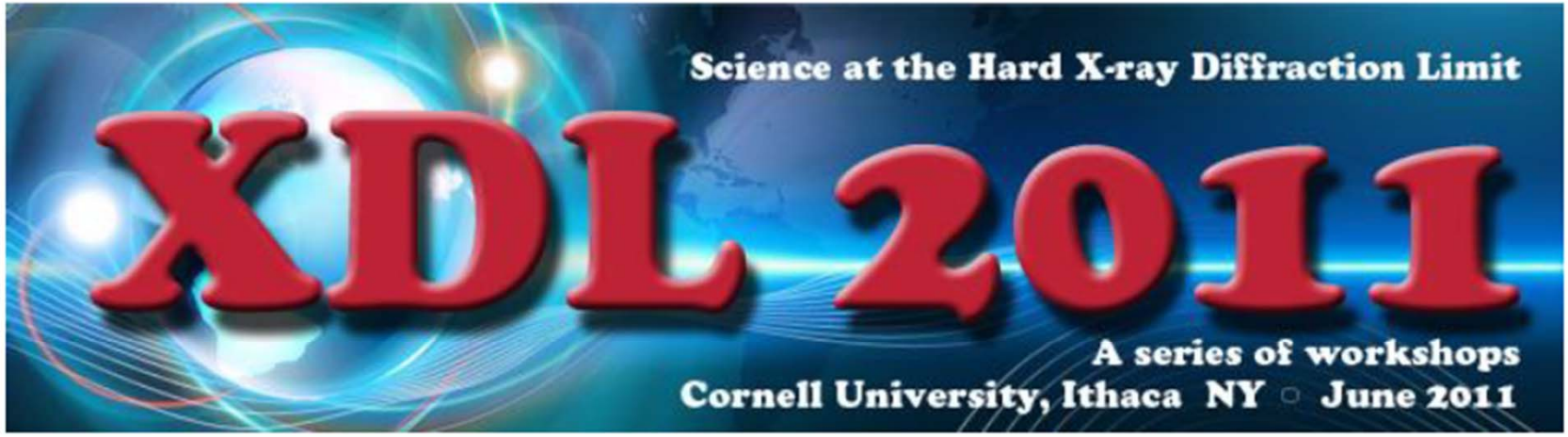
WS3 “Ultra-fast Science with Tickle and Probe” の報告

KEKPF　足立伸一



Ultra-fast Science with “Tickle and Probe”

June 20 & 21, 2011

Robert Purcell Conference Center, Cornell University, Ithaca NY

Shin-ichi Adachi, High Energy Accelerator Research Organization, KEK

"Toward Fourier-limited X-ray Science"

Don Bilderback, Cornell University

"Expected Performance of CW ERL & USR Ultra-fast Hard X-ray Sources"

Christian Bressler, European XFEL GmbH

"Time-resolved X-ray Spectroscopies and Scattering with One Trillion Photons"

Edward Castner, Rutgers University

"Rapid Chemical and Physical Processes in Solution"

Lin Chen, Northwestern University

"X-ray Transient Absorption Spectroscopy: A Decade and Beyond"

Chi-Chang Kao, SLAC National Accelerator Laboratory

"What is the "ideal" X-ray Source? "

Aaron Lindenberg, SLAC National Accelerator Laboratory

"High-repetition-rate Ultrafast X-ray Experiments with Accelerator-based Sources"

Anne Marie March, Advanced Photon Source

"X-ray Probes of Laser-controlled Molecules in Gases and Solutions"

David Reis, SLAC National Accelerator Laboratory

"Time-resolved Diffuse Scattering"

Robert Schoenlein, Lawrence Berkeley National Laboratory

"Ultrafast X-ray Studies of Complex Materials: Science Challenges and Opportunities"

Roseanne Sension, University of Michigan

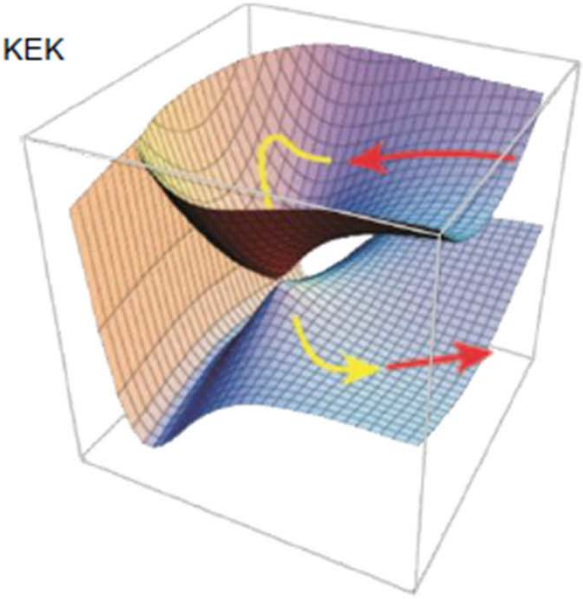
"Using Optical Knobs to Control Photoinitiated Reactions"

Simone Techert, Max Planck Institute, Goettingen

"Molecular Switches and Molecular Machines Investigated with Ultrafast Pulsed X-ray Radiation"

Carol Thompson, Northern Illinois University

"Ferroelectrics at the ERL"

