Introduction to Time-Resolved X-ray Scattering

Opportunities to Resolve Structural Dynamics at the Atomic Scale

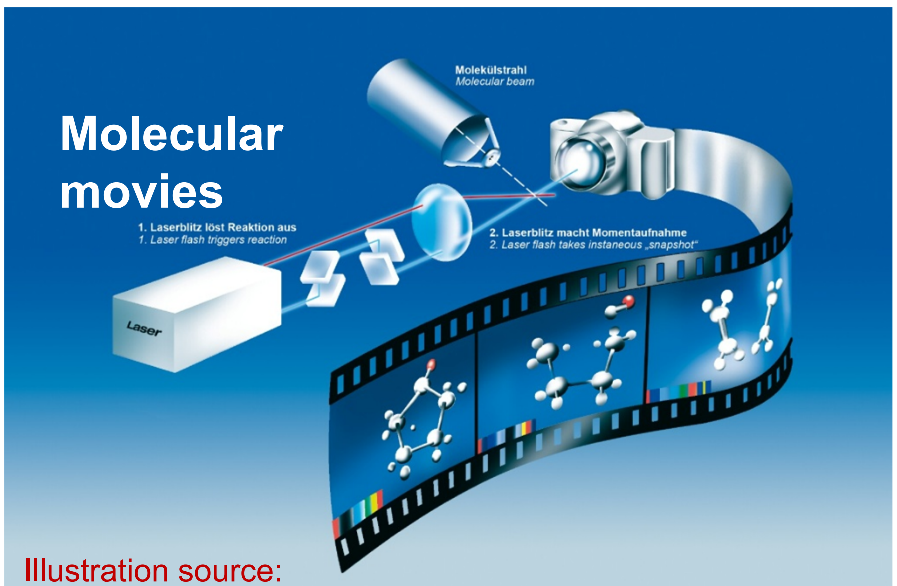

Illustration source:
http://www.xfel.eu/research/examples/chemical_reactions/

David M. Tiede
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13th National School on Neutron & X-ray Scattering
Advanced Photon Source
June 21, 2011

Time-Resolved Techniques Provide Opportunities to Resolve Intermediates in Important, Complex Phenomena

Time-Resolved Techniques Provide Opportunities to Resolve Intermediates in Important, Complex Phenomena

Source: www.electricstuff.co.uk

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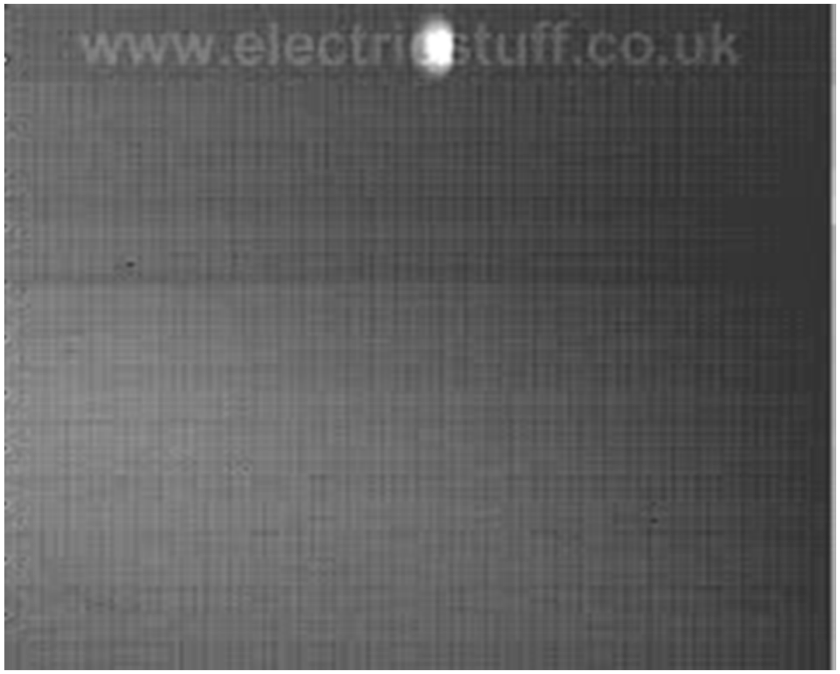

Source: www.electricstuff.co.uk

Time-Resolved Techniques Provide Opportunities to Resolve Intermediates in Important, Complex Phenomena

Philip Anfinrud (NIH): MbCO **SCIENCE (2003) Volume: 300: 1944-1947**

Source:
Schotte, Lim, Jackson, Smirnov, Soman, Olson, Phillips, Wulff, and **Anfinrud**, *Science 2003, 300, (5627), 1944-1947.*

Time-Resolved Techniques Provide Opportunities to Resolve Intermediates in Important, Complex Reactions

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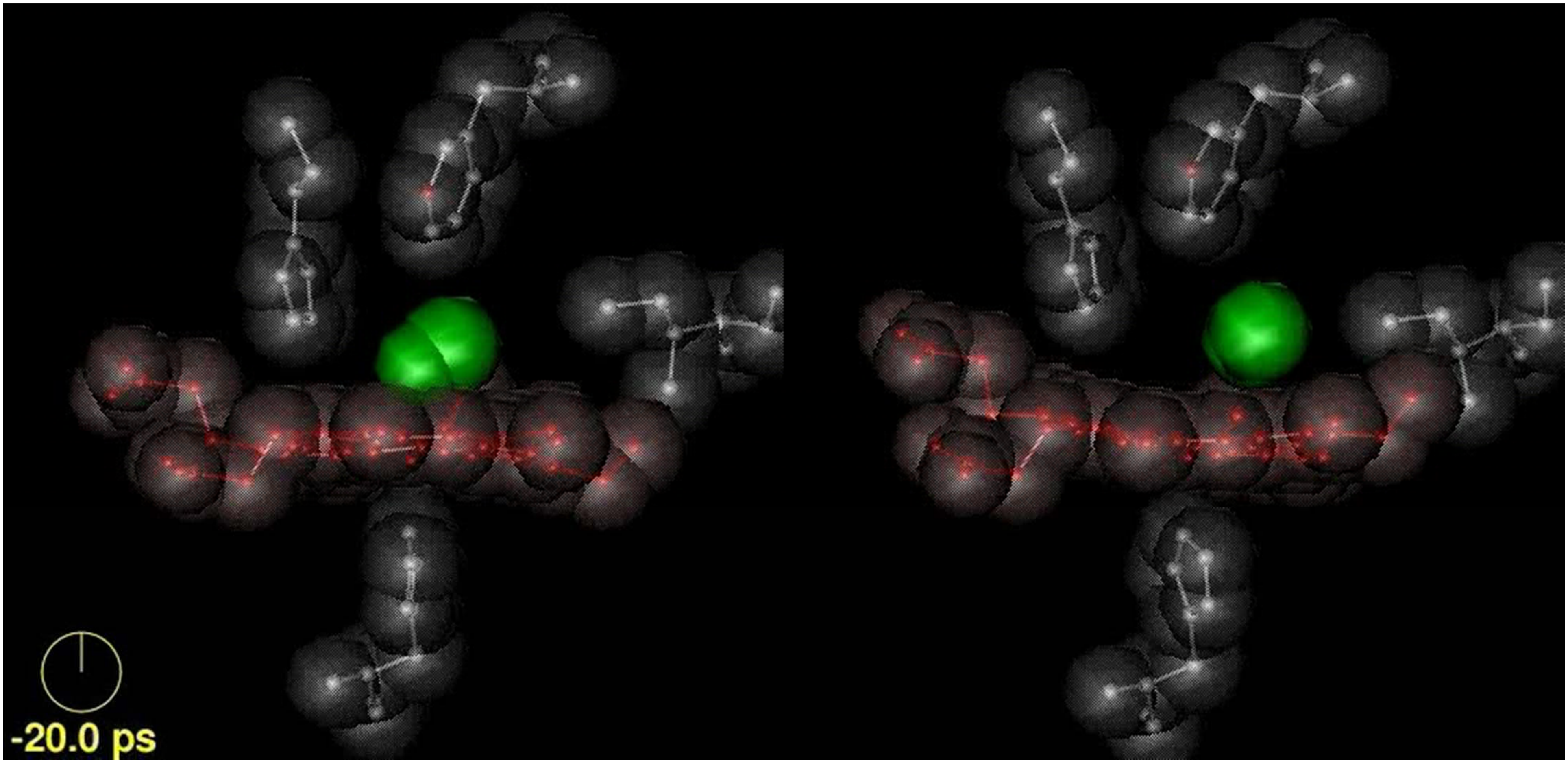
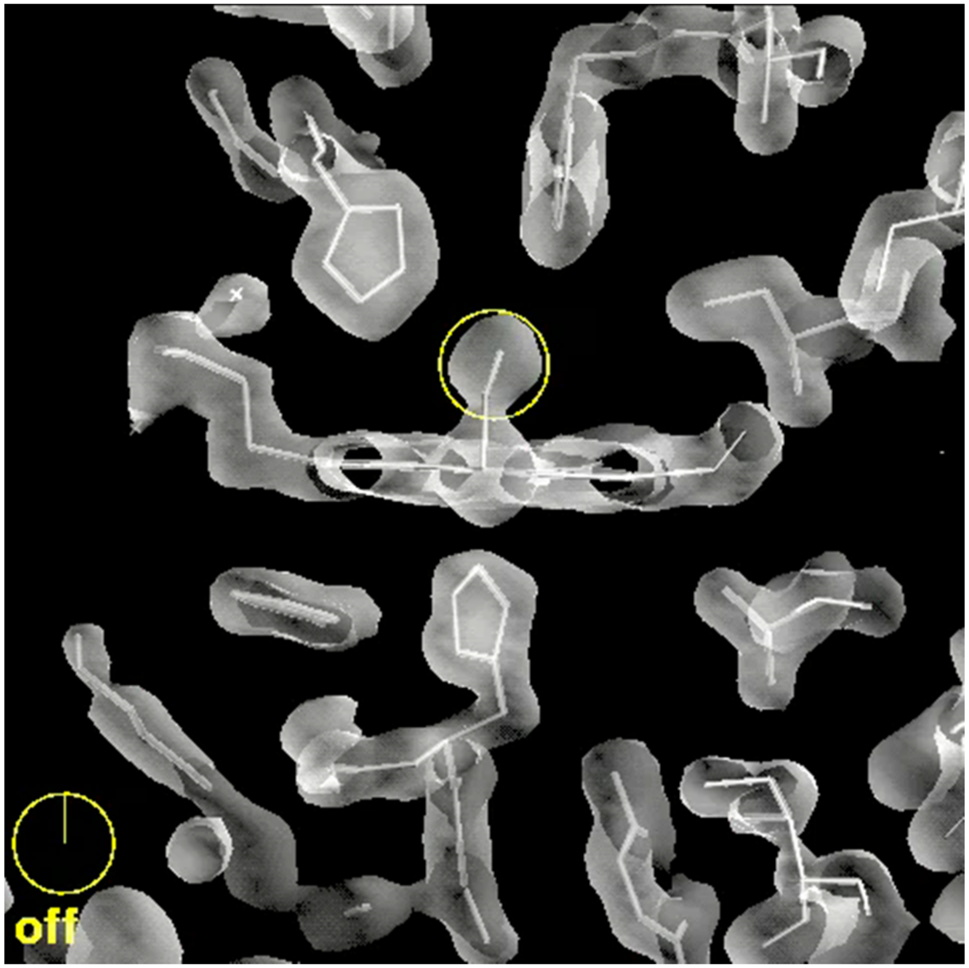


Source:
Schotte, Lim, Jackson, Smirnov, Soman, Olson, Phillips, Wulff, and **Anfinrud**, *Science 2003, 300, (5627), 1944-1947.*

Anfinrud’s Structural dynamics associated with MbCO photo-deligation



Source:
Schotte, Lim, Jackson, Smirnov, Soman, Olson, Phillips, Wulff, and **Anfinrud**, *Science 2003, 300, (5627), 1944-1947.*

Dynamic movies by TR crystallography

Pioneers include:

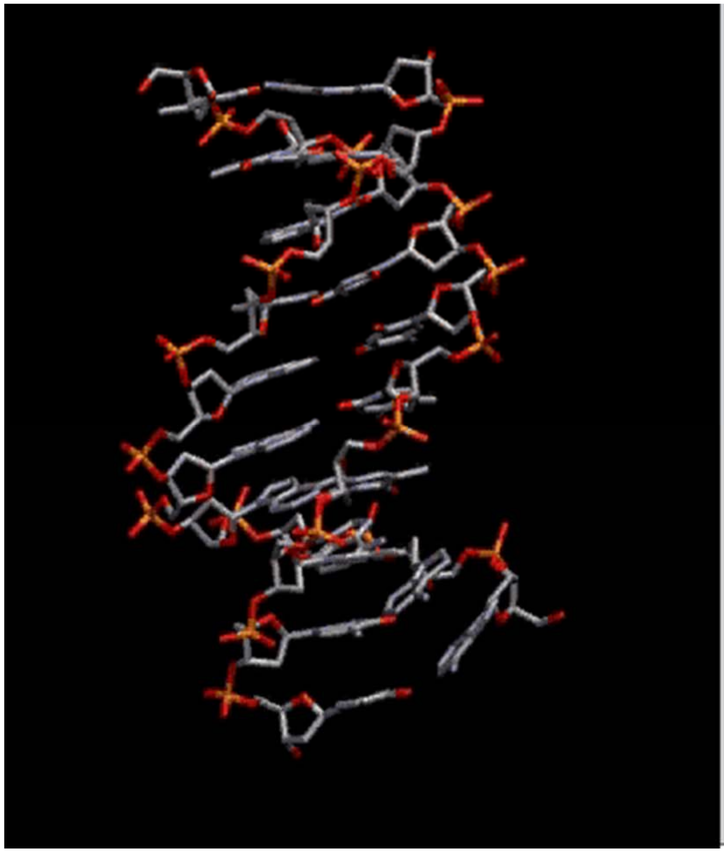
Keith Moffat (U of Chicago),
Philip Anfinrud (NIH),
Philip Coppens (SUNY Buffalo),
, etc., ……

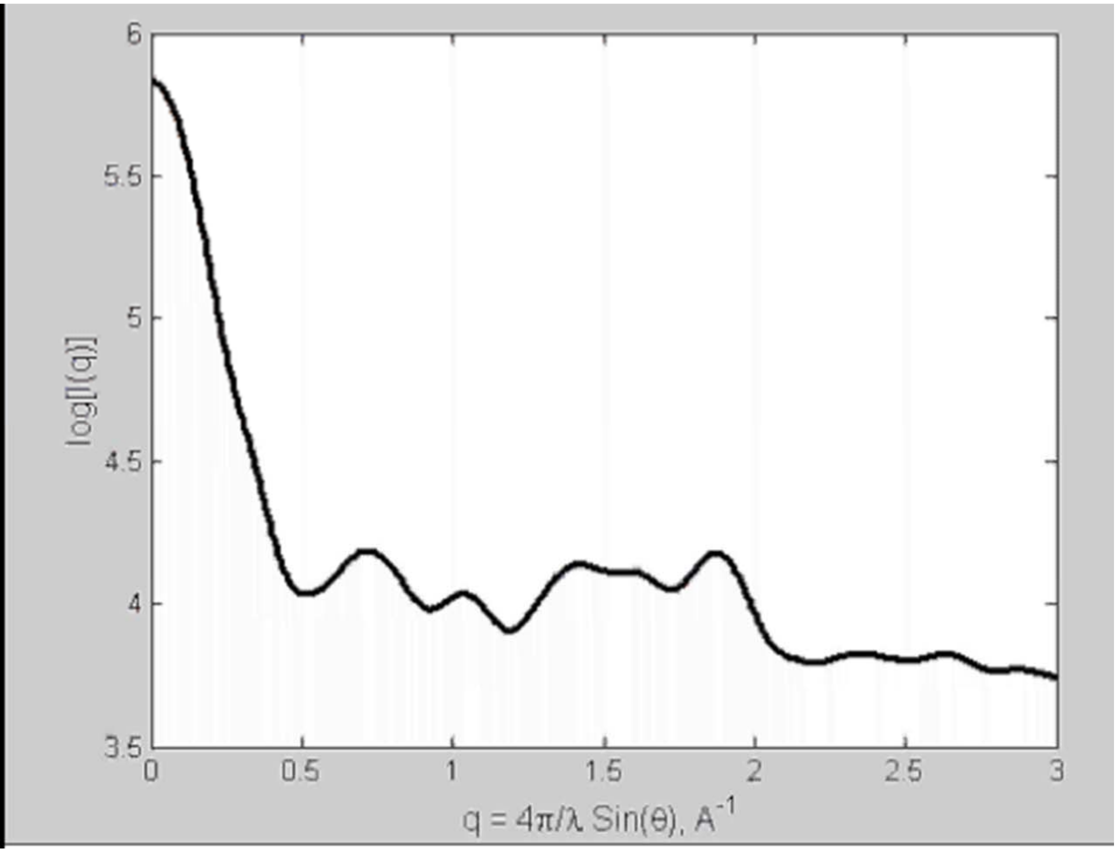
- Crystallographic approaches tend to have:
  - *restricted applicability*
  - *questions about influence of crystal packing forces on dynamics*

- Interest and need for *in-situ* time-resolved measurements
  - *X-ray spectroscopy*
  - *X-ray scattering*

Opportunities to use Solution Scattering for Dynamics Measurements:

Molecular Dynamics Simulation - DNA 5 ps Steps





- WAXS Resolves Individual Time-Jumps (5 ps)
- Implies Time-resolved Opportunity:
  - Synchronized-Ensemble

