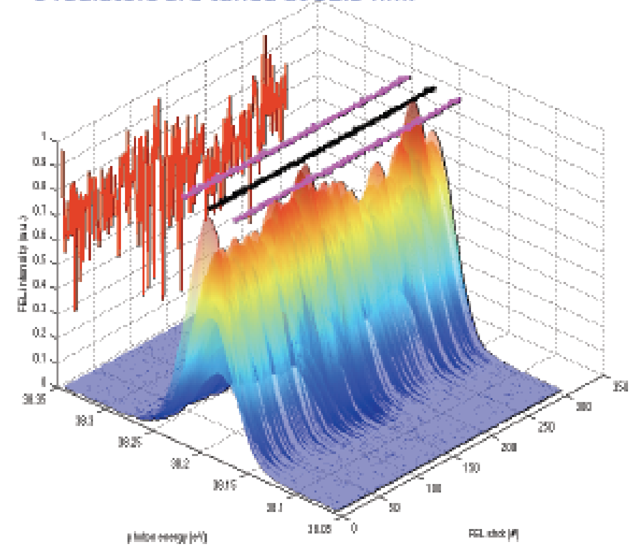
In addition to the very narrow spectrum FERMI is characterized by a very good spectral stability. Both short and long terms measurements show that the spectral peak move less than 10^{-4}.



D. Cocco, C. Svetina, M. Zangrando

courtesy of Fulvio Parmigiani

Reported data refer to an electron beam of 350 pC at 1.24 GeV compressed about a factor 3. The 6 radiators are tuned at 32.5 nm.



FEL photon energy	~ 38.19eV
Photon energy fluctuations	= 1.1meV (RMS)
FEL bandwidth	= 22.5meV (RMS)
	= $5.9e^{-4}$ (RMS)
FEL bandwidth fluctuations	= 3% (RMS)

E. Allaria, W. Fawley

Not viable for hard X-rays.....

Self Seeding: Eliminates Wavelength Jitter

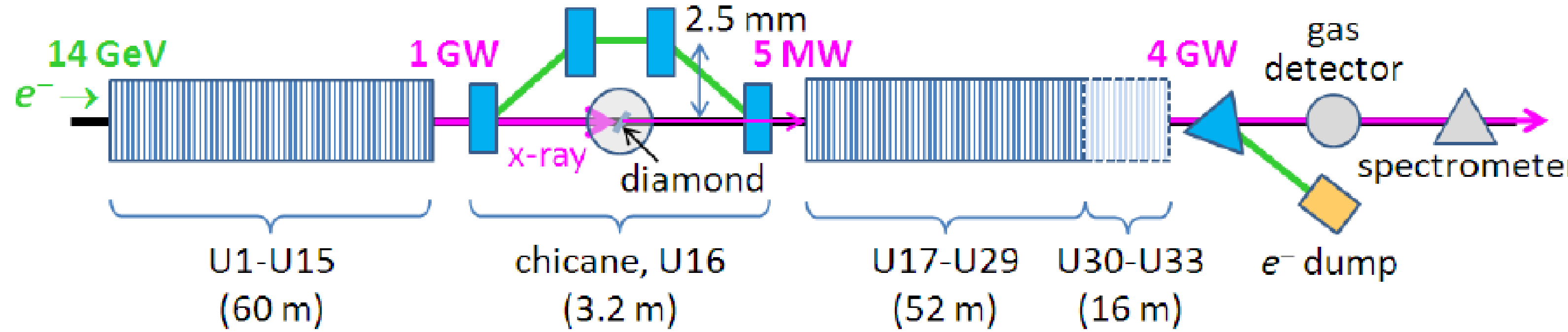
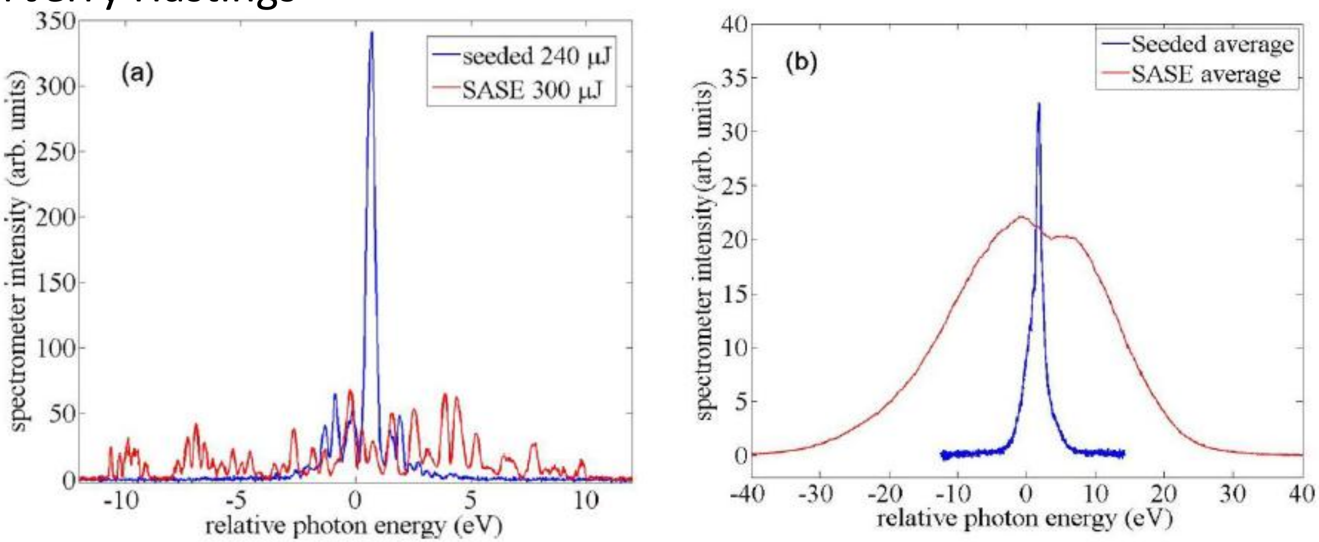