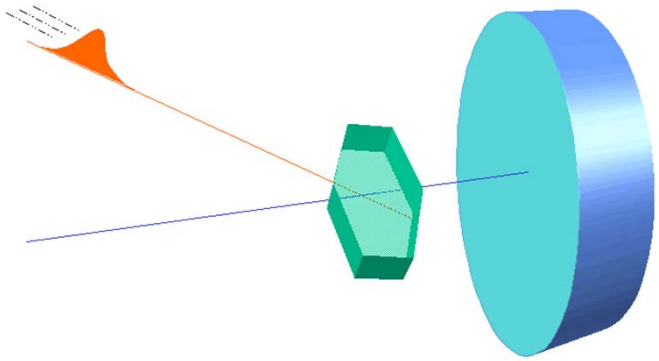


From the BESAC Grand Challenges report (12/20/2007)

CHESS SSRL DESY

High Energy Accelerator Research Organization (KEK)
Institute of Materials Structure Science (IMSS)
PF Photon Factory

Pump and Probe と Tickle and Probe



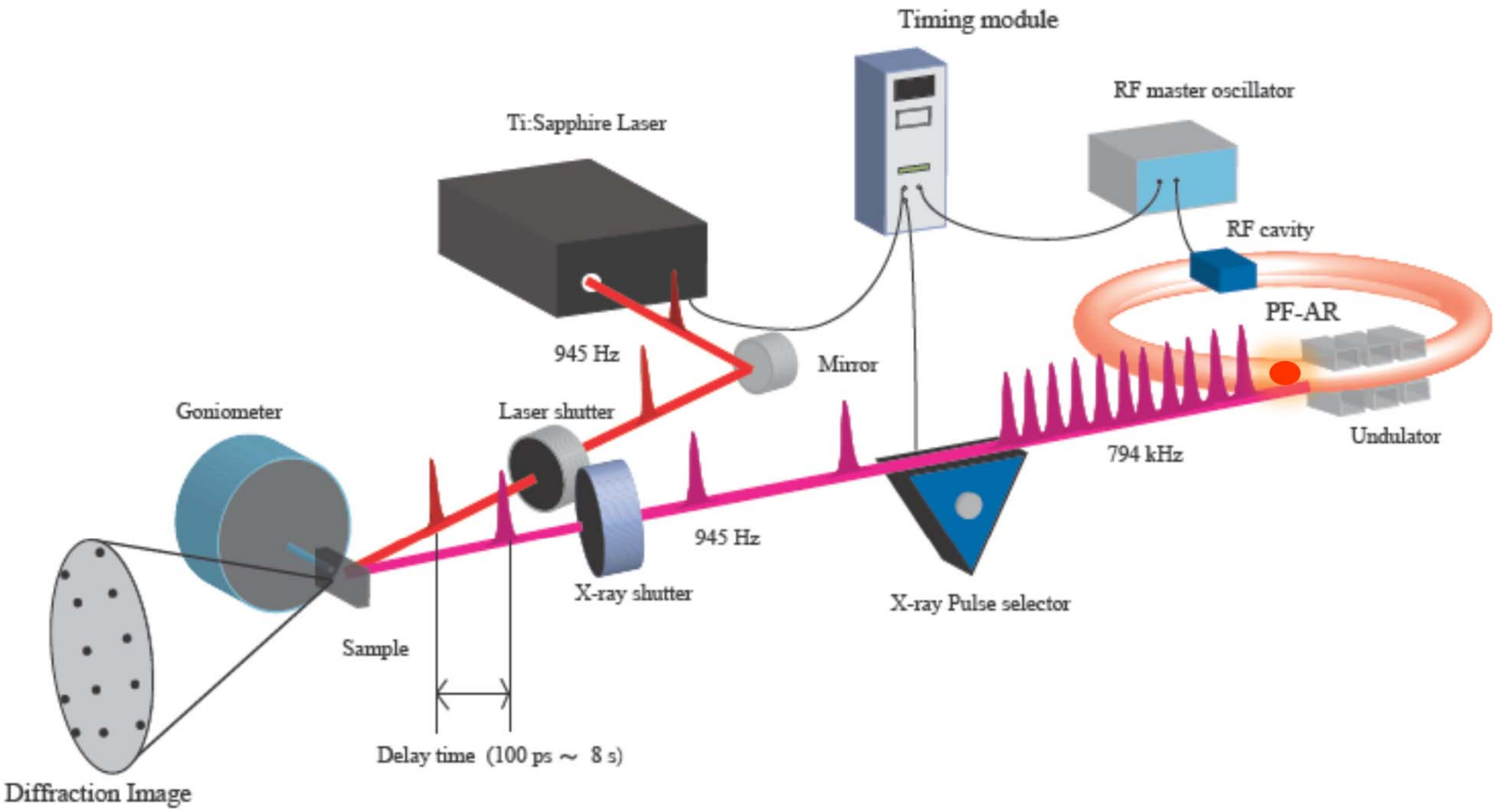
Center for Molecular Movies
http://cmm.risoe.dk/