Zuo, Cui, Mertz, Zhang, Lewis, Tiede, *PNAS. (2006)103: 3534*

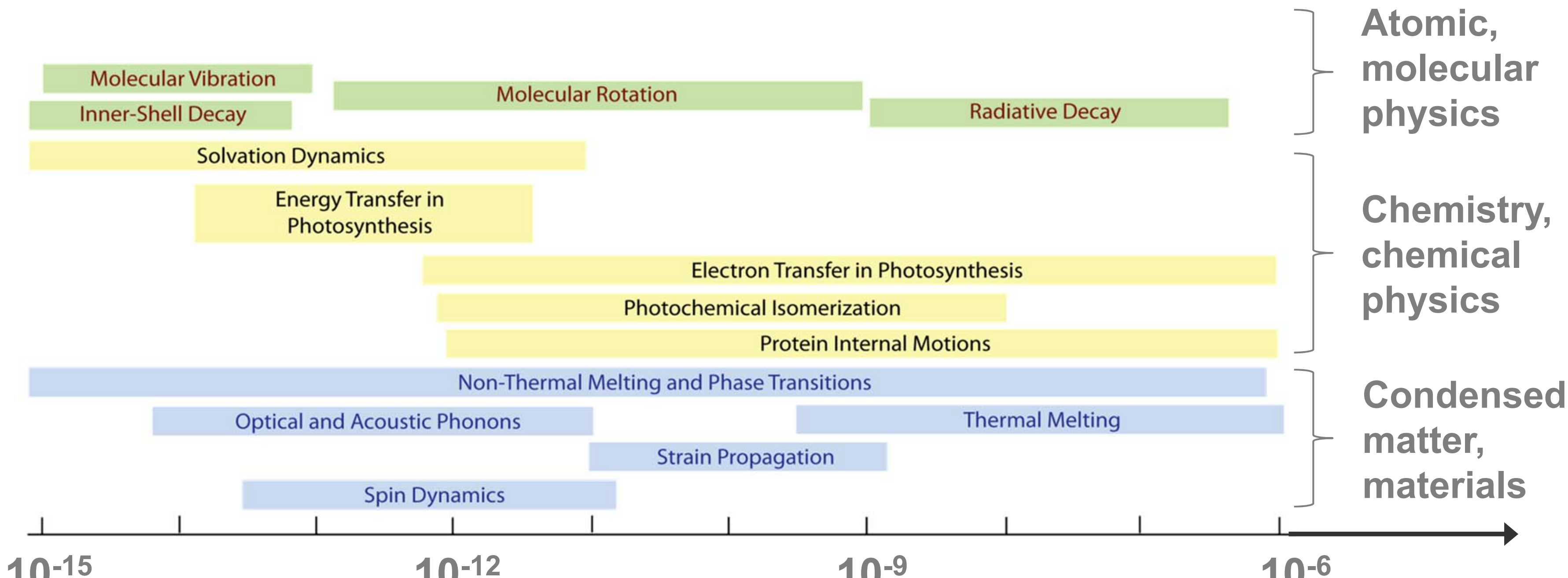
Presentation Outline:

Introduction to time-resolved dynamics

Discussion that follows:

- General Approach,
- Issues for Time-Resolved X-ray (Scattering) Measurements
  - *Choosing your light source*
- Examples from “pink” beam line sources
- Examples from a monochromatic beam line source
- Examples from FEL
- Concluding remarks

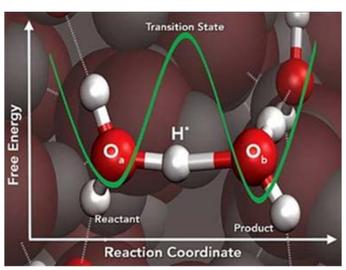
Examples of dynamics spanning ultra-fast time scale:



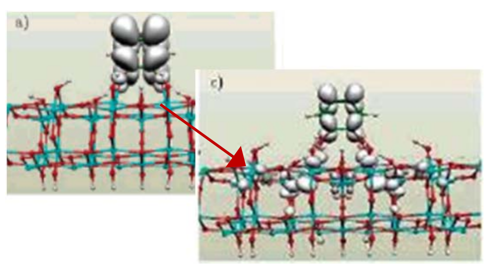
Time line illustration:
P. Evans (U. Wisc), L. Young (APS)

Examples:

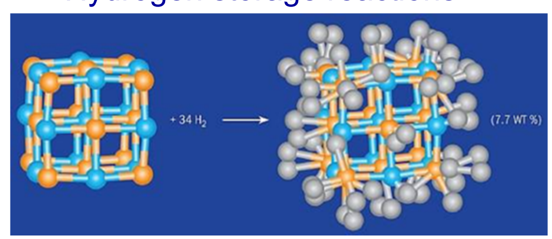
Transition state crossing



Solar-driven interfacial electron transfer

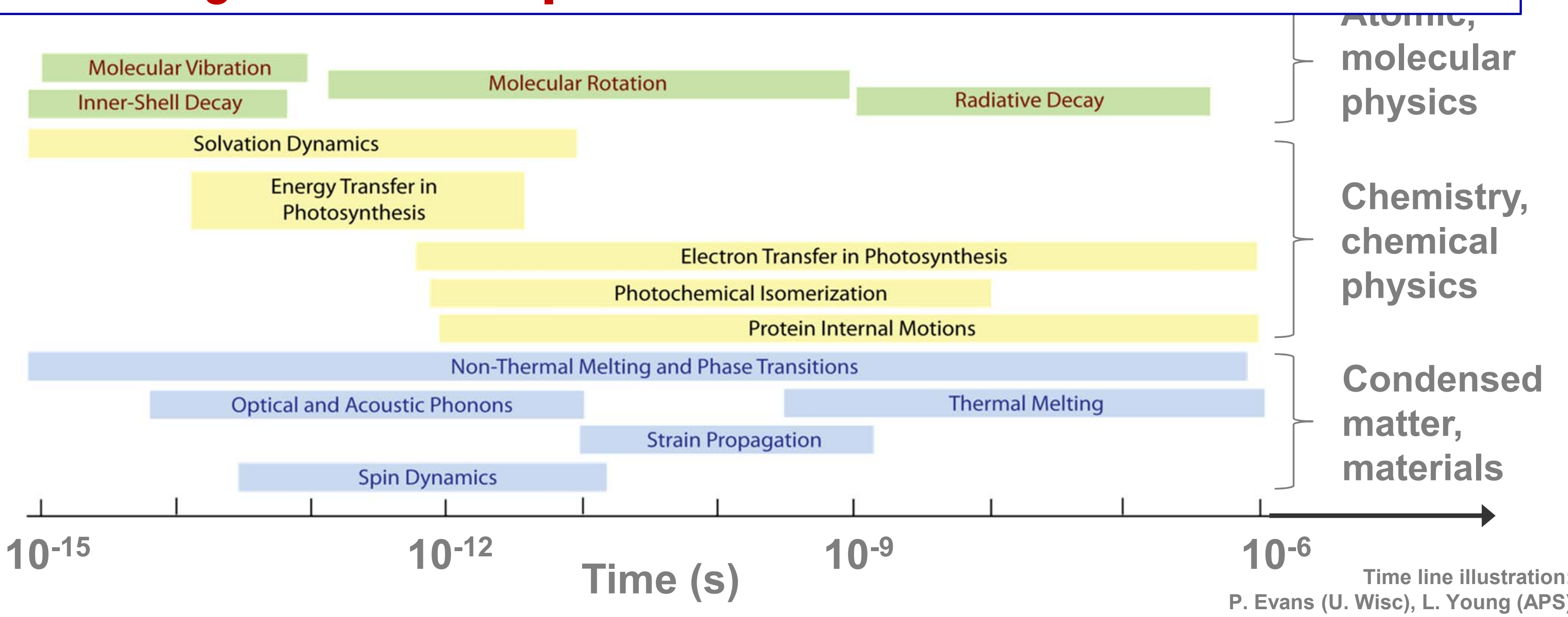


Hydrogen storage reactions



have images from computation, not experiment …..

Challenge: Get Snapshots of these critical events !!!!



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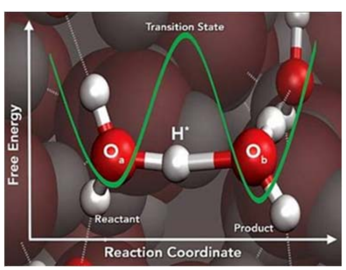

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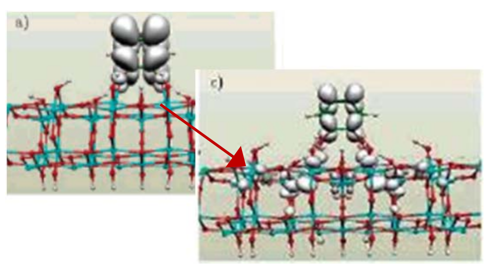

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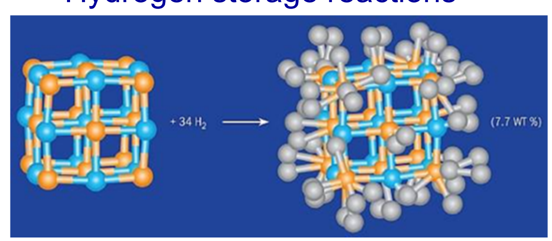


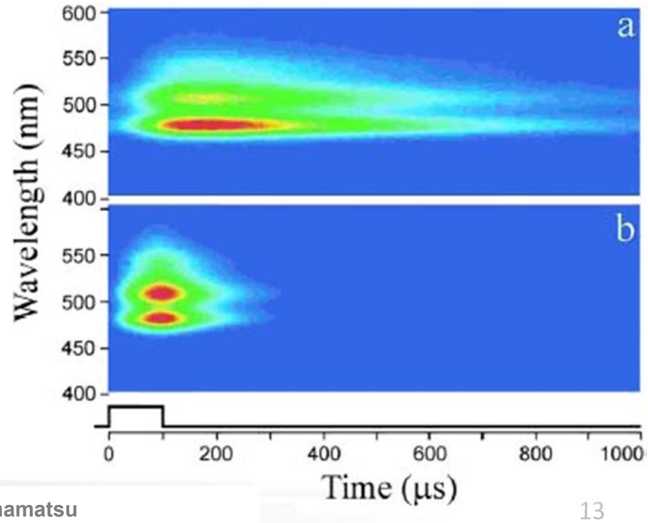
have images from computation, not experiment …..

Time-resolved X-ray measurements

http://people.rit.edu/andpph/text-digital-stroboscopy.html

Two General Approaches:

- Stroboscopic
  - Temporal structure of **probe** pulse (X-ray) determines time resolution
- Fast Detector: rapid gating, streaking
  - Gating or streaking of the **detector** output determines time resolution
- Combination of the two



Source: hamamatsu

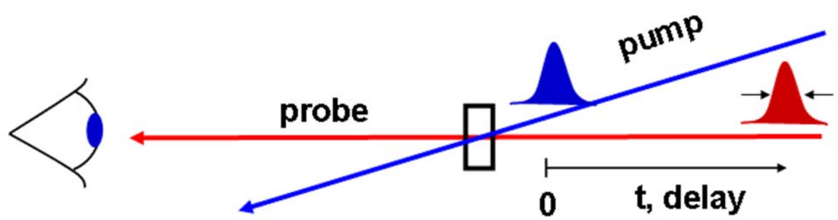
Time-resolved X-ray measurements

Measurements Ultimately:

- Detected X-ray Photon Limited
  - Flux (incident x-ray photons/sec) x time frame (sec) = incident photons per frame
  - Scattering experiments typically need $10^{12} – 10^{14}$ incident x-ray photons

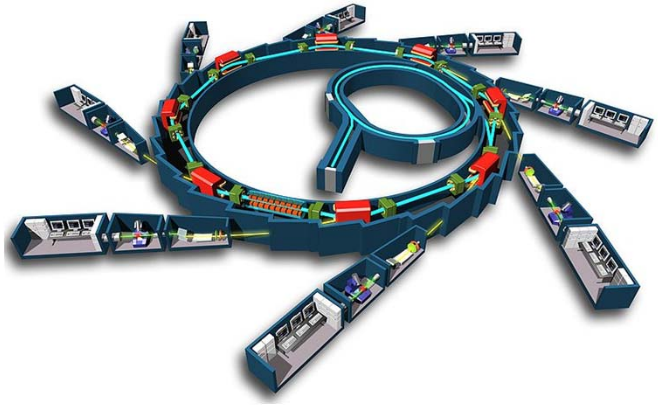
Hence, for TR X-ray Spectroscopy, Scattering

- Need:
  - Bright light sources (3rd, 4th generation: synchrotron, XFEL)
  - Repetitive, cumulative, synchronized measurements
  - Pump-probe approaches (pulsed laser, *or,* pulsed E/H field)



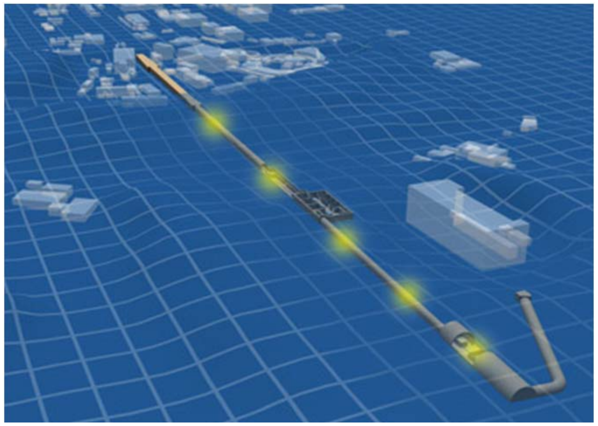
Advanced X-ray light sources: inherently pulsed beams

- Synchrotron Storage Rings
  - Pulse Width:** > 10^{-12} (ps)
  - Intensity, X-ray photons per pulse**
  - Repletion Rate**



Source: EPSIM 3D/JF Santarelli, Synchrotron Soleil

- Free Electron Lasers (XFEL)
  - Pulse Width:** ~ 10^{-15} (fs)
  - Intensity, X-ray photons per pulse:**
  - Repletion Rate**



Source: http://lcls.slac.stanford.edu/images/slac_site.jpg

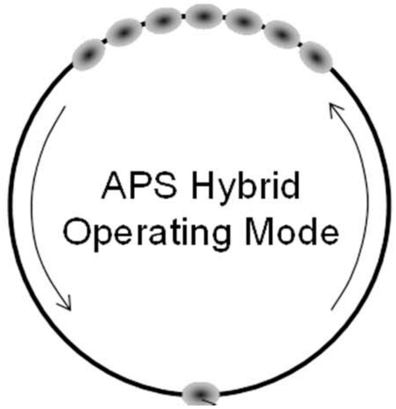
** Depends on light source, mode of operation, etc., …

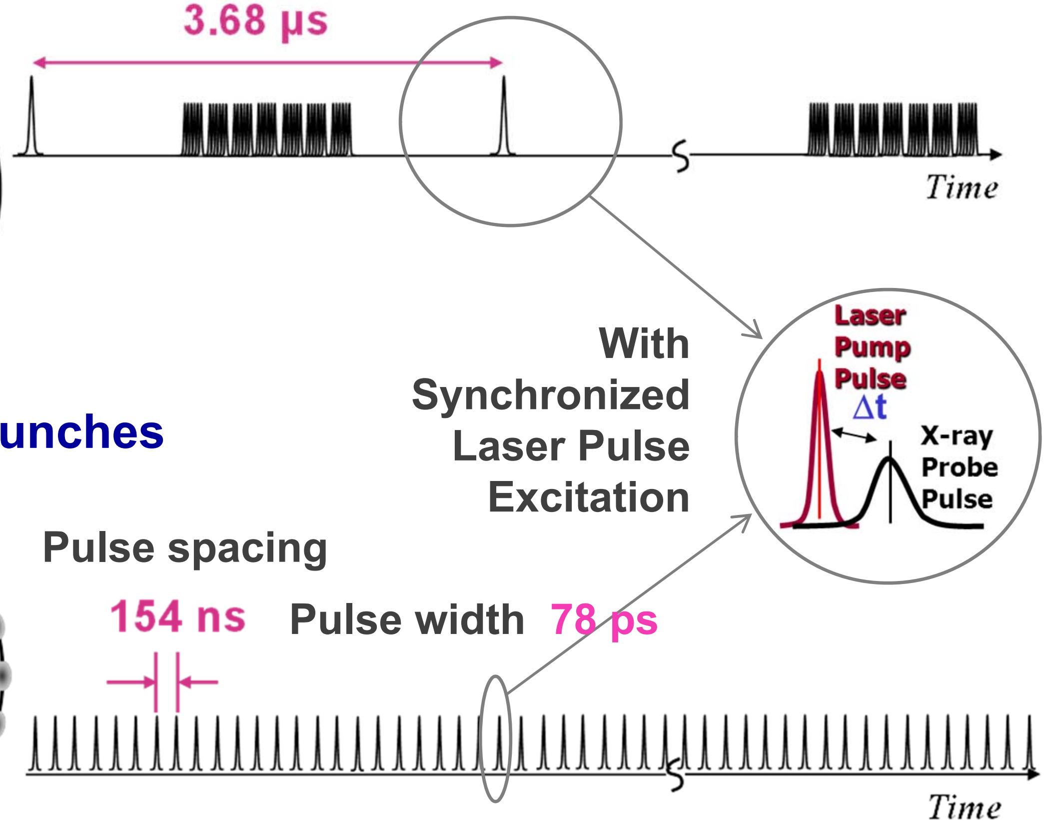
APS Operating Modes: 3 Available

Pulse spacing 3.68 μs

Pulse width 110 ps

X-ray Pulse Frequency

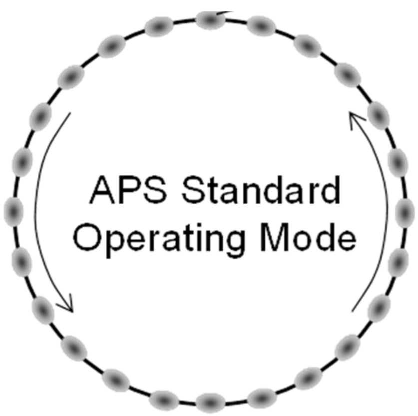




272 kHz

With Synchronized Laser Pulse Excitation

Hybrid Mode: 7 + 1 Bunches



Pulse spacing 154 ns

Pulse width 78 ps

6.5 MHz

24-Bunch Mode ("Standard")