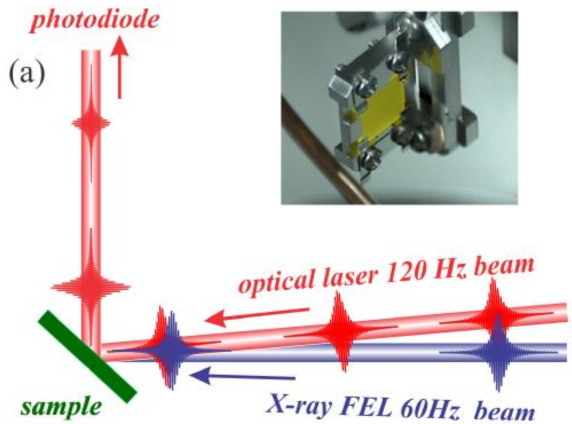
Figure 1. Layout of LCLS undulator with self-seeding chicane, diamond monochromator, gas detector, and hard x-ray spectrometer. The chicane is greatly exaggerated in scale here.

courtesy of Jerry Hastings



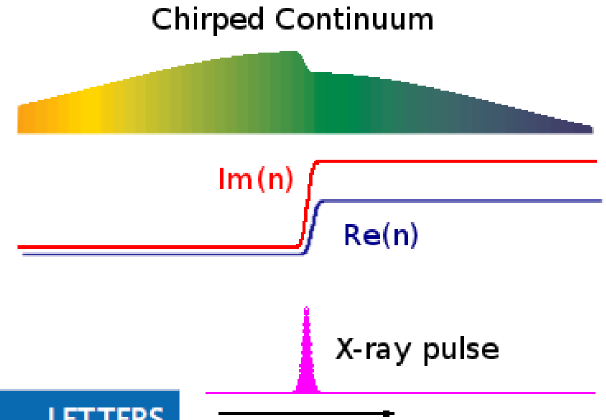
Promising and fixes wavelength jitter, but not temporal jitter…….