放射光X線を用いたポンプ・プローブ実験のイメージ

放射光のパルス性

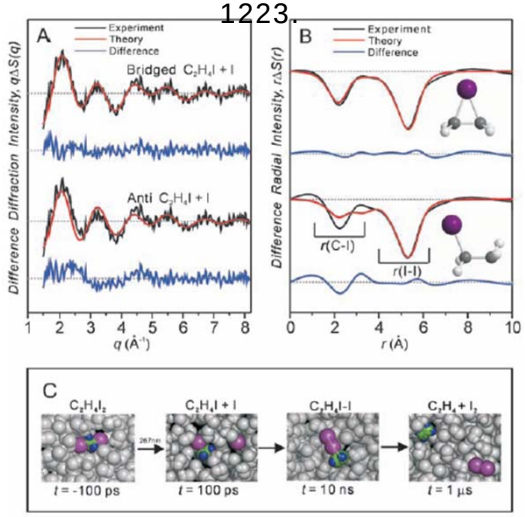
Institute for Storage Ring Facilities http://www.isa.au.dk/
Electron Injection, Storage and Synchrotron Radiation Light Generation in the Storage Ring ASTRID. *(Credit: Coldvision Studio/ISA)*

典型的な実験配置
(NW14A, PF-AR, KEK)

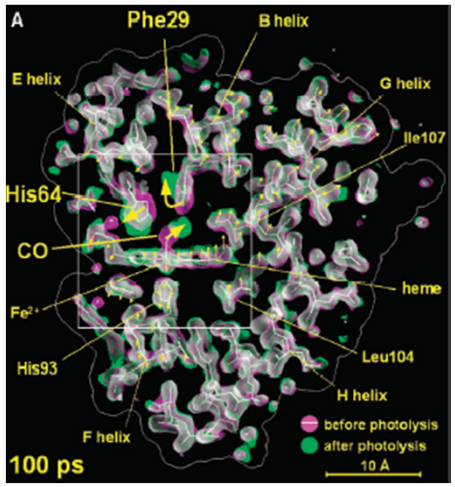


Pump and Probeの実験例

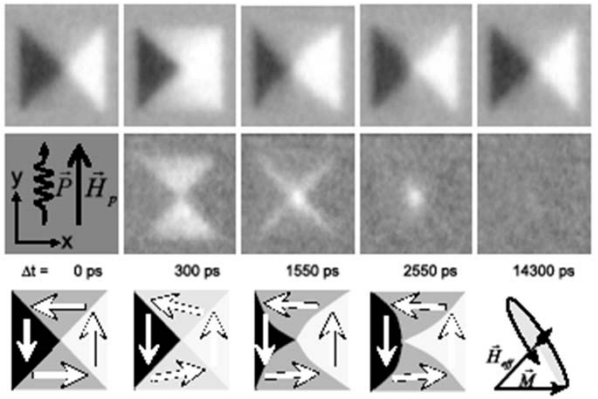
Photochemistry of $C_2H_4I_2$ in methanol (ESRF)
Ihee, et al., (2005) Science 309, 1223.

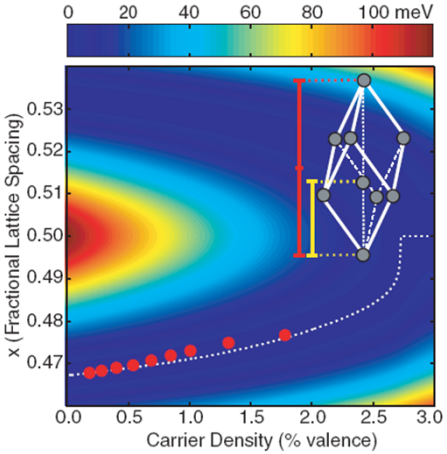


Ligand migration dynamics in myoglobin (ESRF)
Schotte et al.(2003) Science 300, 1944.

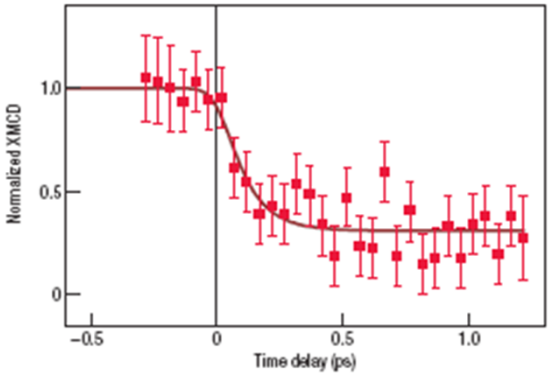


Magnetic excitations in permalloy squares (SLS)
Raabe et al. (2005) Phys. Rev. Lett. 94,217204.

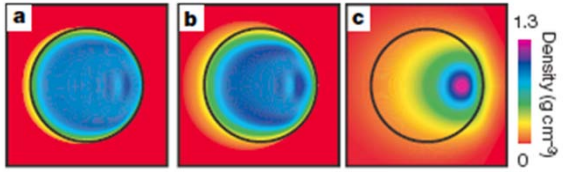




Bond softening in Bismuth (SPPS)
Fritz et al. (2007) Science 315, 633.



Femtosecond magnetization in nickel (BESSY)
Stamm et al. (2007) Nature Mat. 6, 740.



Femtosecond holography of explosion of polystyrene spheres (FLASH at DESY)
Chapman et al. (2007) Nature 448, 676.