324-Bunch Mode

Pulse spacing 11.4 ns

Pulse width 50 ps

88.1 MHz

Critical Parameters For Pump-Probe Experiments:

- **How Many Photons per Pulse?**
  - *Determines flux for single snapshot*

- **How Often Do You Get Them?**
  - *Flux for cw experiment*

- **How Many of Them Can You Use?**
  - *Flux for pump-probe experiment*

Comparison of X-ray pump-probe capabilities at representative light sources

	Source	Photons / bunch[a]	X-ray Repetition Rate	Laser Repetition Rate	Total X-ray Flux [photons/s]		Beamline with X-ay capability		
					Mono-chromatic	Poly-chromatic	XAFS	WAXS	GIXAFS / GIWAXS
XFEL	LCLS	3 x 10^{10}	120 Hz	120 Hz	4 x 10^{12}	1 x 10^{14}	XPP	XPP	?
6-8 GeV high energy storage rings	APS	1 x 10^{7}	6.5 MHz	1 kHz 10 kHz 271 kHz [b]	1 x 10^{10} 1 x 10^{11} 2 x 10^{12} [b]	5 x 10^{11} 5 x 10^{12} [b] 1 x 10^{14} [b]	11-IDD	9-ID/ 11-IDD	11-IDD
	ESRF	1 x 10^{7} [c]	1 kHz[d]	1 kHz	1 x 10^{10}	5 x 10^{11}	-----	ID09	-----
2-3 GeV storage rings	ALS	1 x 10^{4}	420 MHz	4 kHz	4 x 10^{7}	-----	U6.0.1	-----	-----
	SLS	3 x 10^{3}	414 MHz	1 kHz (?)	3 x 10^{6} (?)	-----	MicroXAS	-----	-----
	NSLS II	2 x 10^{3}	414 MHz	10 kHz (?)	2 x 10^{7} (?)	-----	?	?	?

[a]estimate @10 keV monochromatic beam. [b]MTX upgrade. [c]16-bunch special operating mode. [d] Storage ring 5.7 MHz , beamline uses 1 kHz X-ray chopper. ? = Could not be verified or unknown.

representative

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Per pulse basis, LCLS:
$>10^3$ (6-8 GeV)
$>10^6$ (2-3 GeV)
fold better than synchrotrons

How Many Photons per Pulse?

Comparison of X-ray pump-probe capabilities at representative light sources

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How Often Do You Get Them?- cw flux

How Many Photons per Pulse?

Scattering measurements typically ~ 10^{12} to 10^{14} photons

Comparison of X-ray pump-probe capabilities at representative light sources

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[a]estimate @10 keV monochromatic beam. [b]MTX upgrade. [c]16 bunch special operating mode. [d] Storage ring 5.7 MHz , beamline uses 1 kHz X-ray chopper. ?

1 2

Compared to LCLS, 6-8 GeV synchrotrons can catch-up by increase:
1) rep rate; 2) poly-chromaticity

How Many Can You Use?- Pump-probe flux

How Often Do You Get Them?- cw flux

How Many Photons per Pulse?

Scattering measurements typically ~ 10^{12} to 10^{14} photons

Comparison of X-ray pump-probe capabilities at representative light sources

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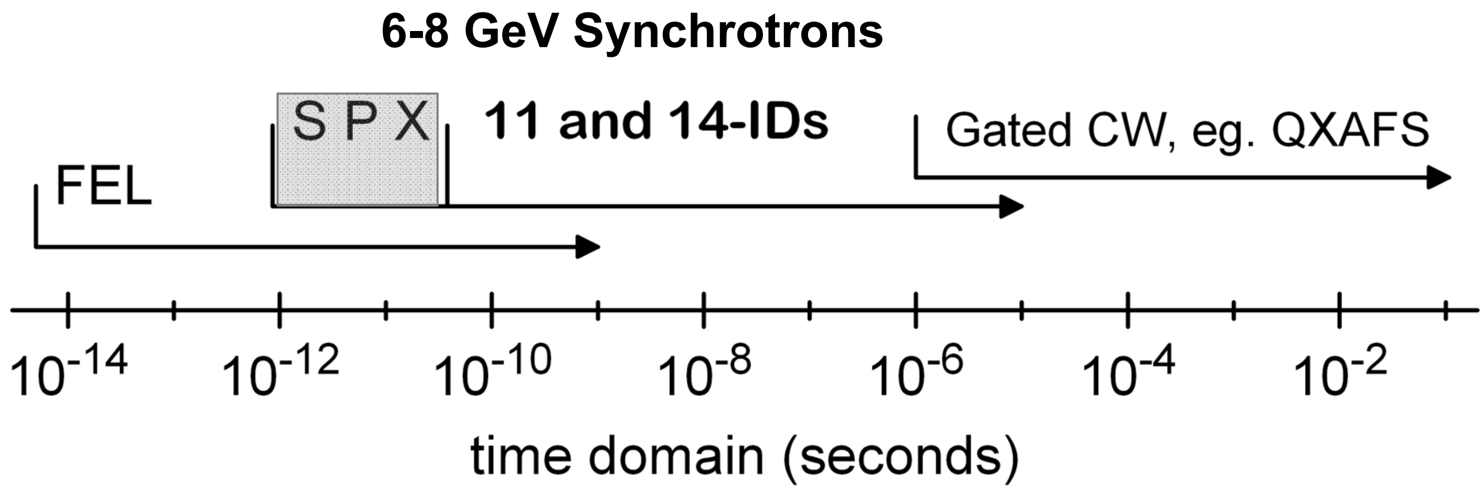
	NSLS II	2×10^{3}	414 MHz	10 kHz (?)	2×10^{7} (?)	-----	?	?	?

- **High Energy 6-8 GeV synchrotrons offer opportunities for state-of-the-art time-resolved X-ray studies**
- **Among the 6-8 GeV synchrotrons, APS standard operating modes well-suited for electronic or mechanical gating critical for pump-probe studies.**
- **2-3 GeV storage rings do not compete with high-energy storage rings as forefront light sources for pump-probe experiments**

Time Domains and Light Sources:

Time domain:



- **Within accessible time-range, 6-8 GeV synchrotrons have advantages compared to XFELs**
  - *higher beam stability*
  - *5 keV to 100 keV tunable X-ray energy range*
  - *Easier user access*
- **APS well-positioned for time-resolved X-ray studies**
  - *Only high energy storage ring in western hemisphere*
  - *Fills critical resources for time-resolved X-ray capabilities*

Presentation Outline:

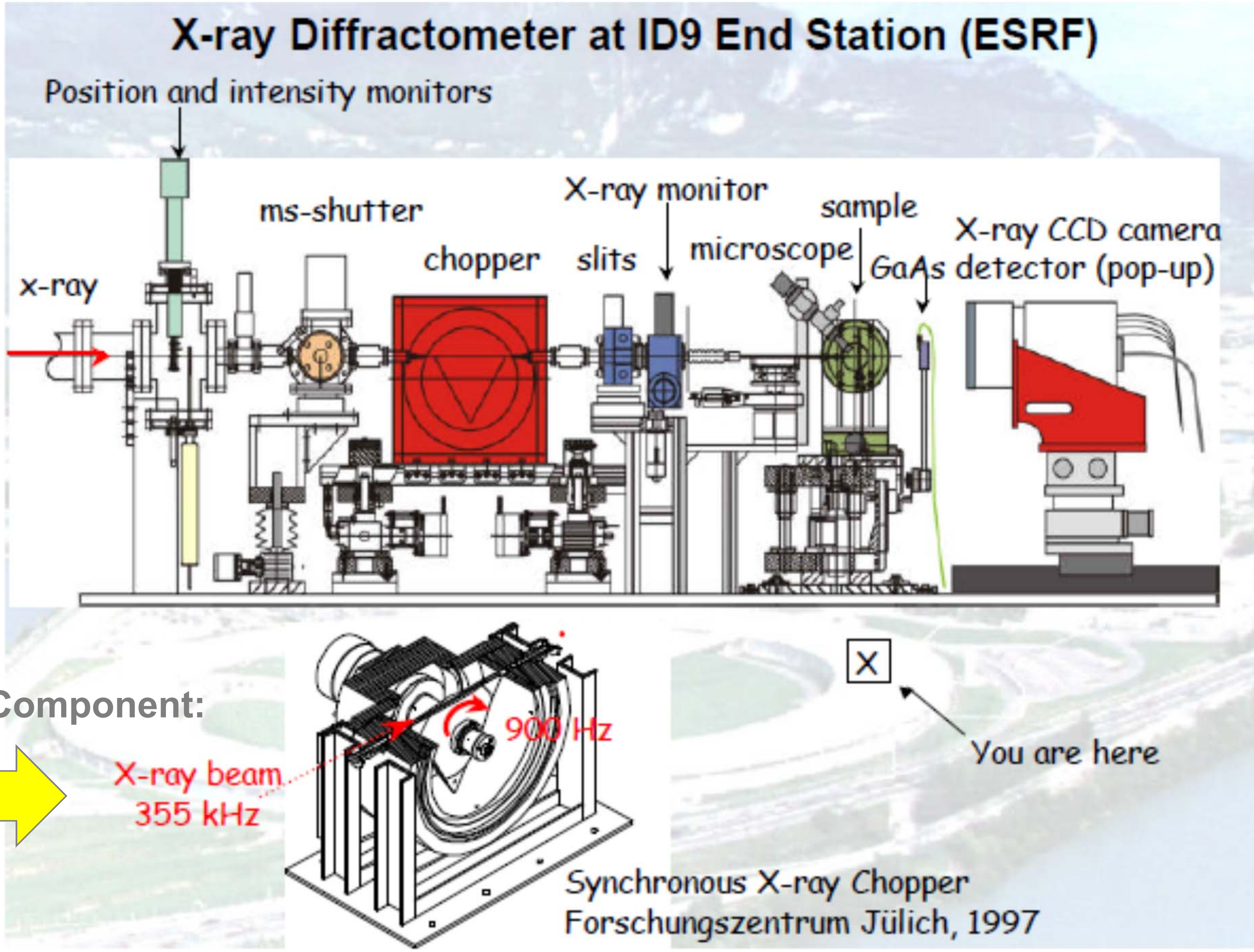
Introduction to time-resolved dynamics

Discussion that follows:

- General Approach and Issues for Time-Resolved X-ray (Scattering) Measurements
  - *Choosing your light source*

- **Examples from:**
  - **"pink" beam line sources**
  - **monochromatic beam line source**
  - **XFEL**

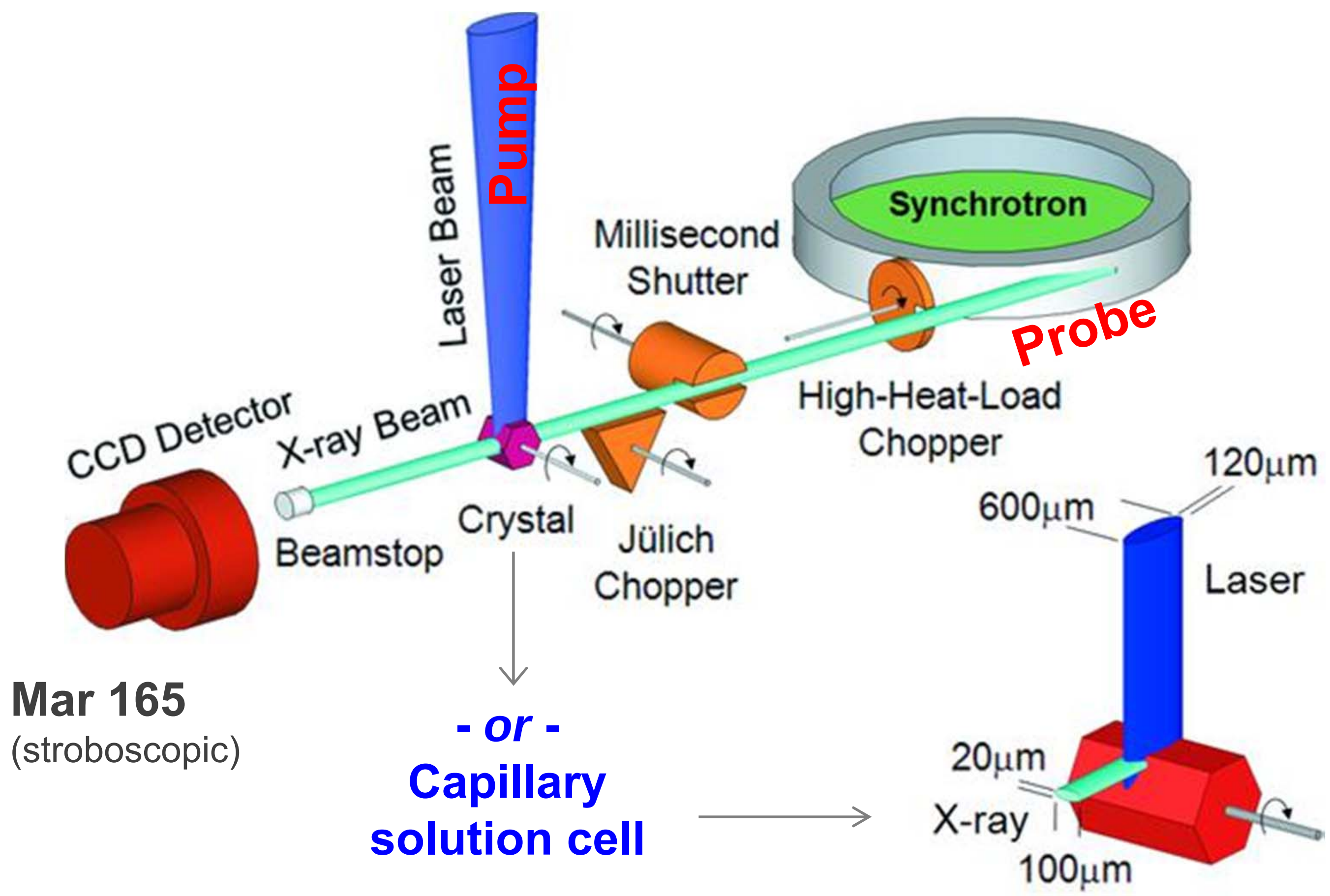
- Concluding remarks



Key Component:

- Allows single X-ray pulse selection

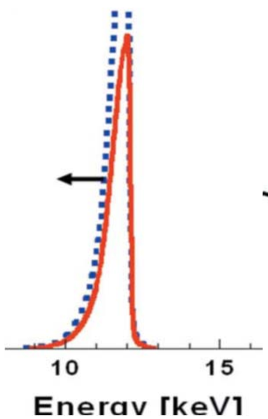
Beamline Diagram for BioCARS APS ID-14



Source: Graber et. al. J. (2011) J. Synchrotron Rad. **18**: *online*

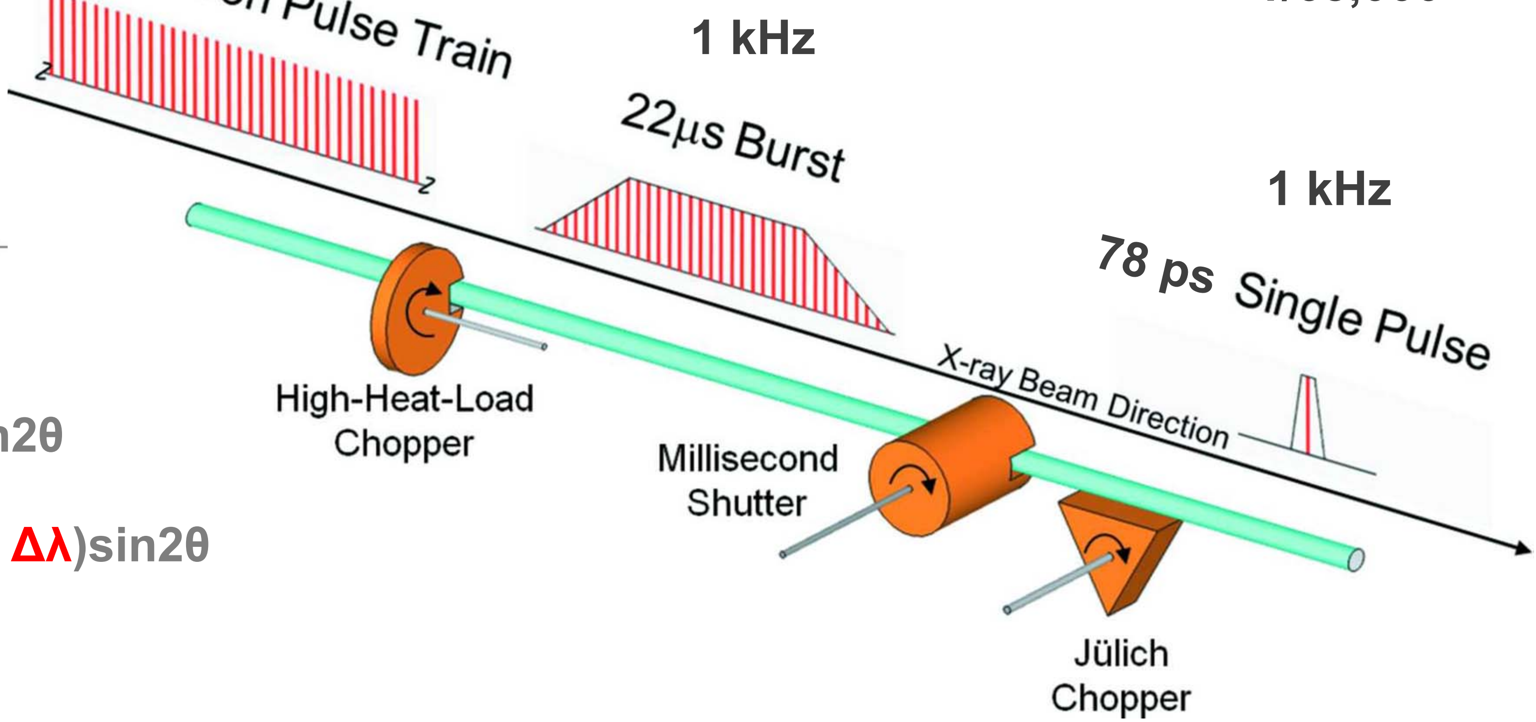
Beamline Diagram for BioCARS APS ID-14

24-bunch Mode
Pink beam



65 MHz

Time Averaged X-ray intensity: 1/65,000



$q = (4\pi/\lambda)\sin 2\theta$

$\Delta q = (4\pi/\Delta\lambda)\sin 2\theta$

Source: Graber et. al. J. (2011) J. Synchrotron Rad. **18**: *online*

Example Pump-probe Pink Beam Experiment

CHEMPHYSCHEM
ChemPhysChem **2009**, 10, 1958 – 1980
DOI: 10.1002/cphc.200900154

REVIEW

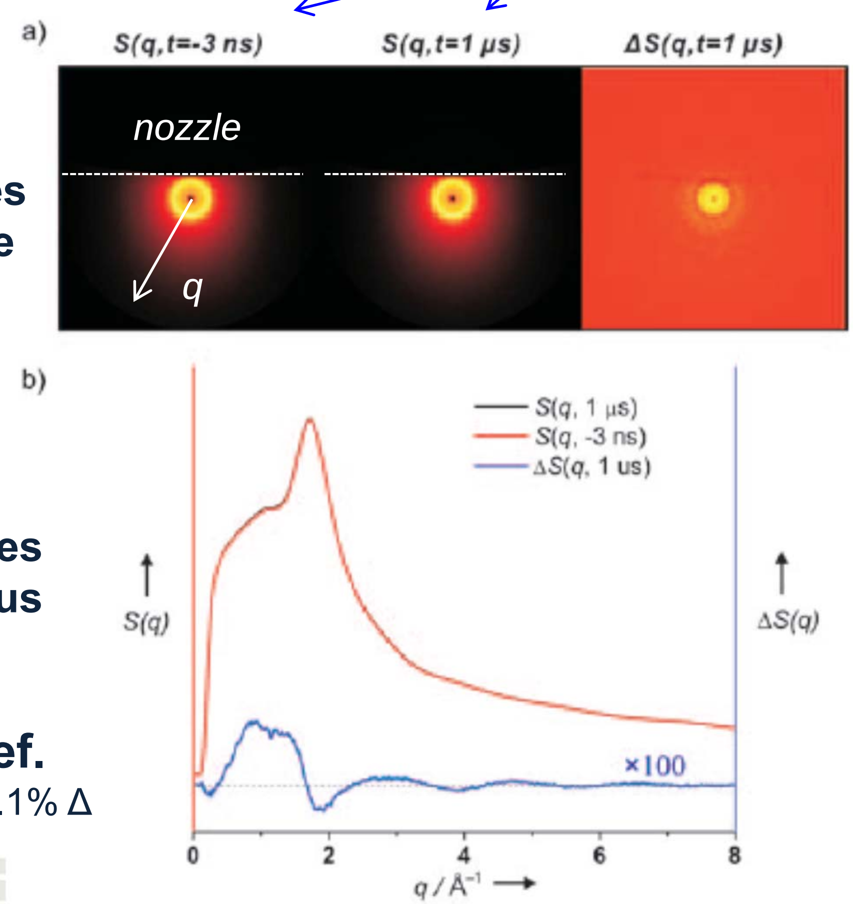
Spatiotemporal Kinetics in Solution Studied by Time-Resolved X-Ray Liquidography (Solution Scattering)

Tae Kyu Kim,[b] Jae Hyuk Lee,[a] Michael Wulff,[c] Qingyu Kong,[d] and Hyotcherl Ihee*[a]

X-ray pulse delay with respect to laser pulse

Detector images
- 3 ns (ref), 1 us, difference

Before, After, Δ



Radial averages
- 3 ns (ref), 1 us

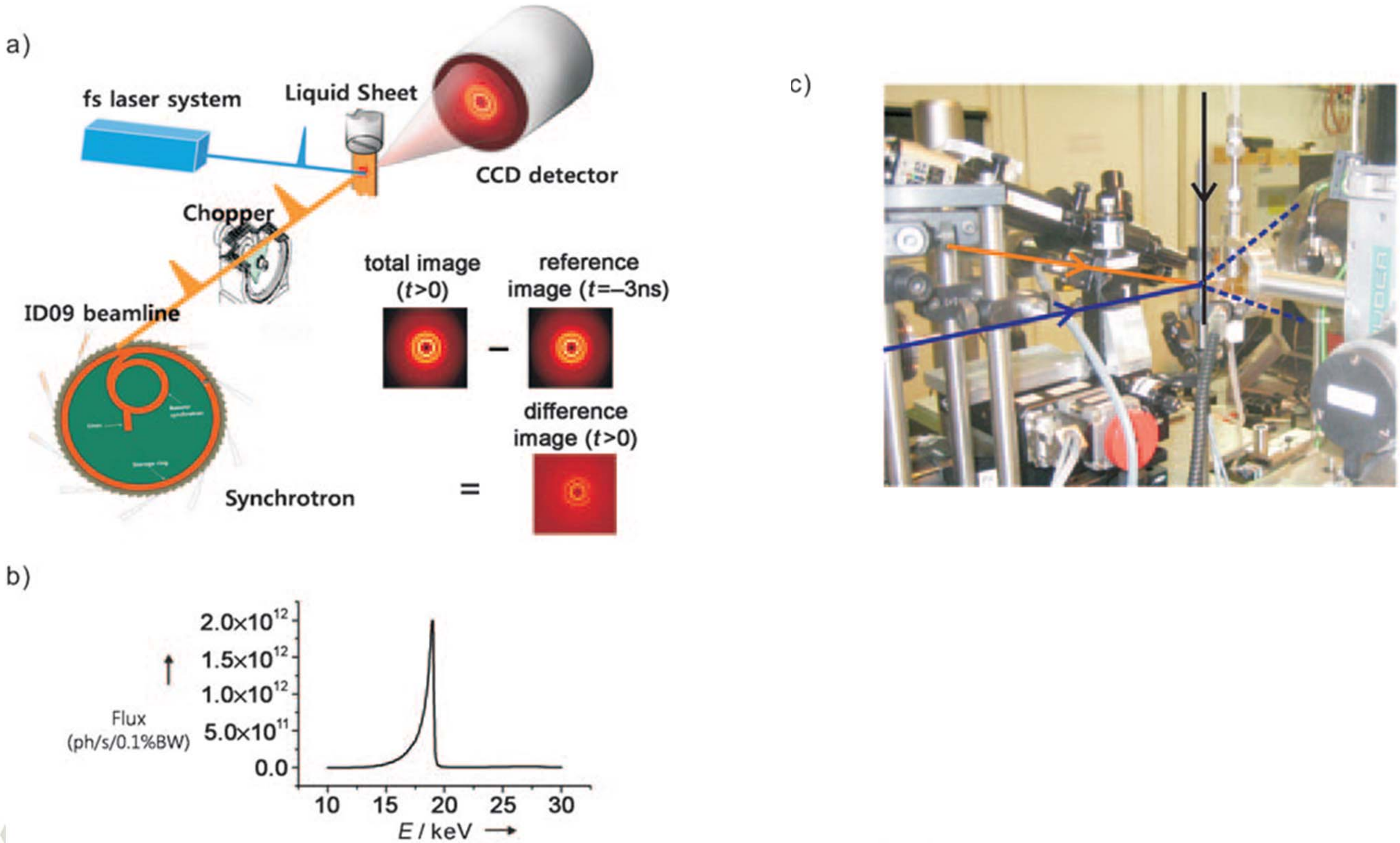
Difference: 1 us – ref.
~ 0.1% Δ

Figure 6:
Raw diffraction pattern pump-probe snapshots at selected time points, and difference patterns for Iodoform, CHI_3, in methanol.

Experimental TRXL Set-up at ID09 ESRF

Kim, Lee, Wulff, Kong, Ihee (2009) ChemPhysChem **10:** 1958-1980

Figure 5.



Identifying excited state reaction pathways.

Example: photo-decomposition of iodoform, CHI_3

(many other examples too!)

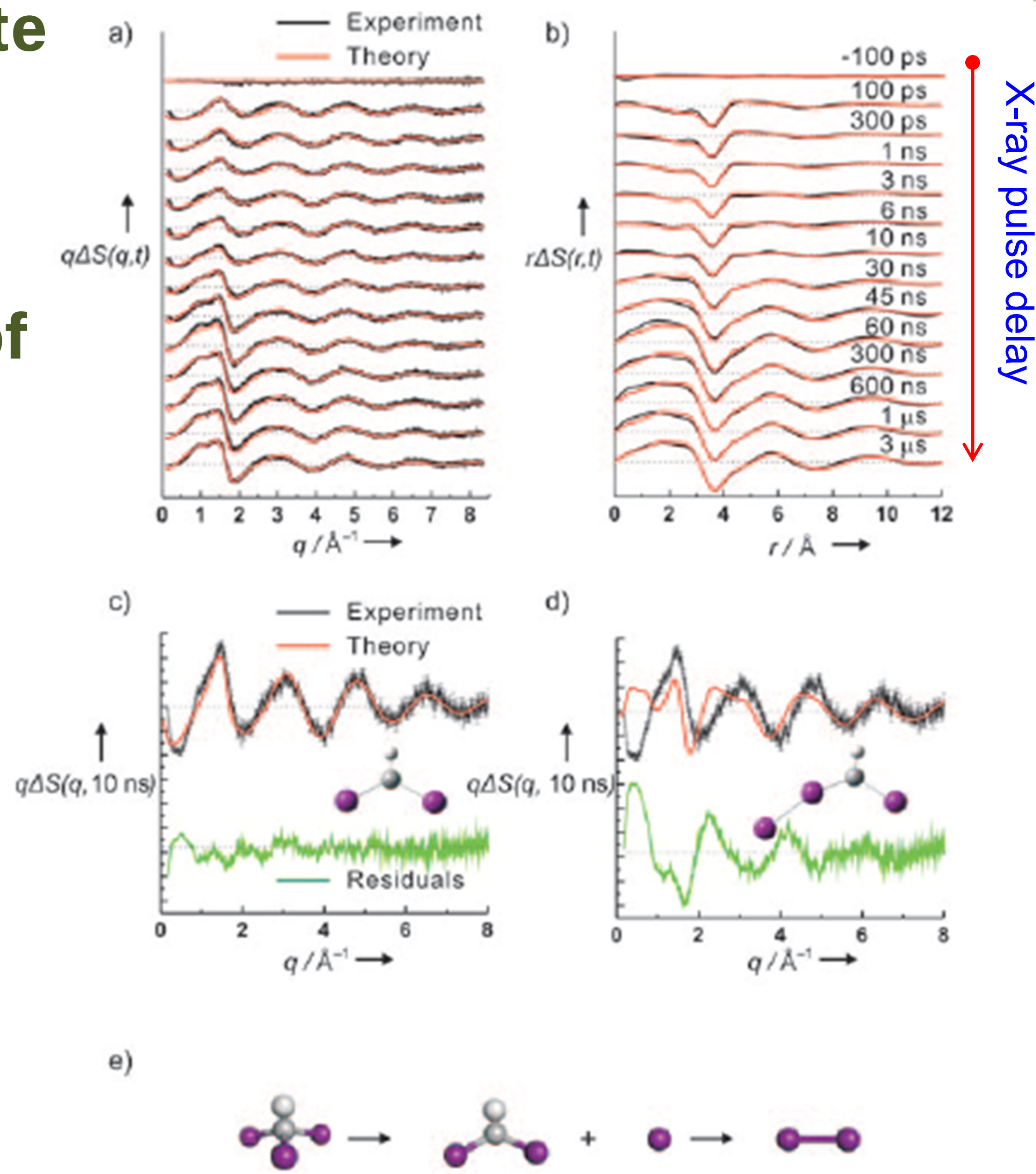
$CHI_3 \xrightarrow{h\nu}$ [CHI_3^*]

or ↓

[CHI_2-I] ?

↓

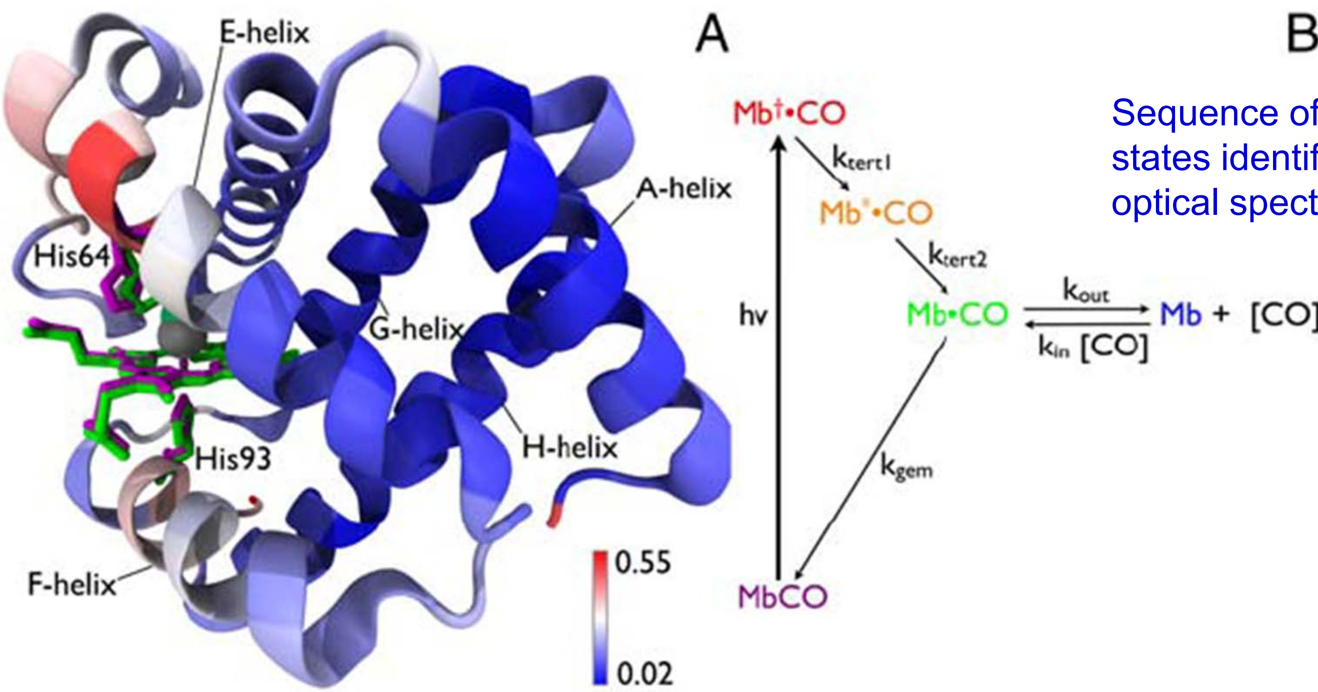
$2CHI_2 + 2I^\bullet \longrightarrow 2CHI_2 + I_2$



Kong, Lee, Plech, Wulff, Ihee, Koch, Angew. Chem. (2008) 120: 5632–5635; Angew. Chem. Int. Ed. (2008) 47: 5550–5553.