Time Stamping



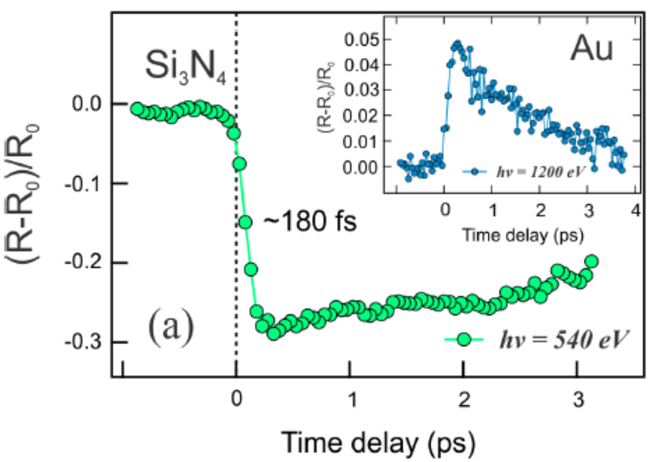
Courtesy of Ryan Coffee

X-ray gated reflectivity

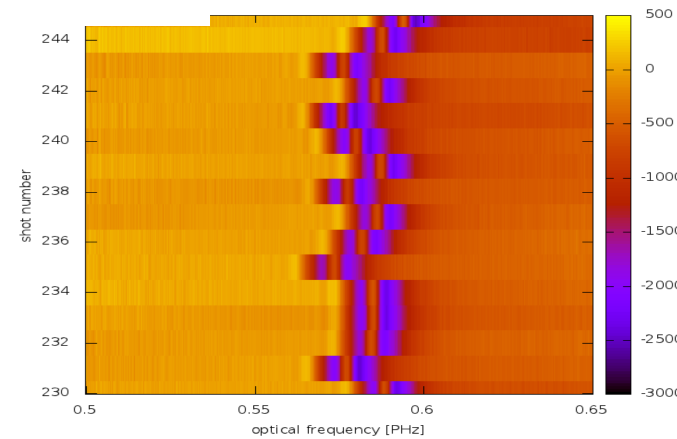


nature photonics
LETTERS
PUBLISHED ONLINE: 17 FEBRUARY 2013 | DOI: 10.1038/NPHOTON.2013.11

Achieving few-femtosecond time-sorting at hard X-ray free-electron lasers



Using chirped pulse for single shot timing measurement – Sub 20fs resolution demonstrated

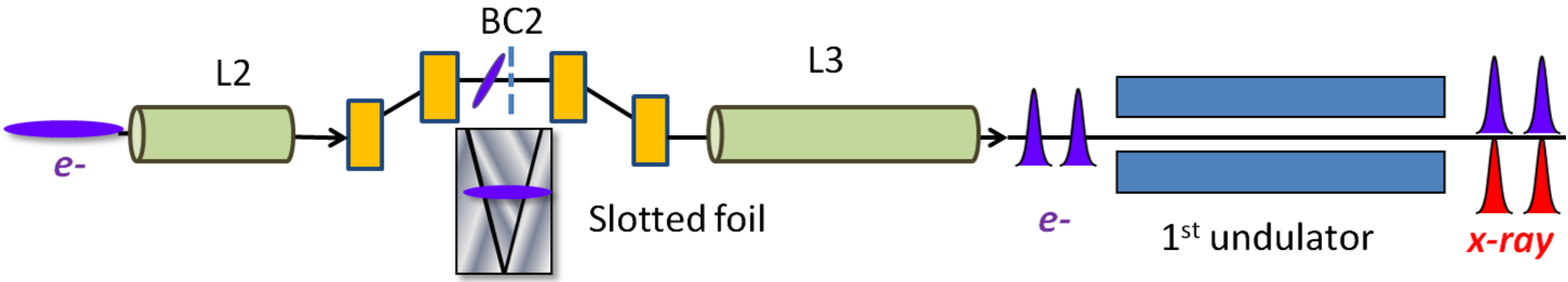


Combined with self seeding this might just do, but still need higher rep-rate to overcome fluctuations (in self seeding spectral fluctuations transferred to intensity fluctuation)….

To eliminate temporal jitter X-ray pump- X-ray probe methods are now being developed

Several options are currently used at LCLS

- Split and delay
- Two-pulse generation at single frequency
- Two-pulse / two-colour generation

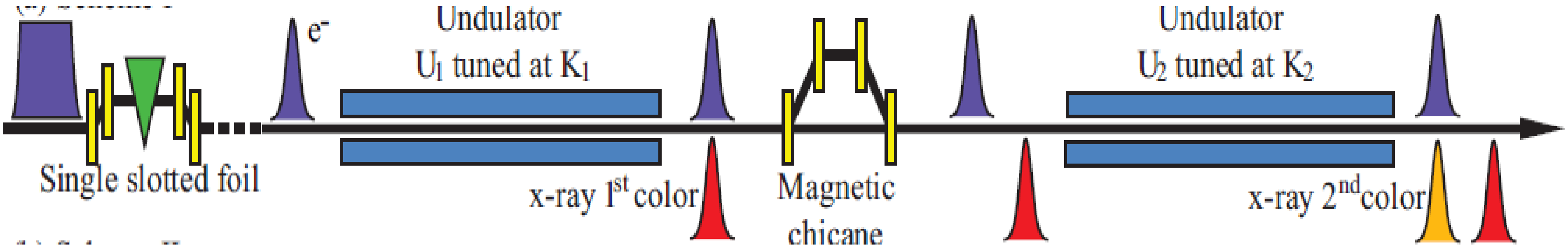


Scheme for two-pulse generation using a slotted foil (PRL 109, 254802):