光源の種類と典型的な繰り返し周波数

光源	繰り返し周波数	1パルスあたりのフォトン数	単位時間当たりのフォトン数	パルス幅
蓄積リング	1MHz-500MHz	10^{6}-10^{9}	10^{12}-10^{15}	~100ps
SASE-XFEL	60-120Hz	~10^{12}	~10^{14}	10-100fs
ERL	1.3GHz	10^{3}-10^{6}	10^{12}-10^{15}	100fs-1ps

What is the 'Ideal' X-ray Source?

Chi-Chang Kao
SLAC National Accelerator Laboratory

The recent successful commissioning of the Linac Coherent Light Source (LCLS) at SLAC has clearly demonstrated the importance of accelerator physics R&D, and stimulated several new free electron laser (FEL) projects worldwide, including a **high repetition rate FEL proposed by LBNL** in the US. In parallel, there also has been significant progress made **in energy recovery linac R&D, and the design of ultimate storage rings**. More importantly, there is a continued growth of photon science in new research directions that demands better sources. So, it is timely to examine **the "ideal" x-ray source** for the main categories of experimental techniques in spectroscopy, scattering and imaging based on these progresses, and provide **critical input** to accelerator physics R&D for future sources.

Chi-Chang Kao

- 将来的にALS（Berkeley）とSSRL（Stanford）を、NGLS（高繰り返しXFEL）とPEP-X（ERLまたはUSR）に置き換えてゆく可能性がある
- 日米欧の放射光施設が協力して、最先端の情報を共有し、各政府に効果的に働きかける仕組みが必要
- SASE-XFELの「1分子イメージング」のような一般に分かりやすいスローガンが必要

High-repetition-rate Ultrafast X-ray Experiments with Accelerator-based Sources

Aaron Lindenberg
SLAC National Accelerator Laboratory

High repetition-rate ultrafast x-ray studies at low peak intensities provide new opportunities for investigating dynamical processes in space and time, complementary to existing free electron laser-based sources. I will discuss recent efforts and results in this **direction at SSRL with few picosecond x-ray pulses at MHz repetition rates** as they relate to the development of ERL and USR sources. Associated scientific opportunities in materials science, and experimental challenges, including sample refreshing, laser technology, and the development of **novel pump sources at THz frequencies** will also be discussed.

Aaron Lindenberg

- 高繰り返し光源
  - SSRL low-αモード、5μA/bunch、1ps RMS
- 低繰り返し光源
  - LCLS、テラヘルツ光の利用
- 強誘電体（$BaTiO_3$）の光誘起構造転移
- Superionic materialの温度誘起構造転移

Time-resolved X-ray Spectroscopies and Scattering with One Trillion Photons

Christian Bressler
European XFEL GmbH

Structural Dynamics with hard x-radiation offers to add new observables for elucidating the detailed steps of chemical reactivity. X-ray absorption fine structure **(XAFS)** spectroscpoy reveals details about the local geometric and electronic structure around selected atoms, where the x-ray absorption near-edge spectroscopy **(XANES)** delivers additional information about unoccipied orbitals (LUMO's). X-ray emission spectroscopy **(XES, RIXS)** reveals details about occupied electronic states including spin-sensitive information, while **x-ray diffuse scattering** of photoexcited molecules in solution can deliver details about the guest-host interactions and the thermal response around the solute. We have recently combined these complementary tools into one single experiment in a time-resolved pump-probe configuration to understand the combined electronic, nuclear and spin degrees of freedom during dynamic processes in molecular systems. **Picosecond studies at 3rd generation synchrotrons at MHz repetition rates** permitted to exploit the full flux available at synchrotrons for time-resolved studies, while **initial femtosecond XANES studies at the LCLS** revealed dynamic processes during the initial steps of photochemical reactivity. Both groups of studies rely on the use of **one trillion (10^{12}) photons** per data point, which is 4-6 oders of magnitude larger than conventional studies with 1 kHz laser systems (100 ps), or femtosecond sliced SR. This talk will present current and future prospects with new femtosecond x-radiation sources.

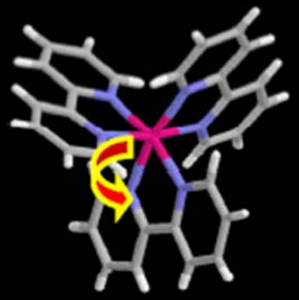
Christian Bressler

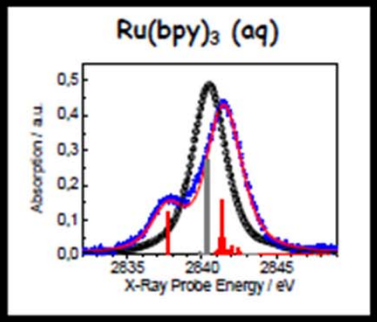
- 第3世代放射光を用いた、金属錯体溶液反応のMHzオーダーX線分光測定
  - 蛍光XAFSだけでなく、発光分光、RIXS測定まで可能
- LCLSを用いた、フェムト秒XAFS
  - 光励起初期過程の観測


Time-Resolved X-Ray
Spectroscopies and Scattering
with
One Trillion Photons
Christian Bressler
European
XFEL
XDL Workshop "tickle and probe", Cornell University, June 21, 2011