Time-resolved applications in macromolecular photochemistry:

Example: Photo-deligation in CO-Mb



Sequence of intermediate states identified by transient optical spectroscopy

Figure source:

Figure 1 *in* Choa, Dashdorj, Schotte, Graber, Henning, and Anfinrud, (2010) PNAS **10**: 7281-7286

Time-resolved approach has applications in macromolecular photochemistry:

Example: Photo-deligation in CO-Mb (APS-BioCARS)

Transient Δ scattering   Decomposition to set of intermediates   Intermediate kinetic sequence

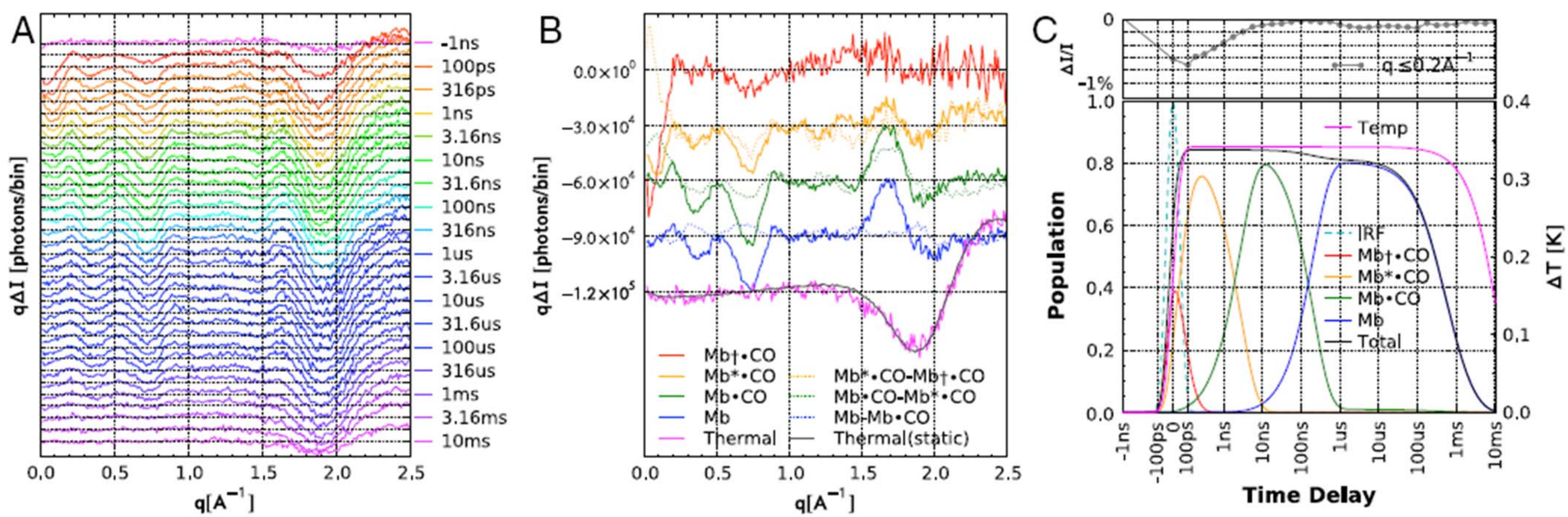


Figure source:

Figure 4 *in* **Choa, Dashdorj, Schotte, Graber, Henning, and Anfinrud, (2010) PNAS 10: 7281-7286**

Also:

Kim, Oang, Kim, Lee, Kim and Ihee (2011) Chem. Commun. **47**: 289–291

Time-Resolved X-ray Scattering:

Permitting Dynamics Resolution of Solution-State Processes

Polychromatic “pink” beamlines:

- ID09 European Synchrotron Radiation Facility (ESRF)
- ID-14 BioCARS APS

Monochromatic/multi-chromatic beamlines

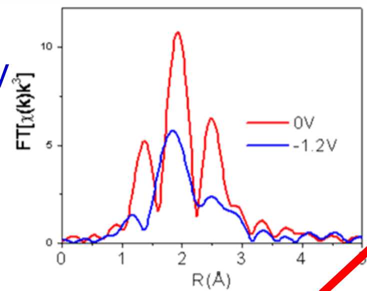
- 11-IDD APS

Combined Pump-Probe X-ray Scattering: Enables Multi-Scale Structure Characterization

TR X-ray Spectroscopy

Probes inner sphere:

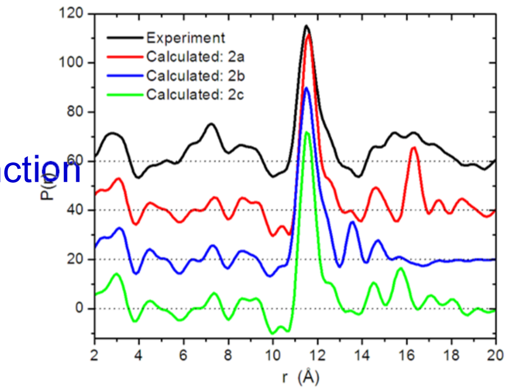
- Metal oxidation state
- Coordination geometry
- Electronic structure

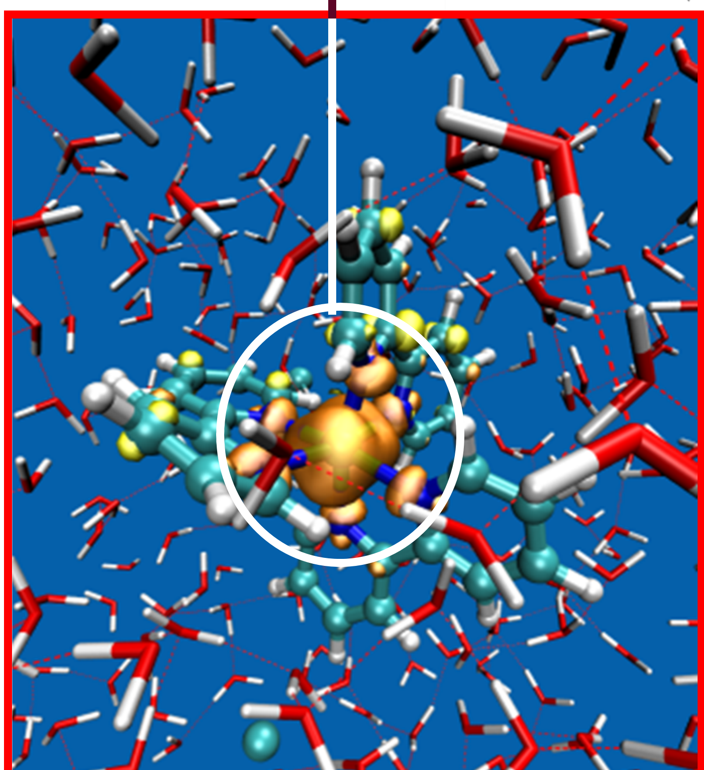


TR X-ray Scattering

Probes outer sphere:

- Molecular shape
- Interactions with solvent
- Pair density distribution function
- PDF





New tool for dynamics characterization for metal complexes across multiple research communities

- Solar energy conversion
- Chemical energy conversion
- Catalysis
- Geochemistry
- Fuel cells

QM/MM-MD Simulation: $Fe(bpy_3)$ solution structure
Daku and Hauser (2010) JPC Letts 1:1830

11-IDD (MTX) Beamline Approach/Capabilities:
Pump-probe, Stroboscopic X-ray Spectroscopy and Scattering

i) **Combined time-resolved X-ray spectroscopy (XANES, XAFS, XES) scattering (WAXS)**
   - Enables resolution across multiple length scales (0.01 Å to 100 nm)

ii) **Tunable monochromatic and polychromatic band-pass X-rays**
   - *Enables opportunities for combined spectroscopy/scattering*
   - *High-resolution PDF analysis*
   - *Anomalous X-ray scattering*
   - *High-flux measurements (multilayer)*

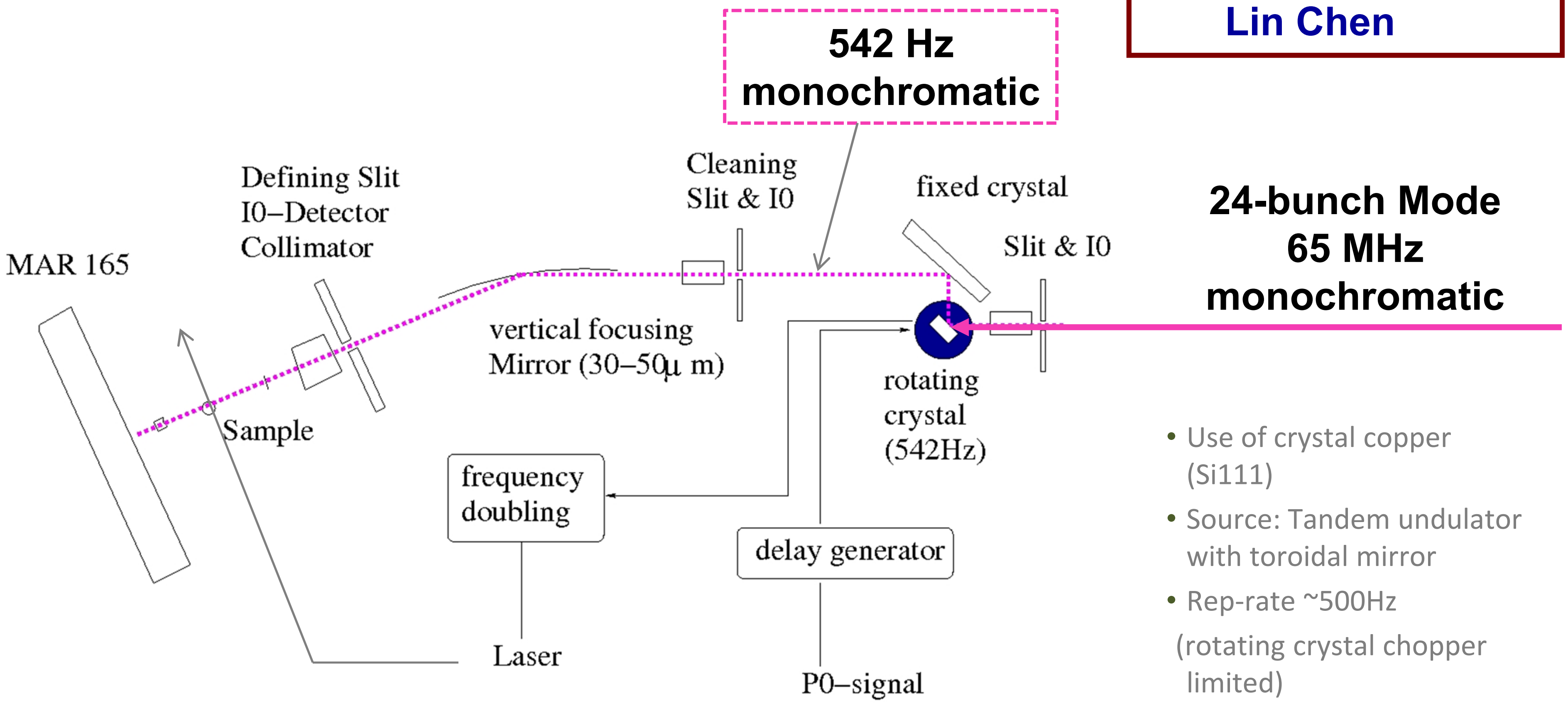
iii) **Grazing incidence scattering (GISAXS) and fluorescence (GIXFS)**
   - *Interfacial processes*
   - *Heterogeneous catalysis*

iv) **Both laser light and pulsed electric field excitation capabilities**
   - *Broadens range of energy-converting processes, enables initiation by:*
     - *Light*
     - *Interfacial electron transfer*
     - *E-Fields*

The Techniques and Methods
Chopping the X-ray Beam Using an Integrating Detector

APS-11-ID

Klaus Attenkofer
Naran Dashdorj
Xiaoyi Zhang
Guy Jennings
Lin Chen

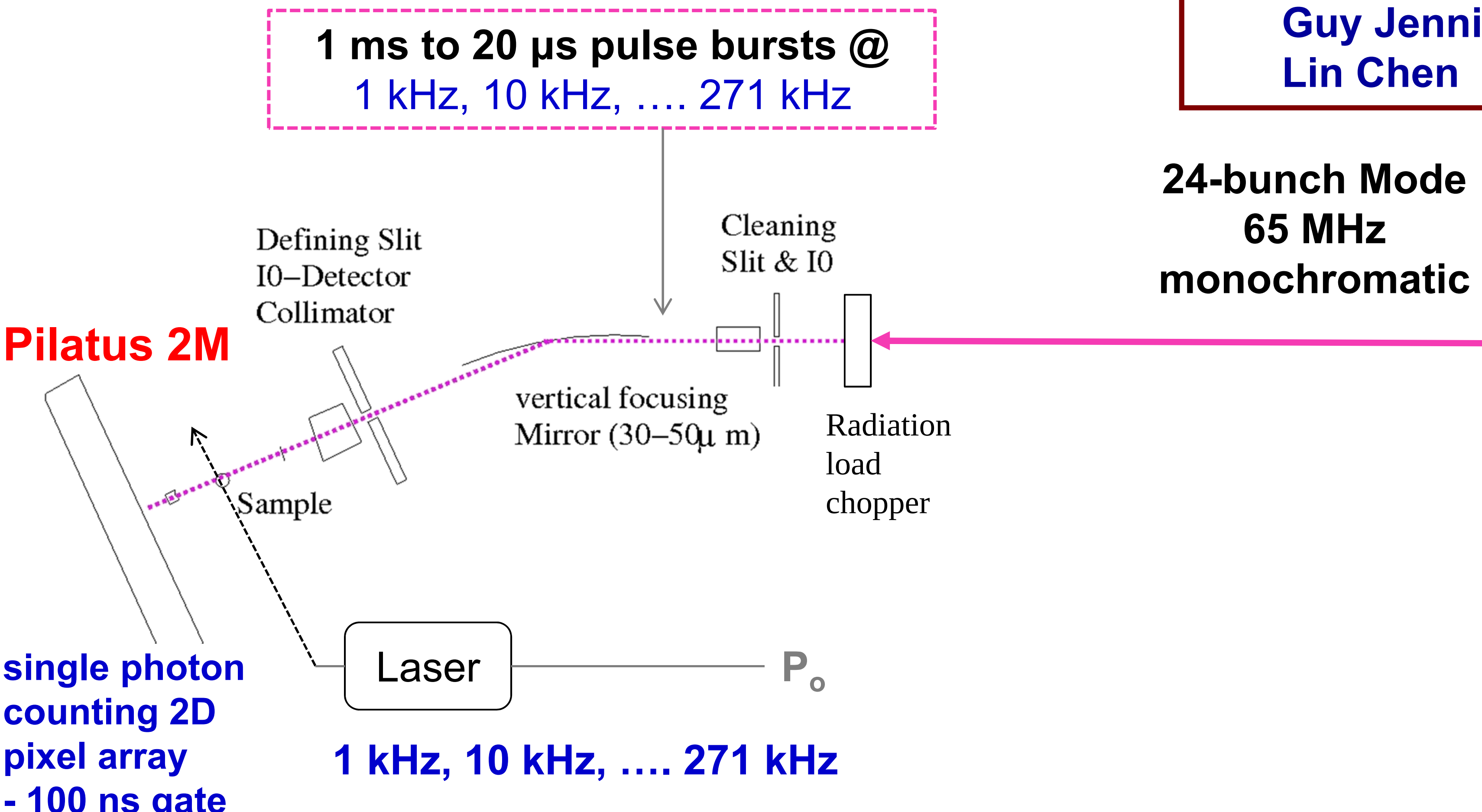


- Use of crystal copper (Si111)
- Source: Tandem undulator with toroidal mirror
- Rep-rate ~500Hz

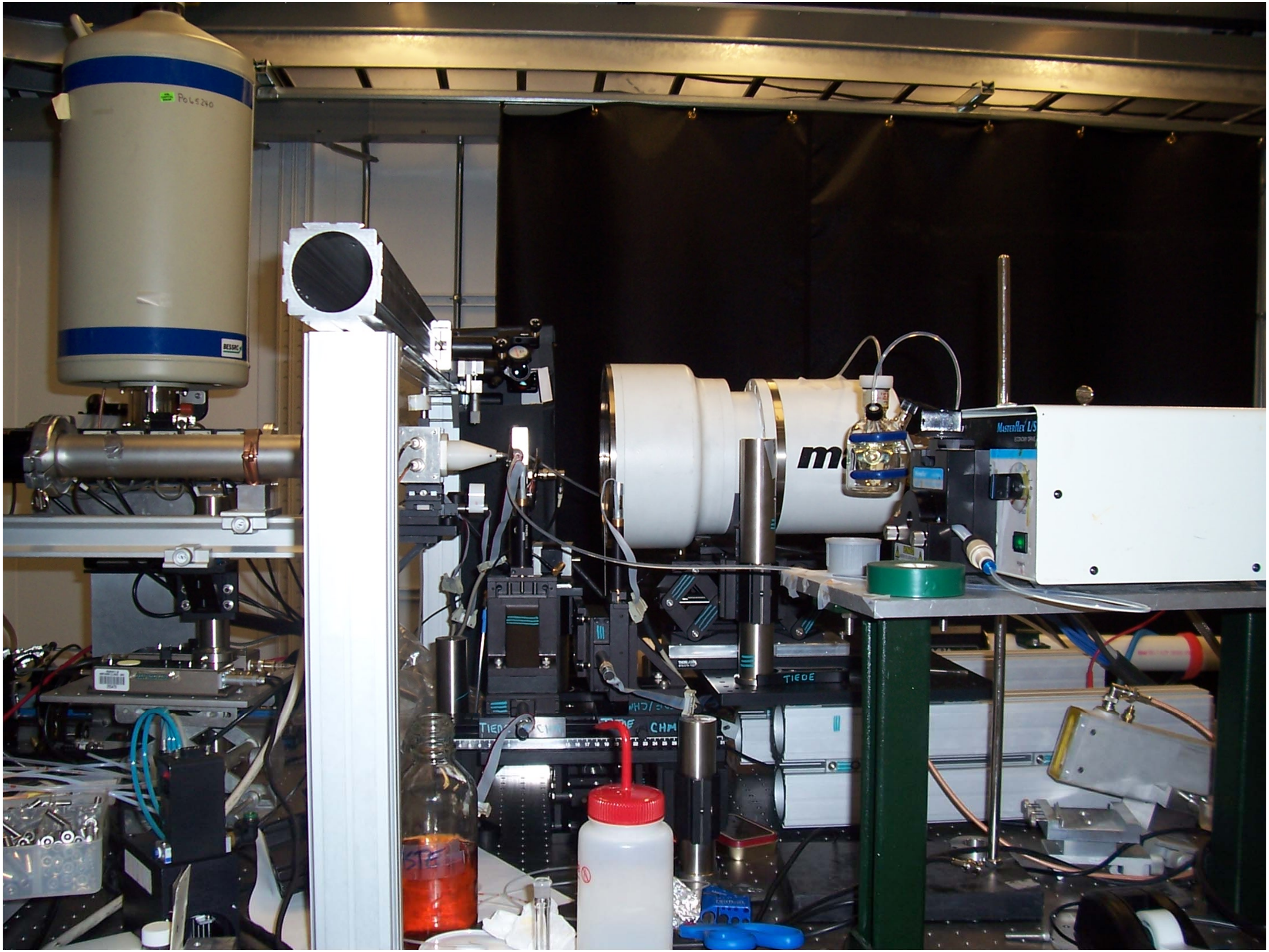
  (rotating crystal chopper limited)
- Efficiency ~70%
- 100 ps time resolution
- 0.3 hr. – 2 hr. data acquisition/time point