Generates two pulses of ~ 3fs each separated by 0-20 fs

Sub-fs jitter

To eliminate temporal jitter X-ray pump- X-ray probe methods are now being developed



Two-colour two-pulse scheme using an intra-undulator chicane and tuning the two undulator sections slightly differently:

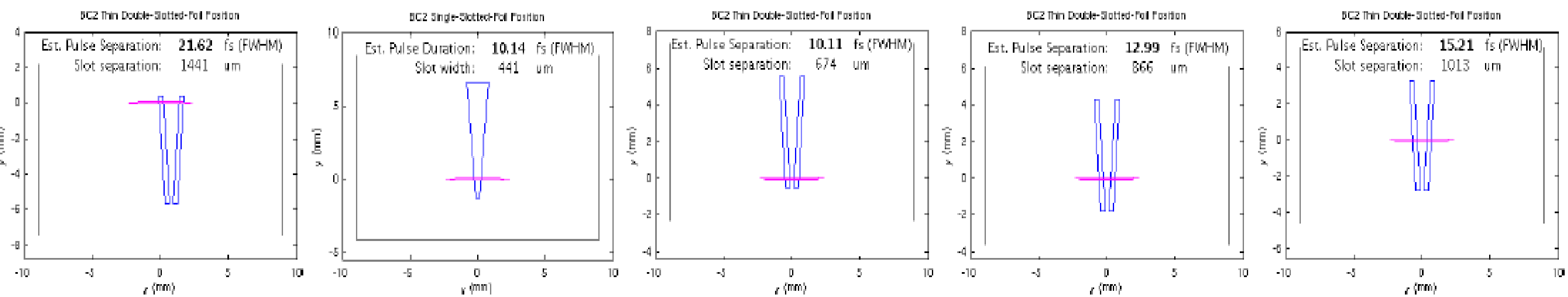
Two pulses of each <3fs

Variable delay 0 to 20 fs

Photon energy difference in pulses of a few percent (e.g at 500eV +/- 10 eV)

X-ray pump-X-ray probe

- Split and delay of X-rays is now being implemented at FLASH and LCLS
- A promising method for high temporal resolution is use of a slotted emittance spoiler placed in the electron beam in a dispersed section:



Creates single or double pulses ~ 5 fs duration with variable delay up to ~50fs

This has recently been used to study ultrafast dynamics triggered by X-ray core exctitation in O_2