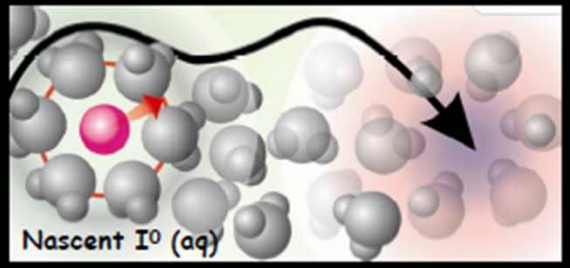
Dynamic Studies in Photochemistry

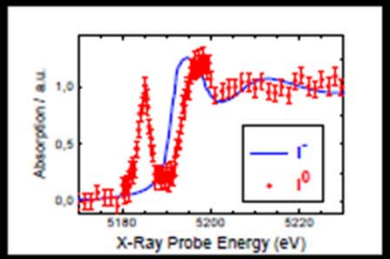
1. Intramolecular Charge Transfer



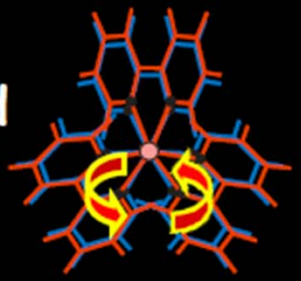


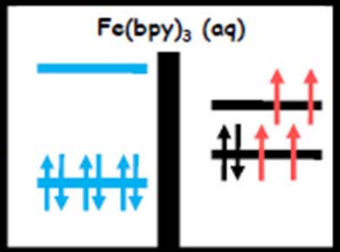
2. Towards Solvation Dynamics

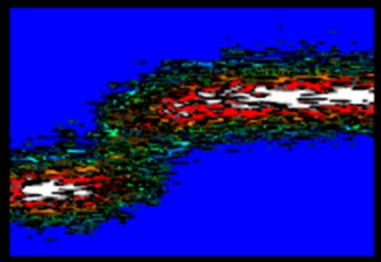




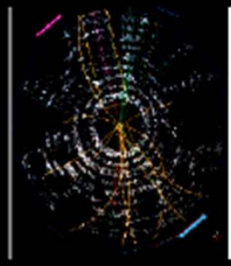
3. Light-Induced Spin Crossover

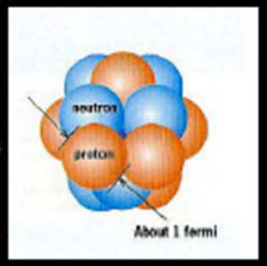






What are the fundamental timescales?