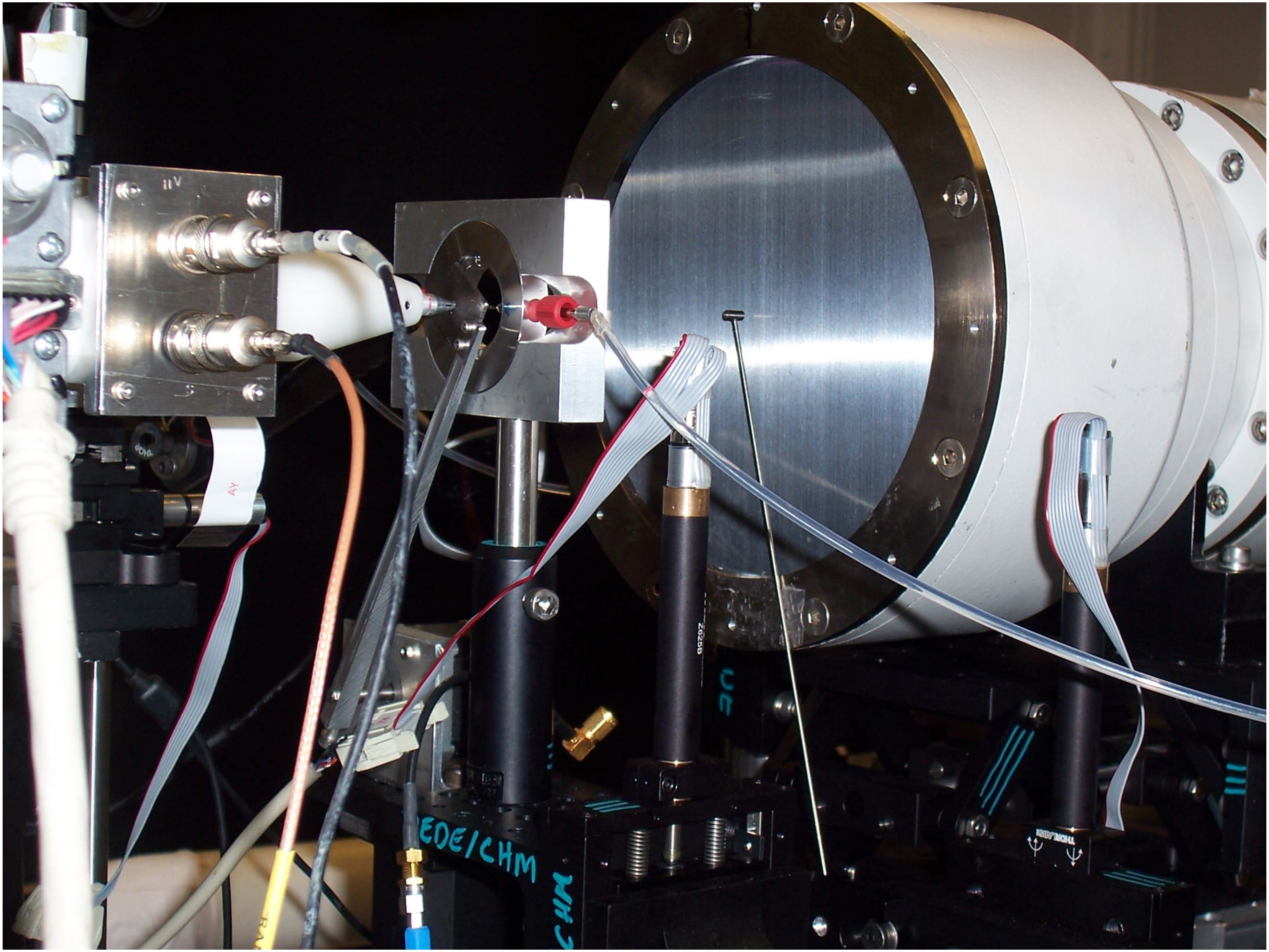
Pump-Probe Using a Gated Detector

APS-11-ID
Naran Dashdorj
Klaus Attenkofer
Xiaoyi Zhang
Guy Jennings
Lin Chen



- **Fast, gated detection is doing X-ray pulse selection**
- **Allows faster data sampling rates**
- **Experiment frequency limited by laser repetition rate, sample exchange**


TIEDE


EDE/CHM
AY

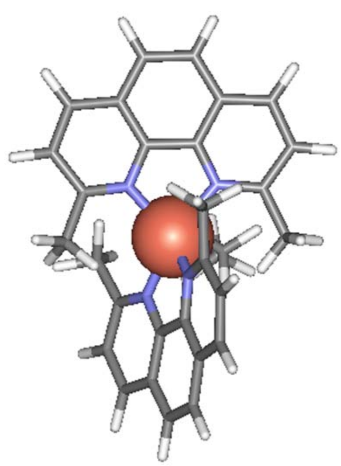
Illustrate with a Scientific Case Example:
Engineering excited-state structure dynamics for photon energy conversion

Metal-to-ligand-charge-transfer, MLCT, complexes

- Broadly investigated for applications in solar energy conversion, alternative lighting, and photo-catalysis

Cu(I) diimide coordination complexes of particular interest

$$\underset{\mathbf{3d^{10}}}{[Cu^{I}(dmp)_2]^+} \xrightarrow{h\nu} \underset{\mathbf{3d^{9}}}{[Cu^{II}(dmp^-)(dmp)]^+}$$



Cu(I)[dimethylphenanthroline]$_2$

- Abundant 1st row transition metal
- Jahn-Teller distortion drives an excited-state change in coordination number and geometry.
- Opportunities for reaction control by:
  - *Structurally gated electron transfer*
  - *Ligand controlled dynamics*

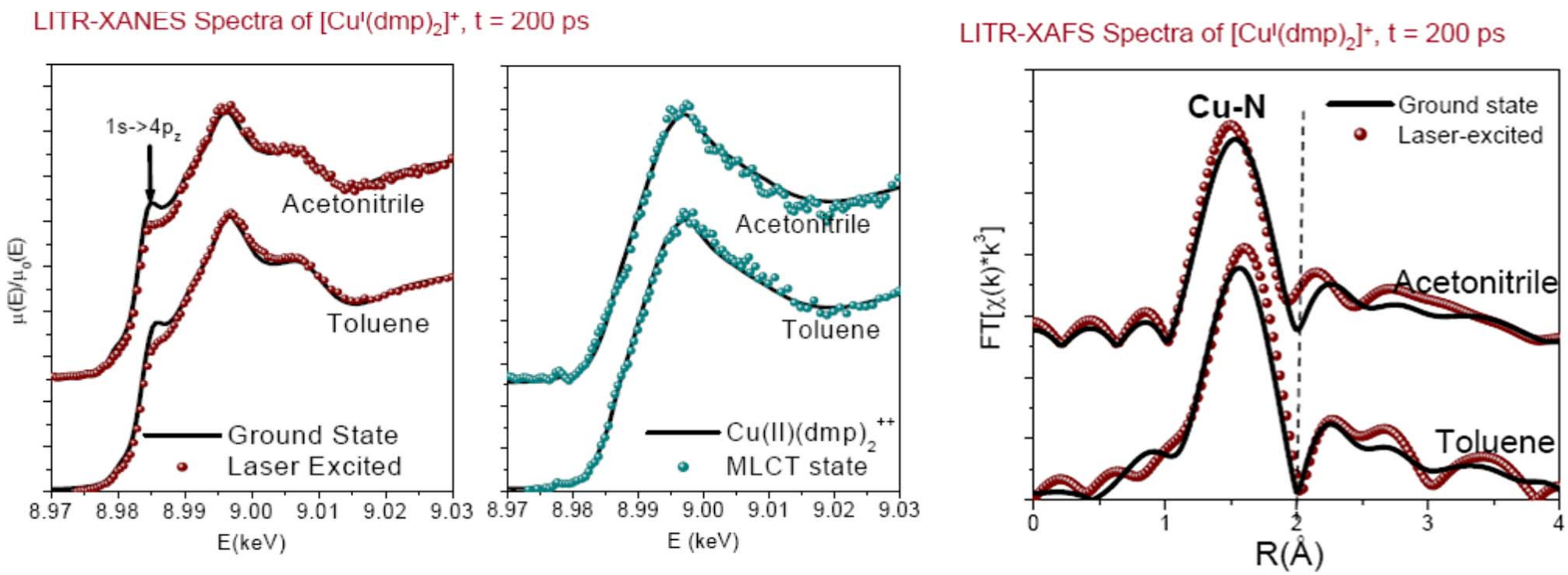
Pioneering example on11-ID-D:
Excited-State Pump-Probe X-ray Spectroscopy:

Lin Chen

$$[Cu^{I}(dmp)_2]^+ \xrightarrow{h\nu} [Cu^{II}(dmp^-)(dmp)]^+$$

$3d^{10}$ → $3d^9$

Science **2001,** 292, 262-264.
Angew. Chem. Int. Ed. **2004,** 43, 2886
Annu. Rev. Phys. Chem **2005,** 56, 221



Pump-probe X-ray spectroscopy track changes in excited-state:

- **Oxidation state,**
- **Coordination geometry,**
- **Coordination number**

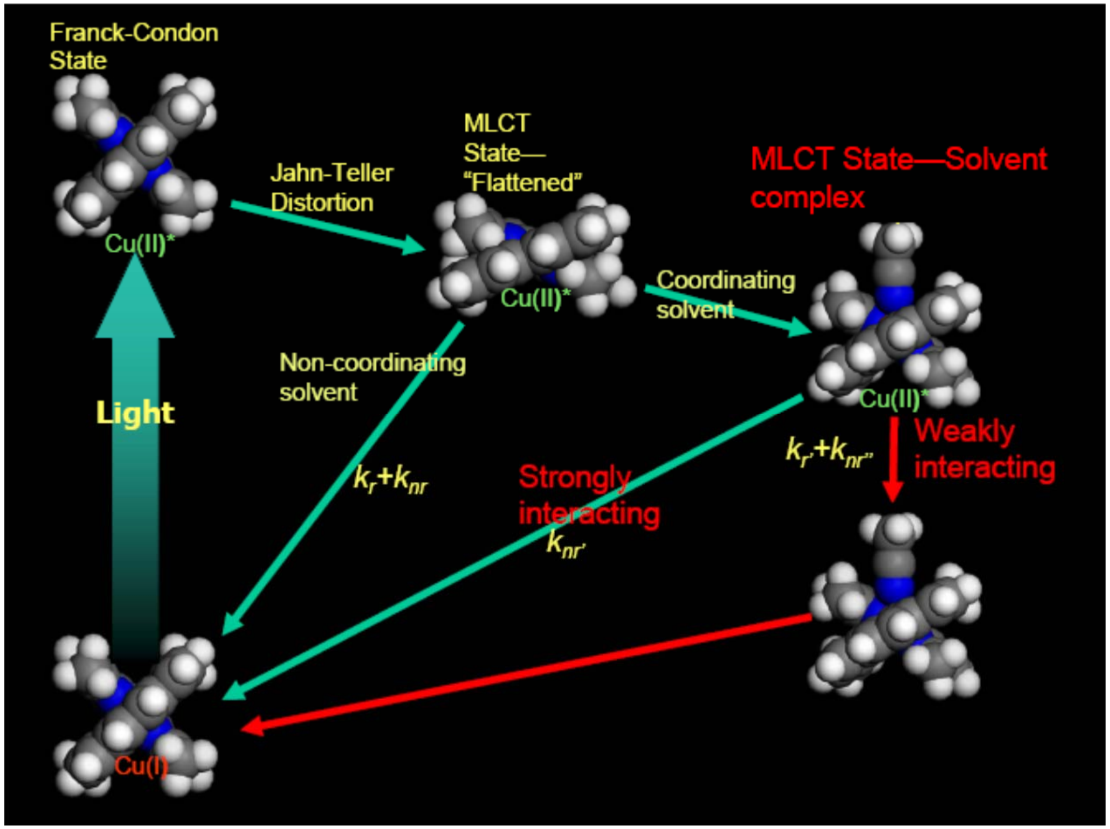
Pump-Probe X-ray Spectroscopy Determined $Cu^{I}DMP_2$ Excited-State Dynamics Scheme

Lin Chen

- TR-XS show excited-state reaction path, kinetics, energies determined by coordination geometry
- Implies converse: ligand geometry control of excited-state chemistry
  - Biological principle: entatic control

New Opportunities:

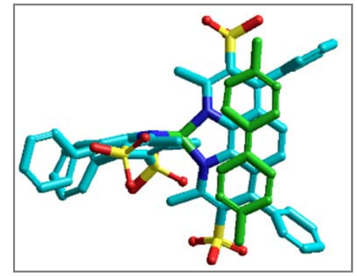
- See excited state structure
- Design molecules for excited-state photochemistry
- Can go beyond 1st coordination shell: X-ray scattering



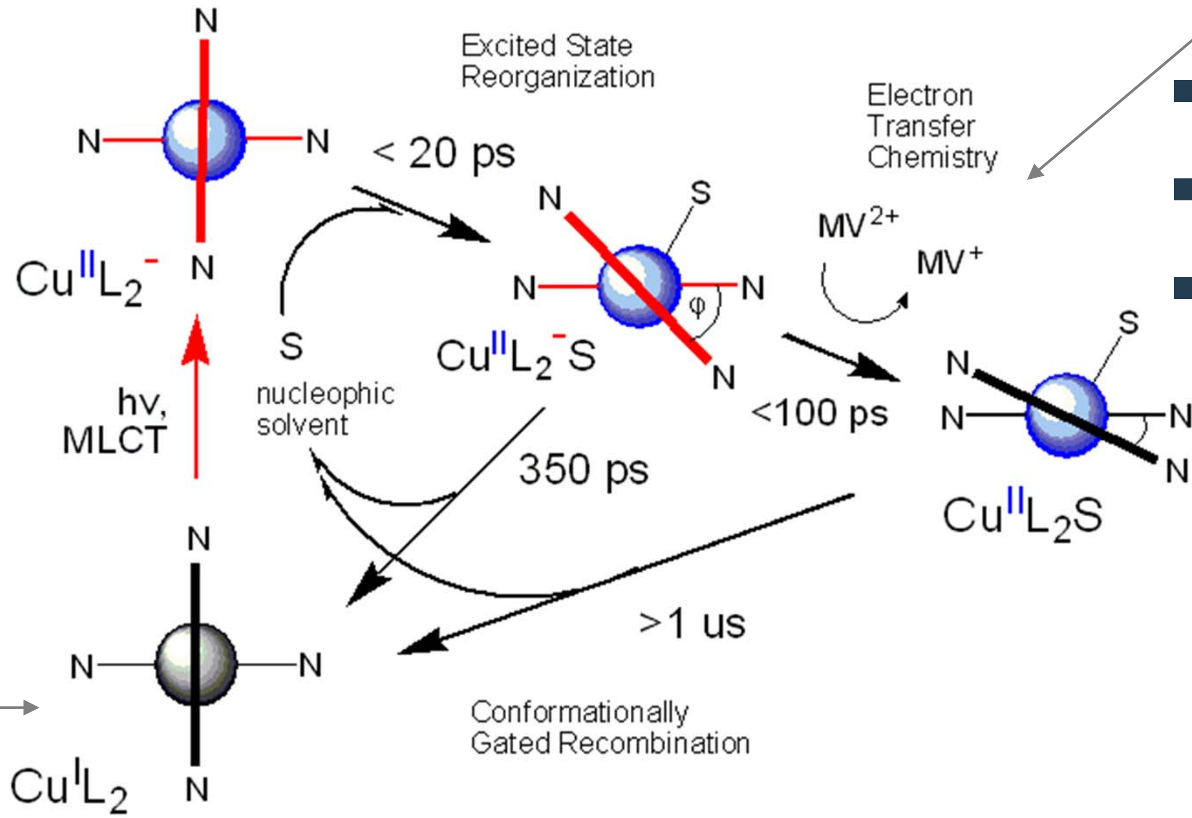
1. Chen, L. X.; Shaw, G. B.; Novozhilova, I.; Liu, T.; Jennings, G.; Attenkofer, K.; Meyer, G. J.; Coppens, P., MLCT state structure and dynamics of a copper(I) diimine complex characterized by pump-probe X-ray and laser spectroscopies and DFT calculations. *J. Am. Chem. Soc* **2003,** 125, 7022-7034.
2. Shaw, G. B.; Grant, C. D.; Shirota, H.; Castner, E. W.; Meyer, G. J.; Chen, L. X., Ultrafast structural rearrangements in the MLCT excited state for copper(I) bis-phenanthrolines in solution. *J. Am. Chem. Soc* **2007,** 129, (7), 2147-2160.
3. Lockard, J. V.; Kabehie, S.; Zink, J. I.; Smolentsev, G.; Soldatov, A.; Chen, L. X., Influence of Ligand Substitution on Excited State Structural Dynamics in Cu(I) Bisphenanthroline Complexes. *J. Phys. Chem. B* **2010,** 114, (45), 14521-14527.