Group of Ryan Coffee LCLS, SLAC Stanford

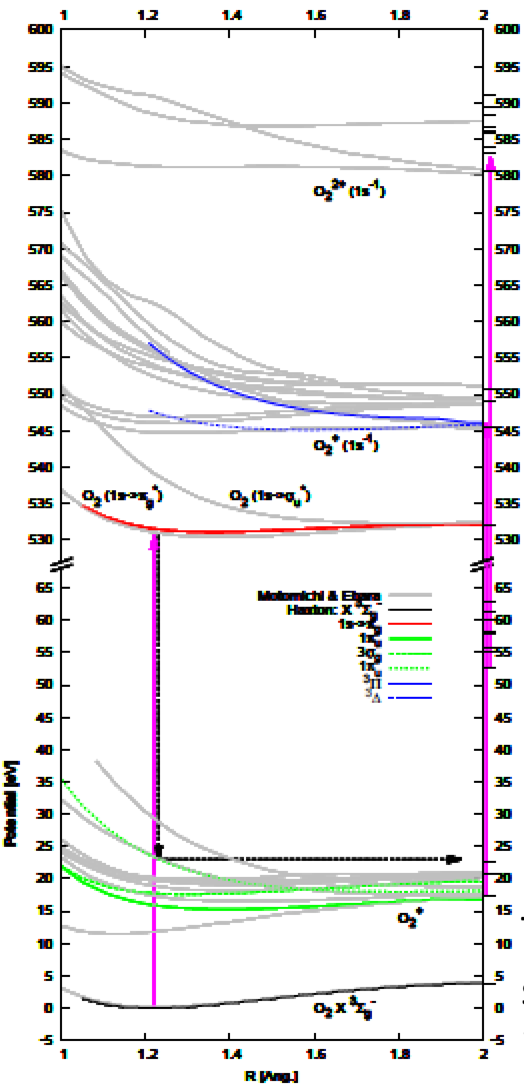
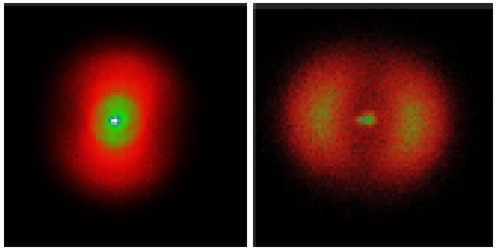
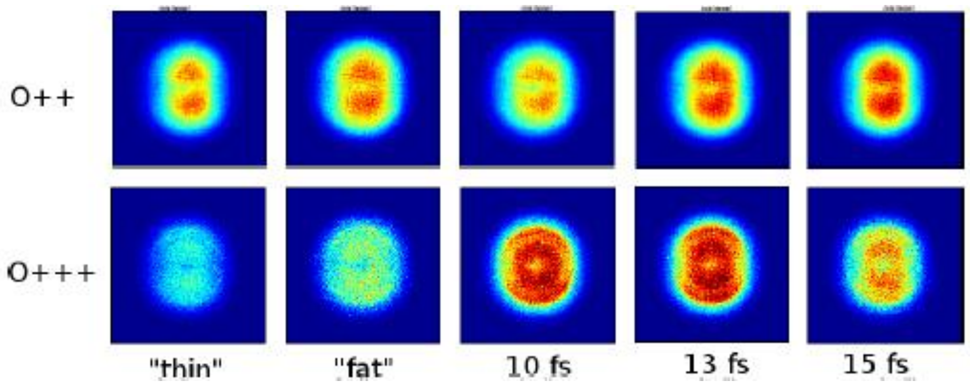


Figure 1: Various potential energy curves. Tashiro Motomichi and Masahiro Ehara produced the gray curves while Dan Haxton produced the symmetry labeled curves.



Left fragment pattern from $\pi *$ resonance, right fragment pattern from σ* resonance



The symmetry goes form π* to convolution of π* with σ* (indicating second absorption is via σ* moment) then recovery of the π* by 15 fs. indicates that the second absorption has become atomic like rather than contributing as a molecular symmetry.

Future Scene

- By 2020 there will be X-ray FELs in USA, Germany (2), Japan, Switzerland, Korea, China + others
- To compete UK will need access to a light source with:
- X-rays 0.1 – 10 keV
- Rep-rate > 100 Hz (preferably >> 100Hz)
- Pulse duration ~10 fs
- ~1mJ pulse energy
- Any ideas how to build one?

UK FEL Meeting
Friday 14th June 2013
Blackett Laboratory, Lecture Theatre 1

0930 Tea & Coffee in level 2 foyer

1000 Sir Peter Knight (Imperial College)
Opening comments

1010 Janos Hajdu (University of Uppsala, Sweden)
"Imaging at High-Energy Densities"

1040 Henry Chapman (CFEL, DESY, Germany)
"Protein Nanocrystallography" TBC

1110 Tea & Coffee in level 2 foyer

1125 Jim Naismith (University of St Andrews)
"UK Life Sciences at XFEL" TBC

1155 Ian Robinson (UCL)
"Direct Imaging of Phonon Modes in Gold Nano-Particles"

1225 Steven Johnson (ETH, Switzerland)
"Controlling Dynamics in Solids: Femtosecond X-ray Diffraction"

1255 Lunch in level 2 foyer

1335 John Costello (Dublin City University, Ireland)
"EUV and X-ray Free Electron Lasers - A New Frontier in AMO Physics"

1405 Jon Marangos (Imperial College)
"Ultrafast Molecular Dynamics with X-Ray FELs"

1435 Robin Santra (CFEL DESY, Germany)
"High-Intensity X-ray Interactions with Heavy Atomic Species"

1505 Tea & Coffee in level 2 foyer

1520 Malcolm McMahon (University of Edinburgh)
"Accessing Extreme States of Matter on X-FELS"

1550 Thomas Cowan (Helmholtz Institute, Germany)
"The Helmholtz Beamline at XFEL "

1620 Justin Wark (Oxford University)
"Solid Density Plasmas Created and Diagnosed with X-ray Lasers"

1650 John Womersley (STFC)
Closing remarks