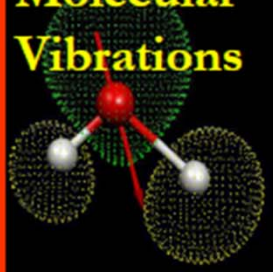


Strings,
Cosmology

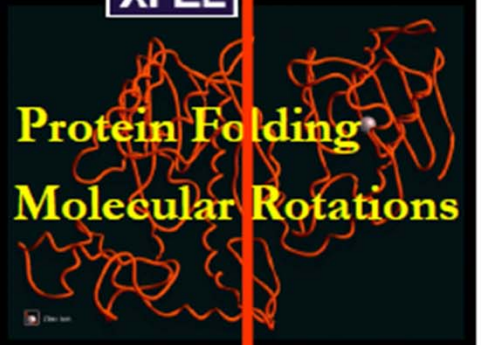
Particle
Collisions

Chemistry and Biochemistry

Photosynthesis
Vision
Molecular
Vibrations



European
XFEL

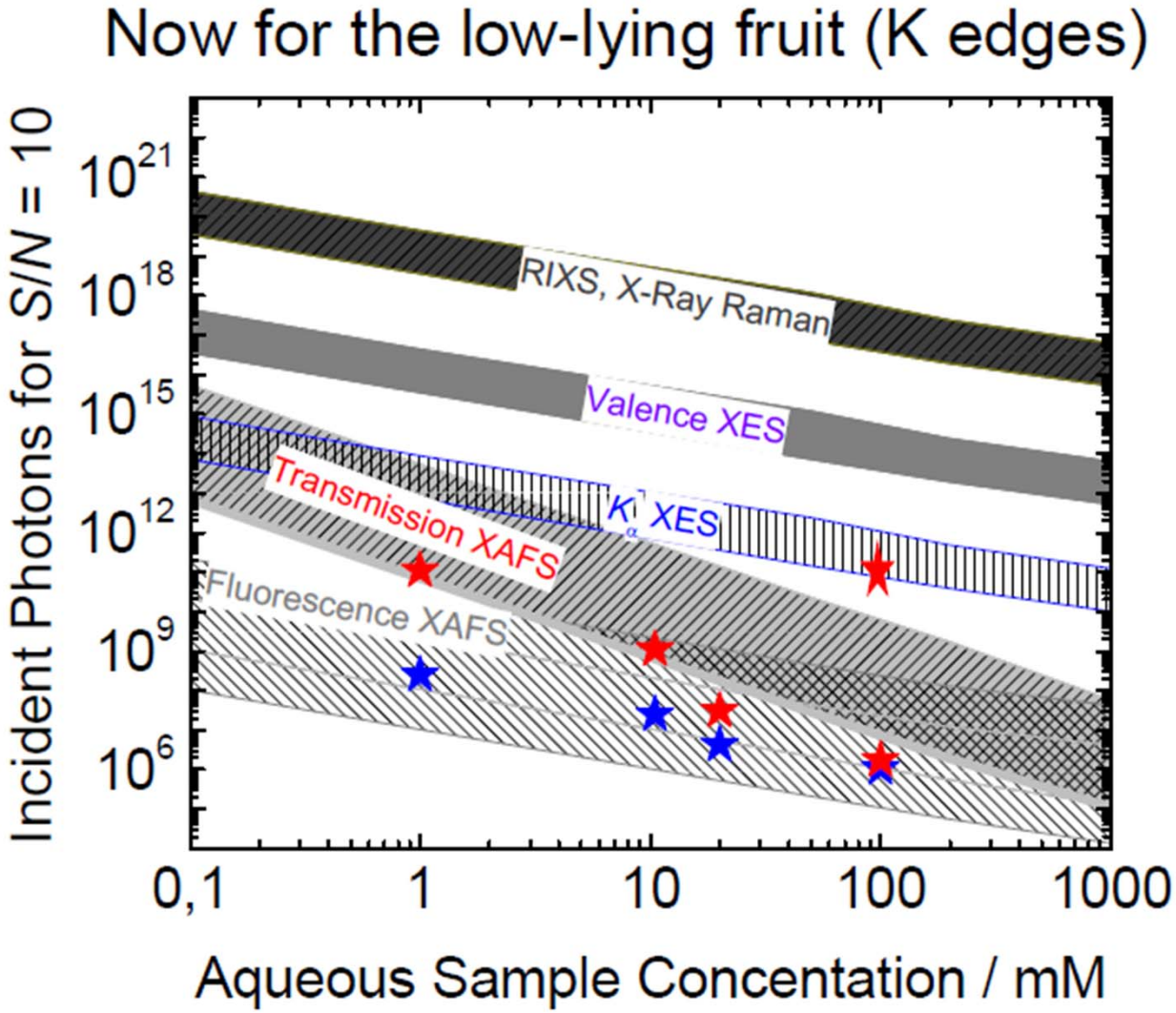


Protein Folding
Molecular Rotations

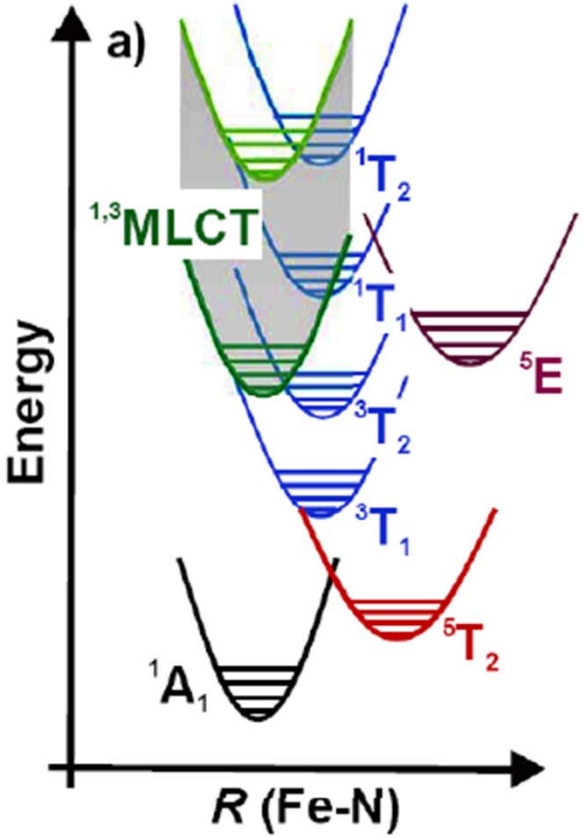
Electron dynamics

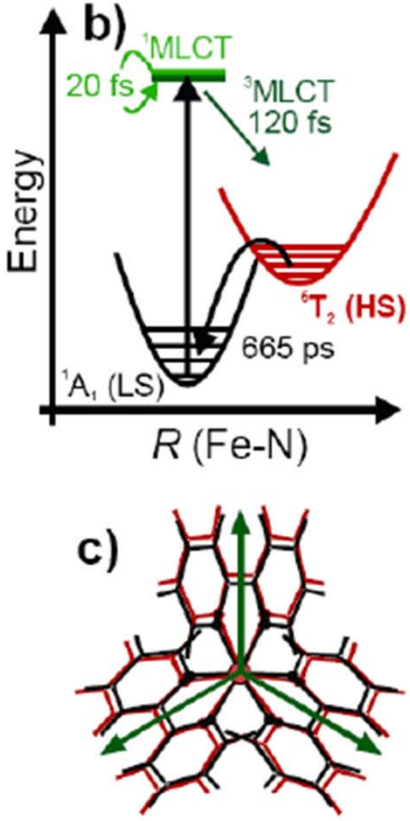
harpo 10^{-27} yacto 10^{-24} zepto 10^{-21} atto 10^{-18} femto 10^{-15} pico 10^{-12} nano 10^{-9} micro 10^{-6} milli 10^{-3}