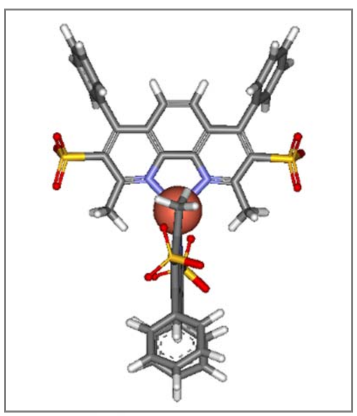
Elaboration on Cu(I) diimide excited-state scheme for electron transfer:
Need for multiple time scales

ET complex



- Molecular recognition
- ET complex formation
- Cage escape

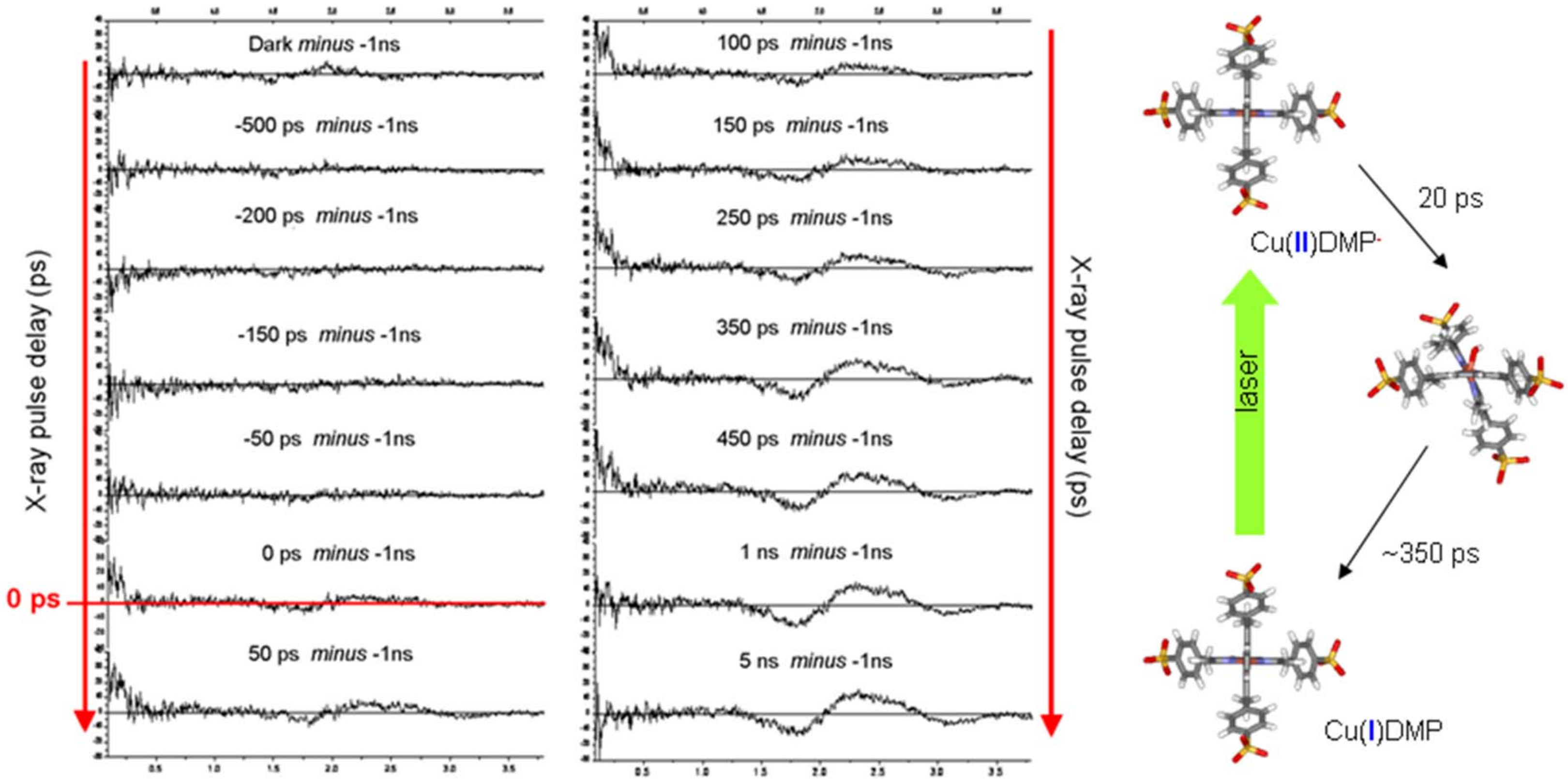




- Inner and outer shell structural events control efficiency of electron transfer
- Dynamic processes cover ultrafast photophysics to multi-scale chemistry
- Model for novel and biomimetic solar conversion

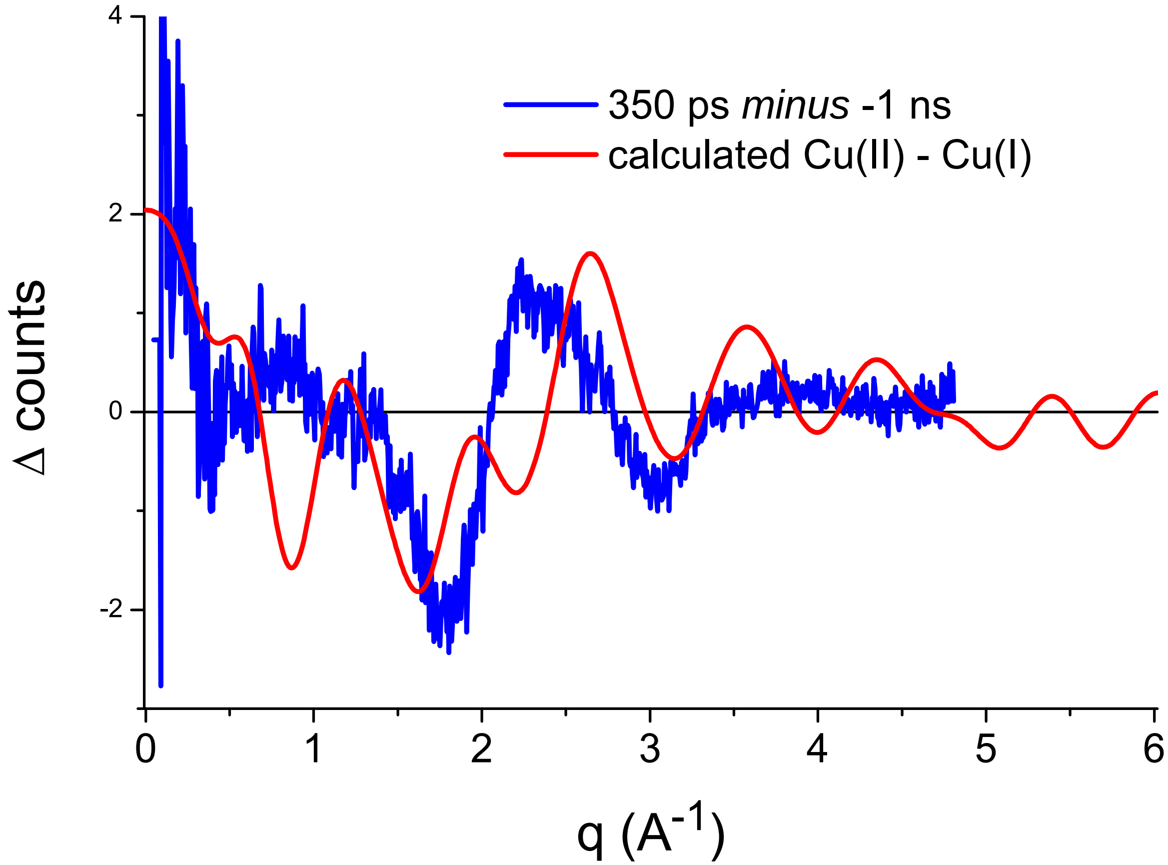
First Pump-Probe Scattering on 11-ID-D using Monochromatic X-rays :

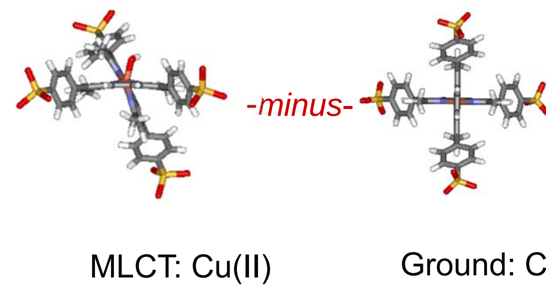
Cu(I) diimide excited-state reaction dynamics



- Demonstration feasibility to do pump-probe TR-scattering experiment using **monochromatic X-rays** at synchrotron light-source
  - **Dilute (6 mM) 1st row transition metal complex**

Comparison of model and TR experiment





- Instantaneous change small angle consistent with change in coordination in MLCT
- Small angle change tracks changes Cu(II) lifetime
- Non-emissive energy transfer between the molecular excited states and the solvent cause heating effects to grow in at longer times.
- Transient difference pattern differs from ground state models: implies new structures

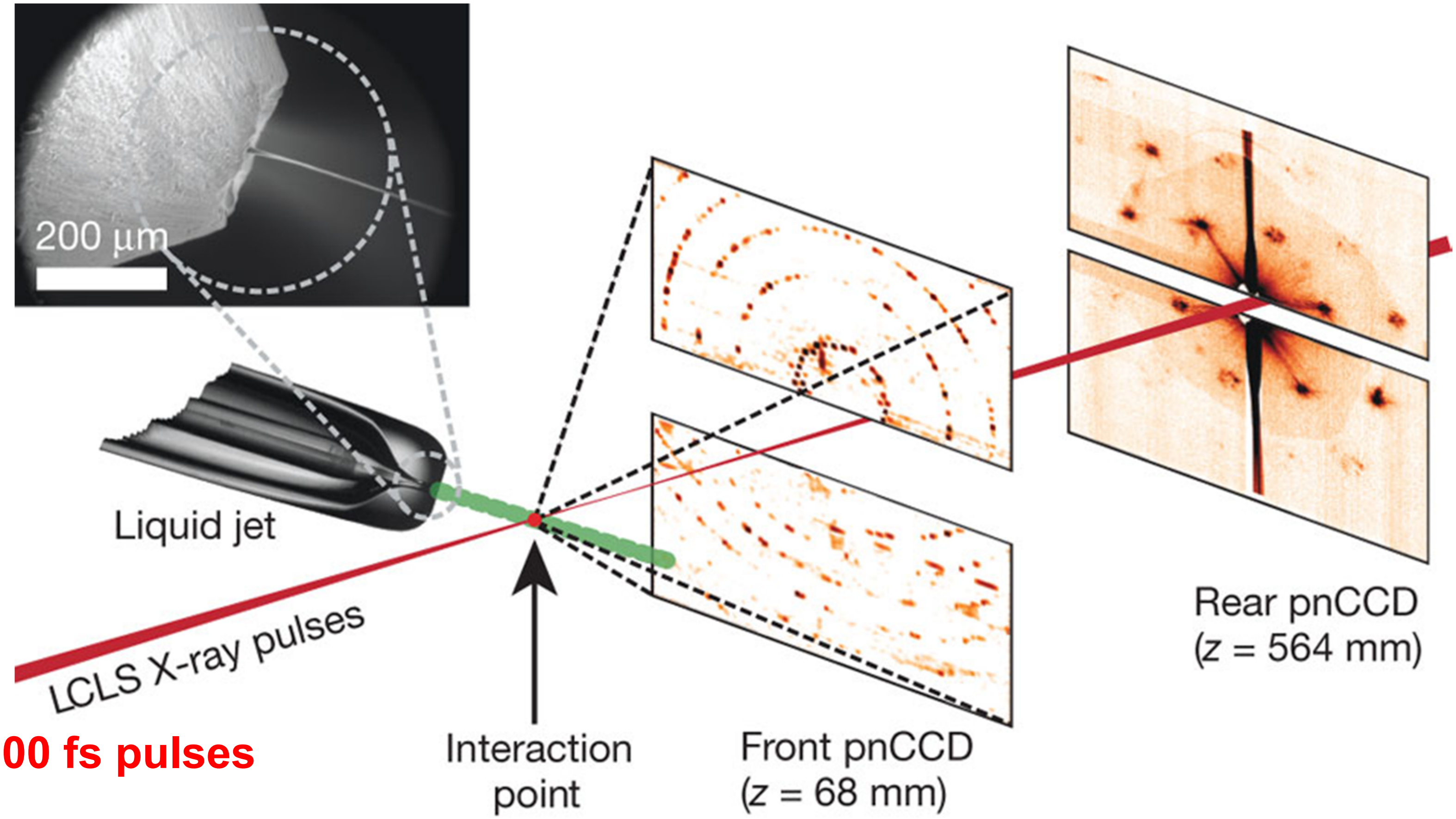
- **Demonstrates opportunity to do combined TR spectroscopy/scattering……., both using monochromatic X-rays**
- **Opportunity to extend to *anomalous* TR scattering**
- **Opportunity to achieve 10- to 50-fold improved intensity with multilayer monochromator (MTX upgrade)**

Pump-probe X-ray Scattering with XFEL:

First Publications:

- Stanford Linac Coherent Light Source (LCLS)

Femtosecond nanocrystallography at LCLS: Photosystem I crystals



HN Chapman *et al. Nature* 470, 73-77 (2011) doi:10.1038/nature09750

nature

LETTER

doi:10.1038/nature09750

Femtosecond X-ray protein nanocrystallography

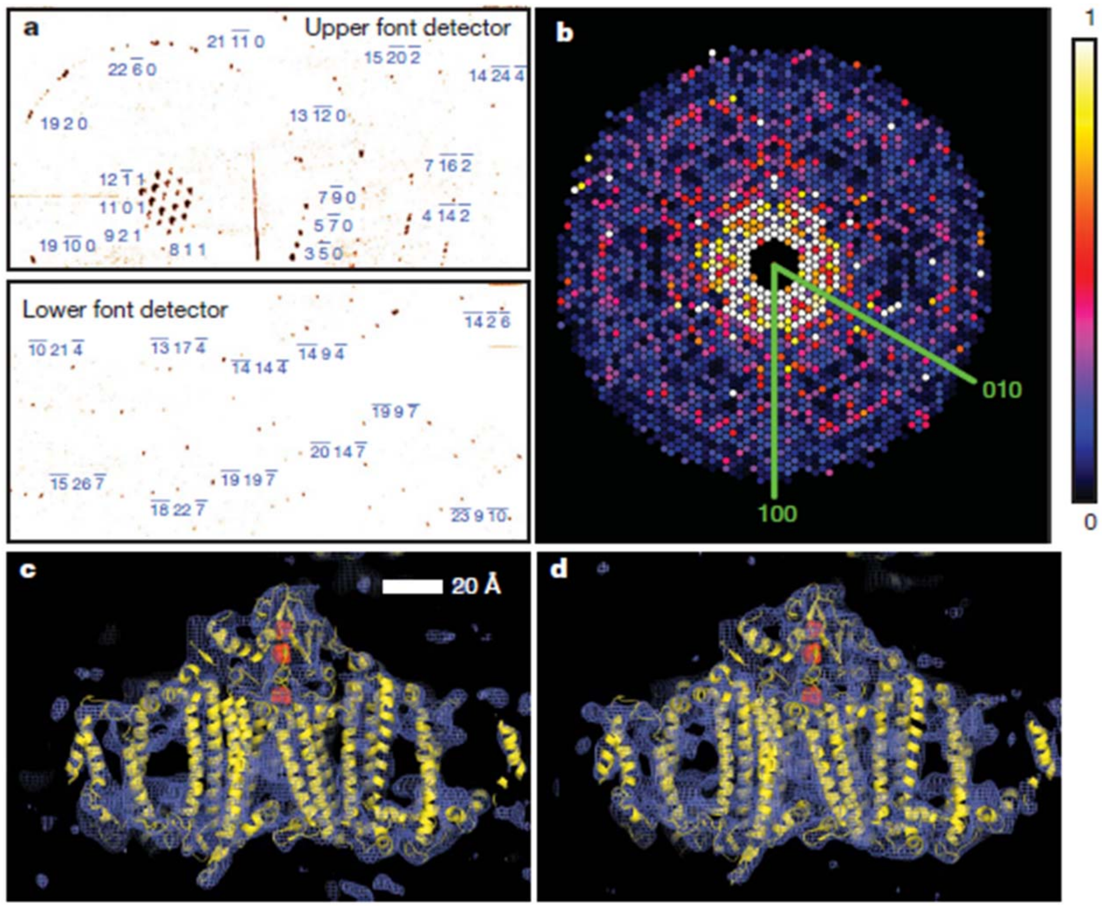
Henry N. Chapman[1,2], Petra Fromme[3], Anton Barty[1], Thomas A. White[1], Richard A. Kirian[4], Andrew Aquila[1], Mark S. Hunter[3], Joachim Schulz[1], Daniel P. DePonte[1], Uwe Weierstall[4], R. Bruce Doak[4], Filipe R. N. C. Maia[5], Andrew V. Martin[1], Ilme Schlichting[6,7], Lukas Lomb[7], Nicola Coppola[1{], Robert L. Shoeman7, Sascha W. Epp[6,8], Robert Hartmann[9], Daniel Rolles[6,7], Artem Rudenko[6,8], Lutz Foucar[6,7], Nils Kimmel[10], Georg Weidenspointner[11,10], Peter Holl[9], Mengning Liang[1], Miriam Barthelmess[12], Carl Caleman[1], Se´bastien Boutet[13], Michael J. Bogan[14], Jacek Krzywinski13, Christoph Bostedt[13], Sasˇa Bajt[12], Lars Gumprecht[1], Benedikt Rudek[6,8], Benjamin Erk[6,8], Carlo Schmidt[6,8], Andre´ Ho¨mke[6,8], Christian Reich[9], Daniel Pietschner[10], Lothar Stru¨der[6,10], Gu¨nter Hauser[10], Hubert Gorke[15], Joachim Ullrich[6,8], Sven Herrmann[10], Gerhard Schaller[10], Florian Schopper[10], Heike Soltau[9], Kai-Uwe Ku¨hnel[8], Marc Messerschmidt[13], John D. Bozek[13], Stefan P. Hau-Riege[16], Matthias Frank[16], Christina Y. Hampton[14], Raymond G. Sierra[14], Dmitri Starodub[14], Garth J.Williams[13], Janos Hajdu[5], Nicusor Timneanu[5], M. Marvin Seibert[5{], Jakob Andreasson[5], Andrea Rocker[5], Olof Jo¨nsson[5], Martin Svenda[5], Stephan Stern[1], Karol Nass[2], Robert Andritschke[10], Claus-Dieter Schro¨ter[8], Faton Krasniqi[6,7], Mario Bott[7], Kevin E. Schmidt[4], XiaoyuWang[4], Ingo Grotjohann[3], James M. Holton[17], Thomas R. M. Barends[7], Richard Neutze[18], Stefano Marchesini[17], Raimund Fromme[3], Sebastian Schorb[19], Daniela Rupp[19], Marcus Adolph[19], Tais Gorkhover[19], Inger Andersson[20], Helmut Hirsemann[12], Guillaume Potdevin[1]2, Heinz Graafsma[12], Bjo¨rn Nilsson[12] & John C. H. Spence[4]