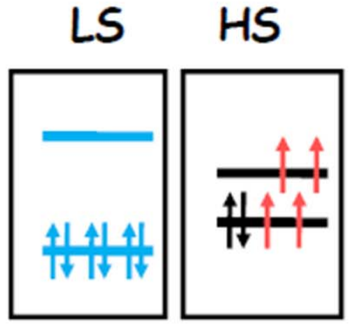
Time /seconds

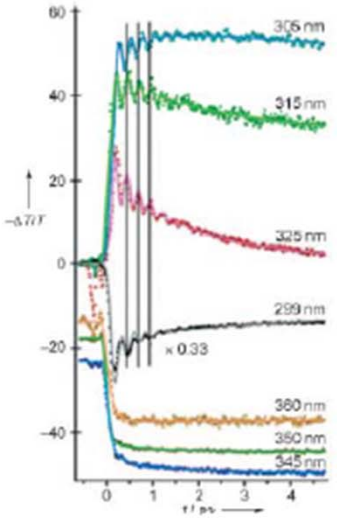

Now for the low-lying fruit (K edges)
Incident Photons for S/N = 10
10^21
10^18
10^15
10^12
10^9
10^6
RIXS, X-Ray Raman
Valence XES
Kα XES
Transmission XAFS
Fluorescence XAFS
0,1
1
10
100
1000
Aqueous Sample Concentation / mM

Now to something completely different….



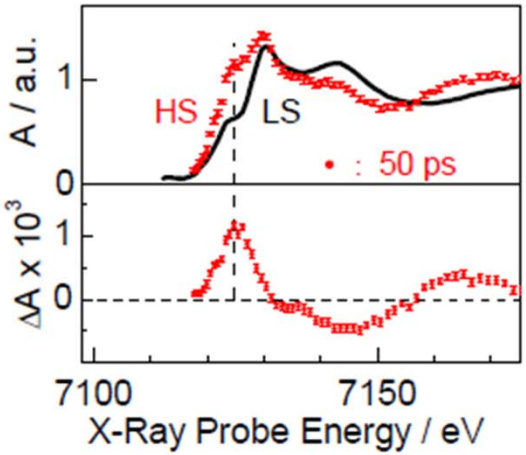


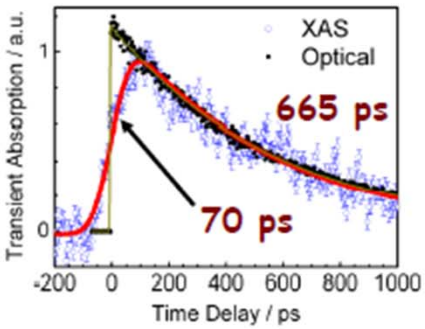




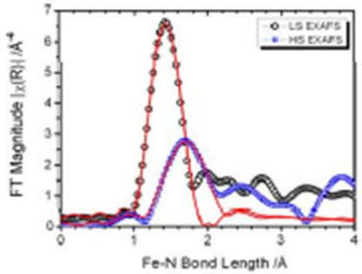
C. Consani *et al.*
Angew Chem (2009)

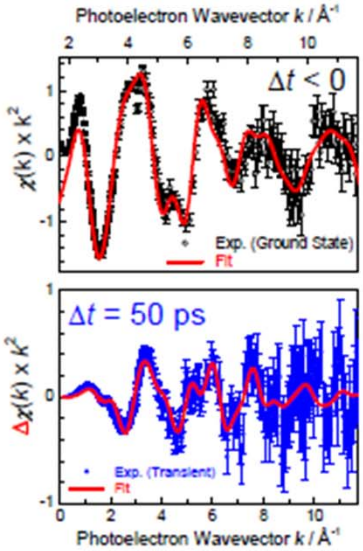
Towards Transient Structures via TR-XAFS