HN Chapman *et al.* *Nature* 470, 73-77 (2011)

nature

Femtosecond nanocrystallography at LCLS: Photosystem I

100 fs, 8.5 Å resolution electron density map

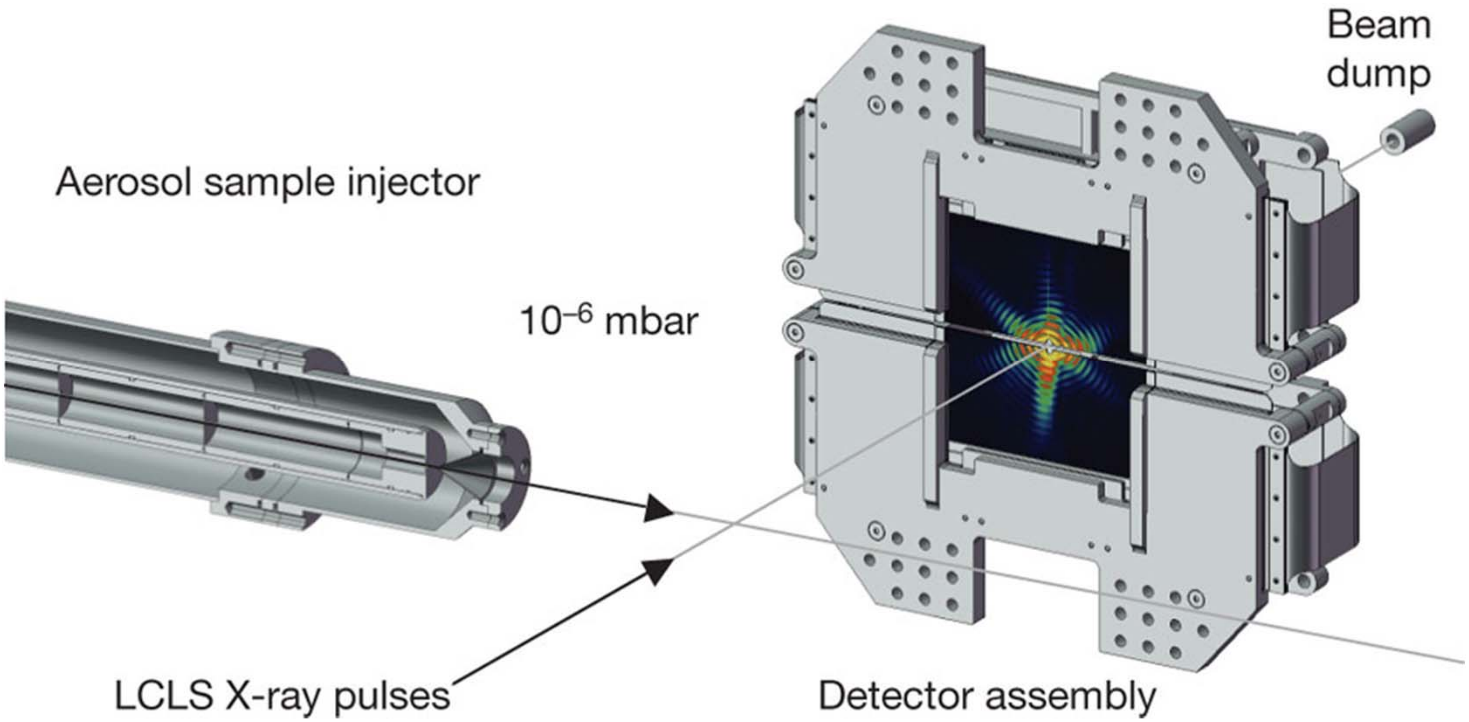


cw, 8.5 Å resolution, 100K electron density map

HN Chapman *et al.* *Nature* 470, 73-77 (2011) doi:10.1038/nature09750

nature

Single LCLS X-ray Pulse, Single Particle Imaging-Obtaining structure without crystals: Mimivirus



MM Seibert *et al. Nature* 470, 78-81 (2011) doi:10.1038/nature09748

nature

LETTER

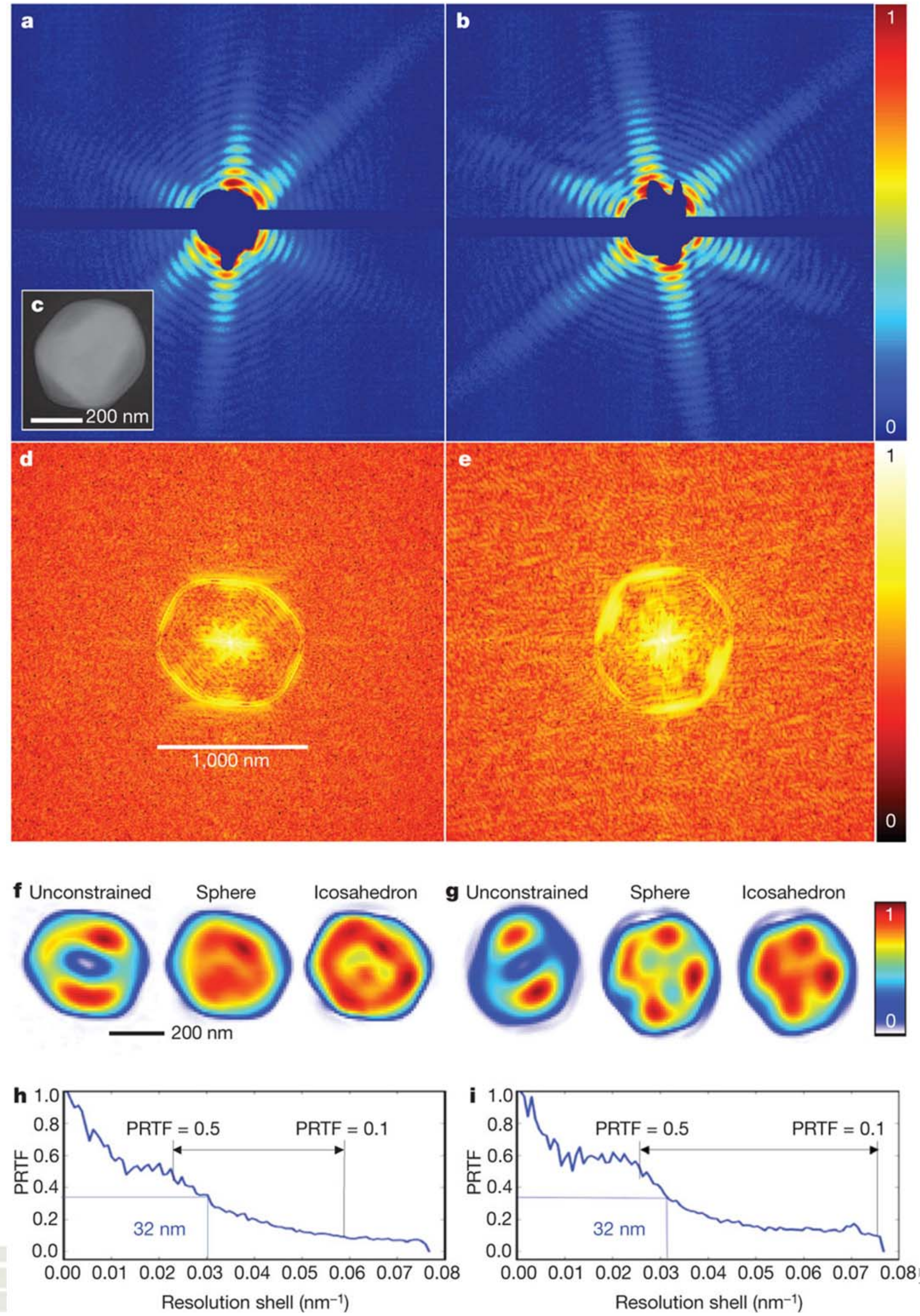
nature 470, 78-81 (2011)

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

M. Marvin Seibert[1*], Tomas Ekeberg[1*], Filipe R. N. C. Maia[1*], Martin Svenda1, Jakob Andreasson[1], Olof Jo¨nsson[1], Dus˘ko Odic´[1], Bianca Iwan[1], Andrea Rocker[1], Daniel Westphal[1], Max Hantke[1], Daniel P. DePonte[2], Anton Barty[2], Joachim Schulz[2], Lars Gumprecht[2], Nicola Coppola[2], Andrew Aquila[2], Mengning Liang[2], Thomas A. White[2], Andrew Martin[2], Carl Caleman[1,2], Stephan Stern[2,3], Chantal Abergel[4], Virginie Seltzer[4], Jean-Michel Claverie[4], Christoph Bostedt[5], John D. Bozek[5], Se´bastien Boutet[5], A. Alan Miahnahri[5], Marc Messerschmidt[5], Jacek Krzywinski[5], Garth Williams[5], Keith O. Hodgson[6], Michael J. Bogan[6], Christina Y. Hampton[6], Raymond G. Sierra[6], Dmitri Starodub[6], Inger Andersson[7], Sas˘a Bajt[8], Miriam Barthelmess[8], John C. H. Spence[9], Petra Fromme[10], Uwe Weierstall[9], Richard Kirian[9], Mark Hunter[10], R. Bruce Doak[9], Stefano Marchesini[11], Stefan P. Hau-Riege[12], Matthias Frank[12], Robert L. Shoeman[13], Lukas Lomb[13], Sascha W. Epp[14,15], Robert Hartmann[16], Daniel Rolles[13,14], Artem Rudenko[14,15], Carlo Schmidt[14,15], Lutz Foucar[13,14], Nils Kimmel[17,18], Peter Holl[16], Benedikt Rudek[14,15], Benjamin Erk[14,15], Andre´ Ho¨mke[14,15], Christian Reich[16], Daniel Pietschner[17,18], Georg Weidenspointner[17,18], Lothar Stru¨der[14,17,18,19], Gu¨nter Hauser[17,18], Hubert Gorke[20], Joachim Ullrich[14,15], Ilme Schlichting[13,14], Sven Herrmann[17,18], Gerhard Schaller[17,18], Florian Schopper[17,18], Heike Soltau[16], Kai-Uwe Ku¨hnel[15], Robert Andritschke[17,18], Claus-Dieter Schro¨ter[15], Faton Krasniqi[13,14], Mario Bott[13], Sebastian Schorb[21], Daniela Rupp[21], Marcus Adolph[21], Tais Gorkhover[21], Helmut Hirsemann[8], Guillaume Potdevin[8], Heinz Graafsma[8], Bjo¨rn Nilsson[8], Henry N. Chapman[2,3] & Janos Hajdu[1]

Single-shot, coherent diffraction patterns on single virus particles

- 70 fs, 1.8 keV pulse
- 8 x 10^{11} photons per pulse
- Single particle, single x-ray pulse exposure s
- Structure reconstruction yielded 32-nm resolution
- No measurable damage
- Reconstruction indicates inhomogeneous arrangement of dense material inside the virion.

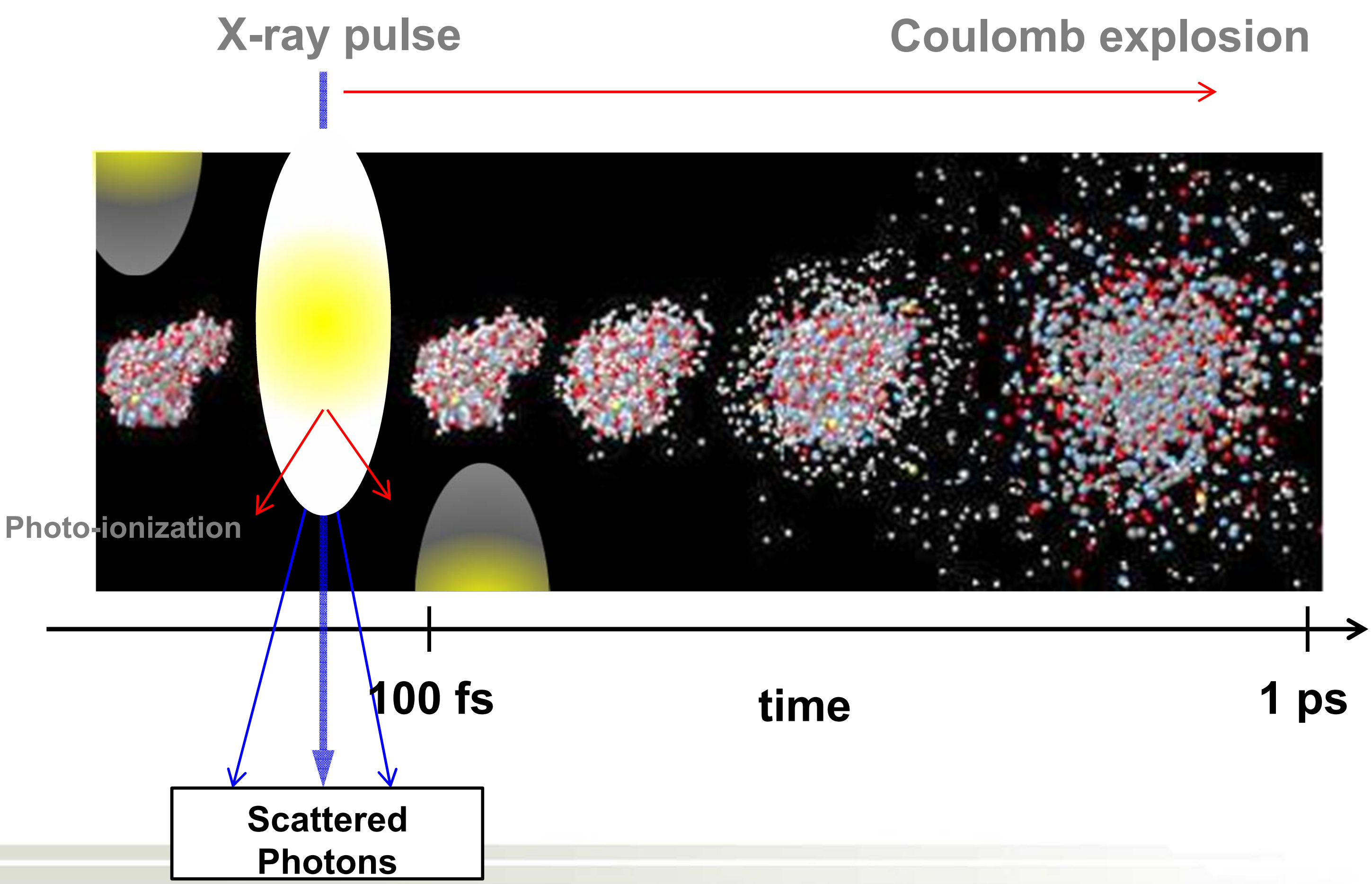


nature

MM Seibert *et al. Nature* 470, 78-81 (2011)

XFELs offer new type of X-ray measurement:

- Detection avoiding convolution with damage
- Extreme peak intensity, coherence, ultra-short pulses
- Single particle detection limit



Concluding Remarks

Combined Advances in:

- X-ray light sources
  - Pulsed, brilliant, coherent
- Detectors
  - Fast gating, direct X-ray detection, efficient, large area pixel arrays
- Pulsed excitation sources
  - High repetition rate, high intensity, compact

Create new, frontier opportunities to resolve ultrafast dynamics associated with critical physical, chemical, biological phenomena at the atomic level

- New frontier for X-ray science

Thanks,

Questions, comments?

Contacts 11-IDD:

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Klaus Attenkofer:	attenkofer@anl.gov
David Tiede:	tiede@anl.gov