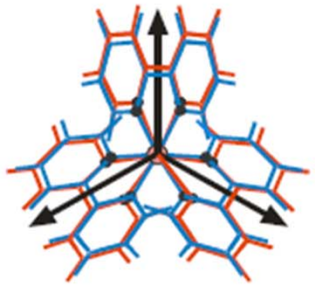




W. Gawelda *et al.*
Phys. Rev. Lett. (2007)

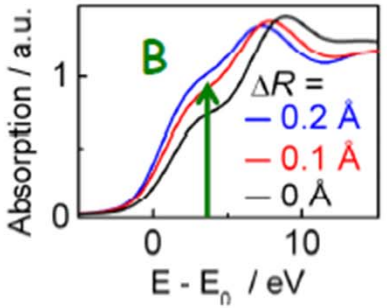






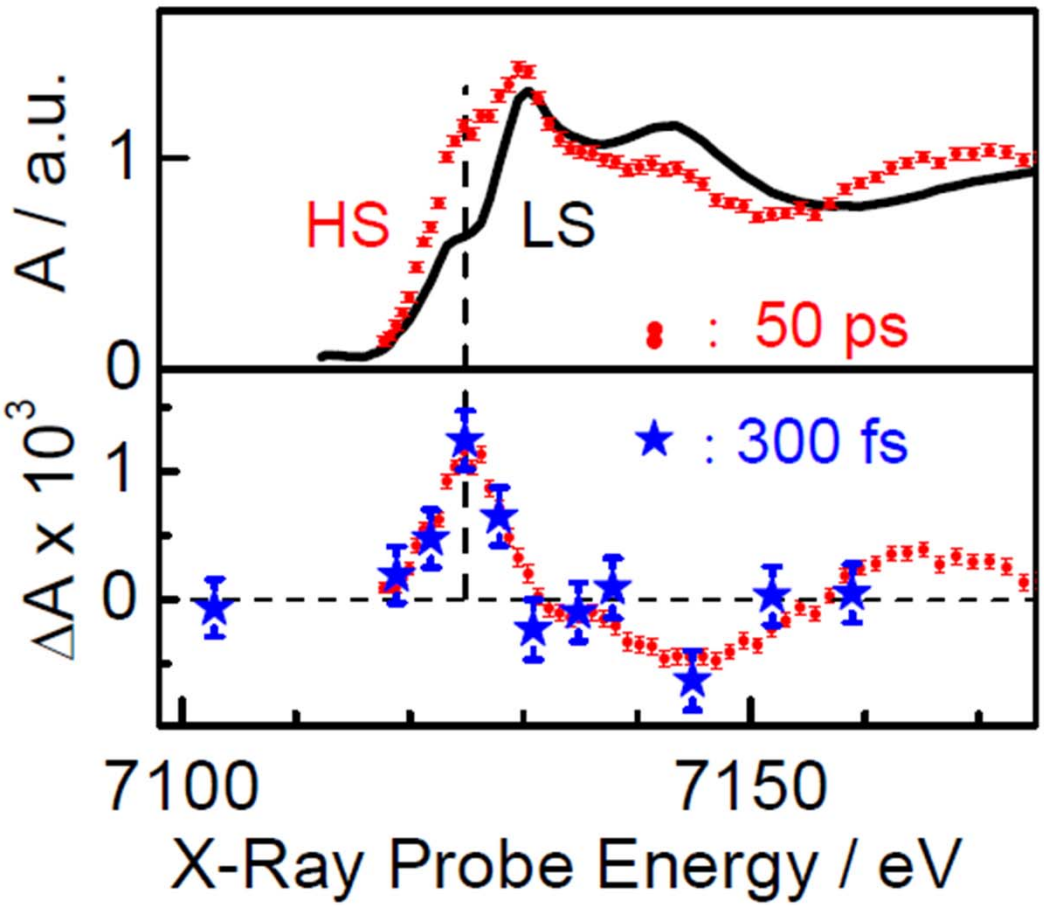
$\Delta R_{Fe\text{-}N}$= 0.2 ±0.008 Å

M. Benfatto (INFN Rome)



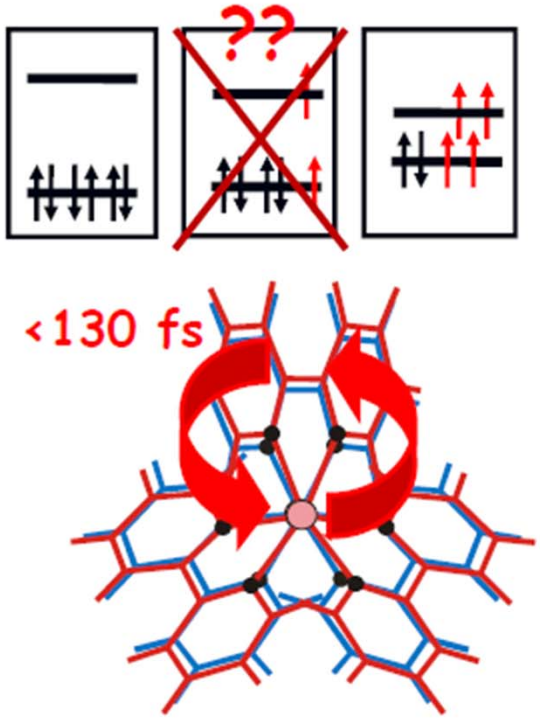
W. Gawelda *et al.*
J. Chem. Phys. (2009)

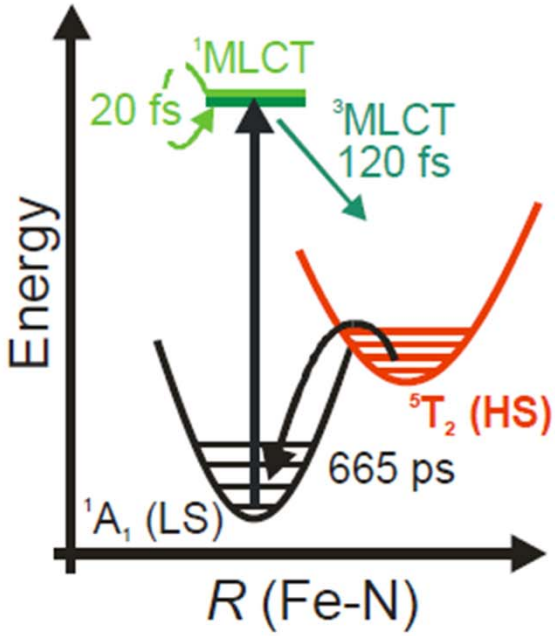
ps and fs XANES (Synchrotron)



C. Bressler *et al.*, Science (2009)

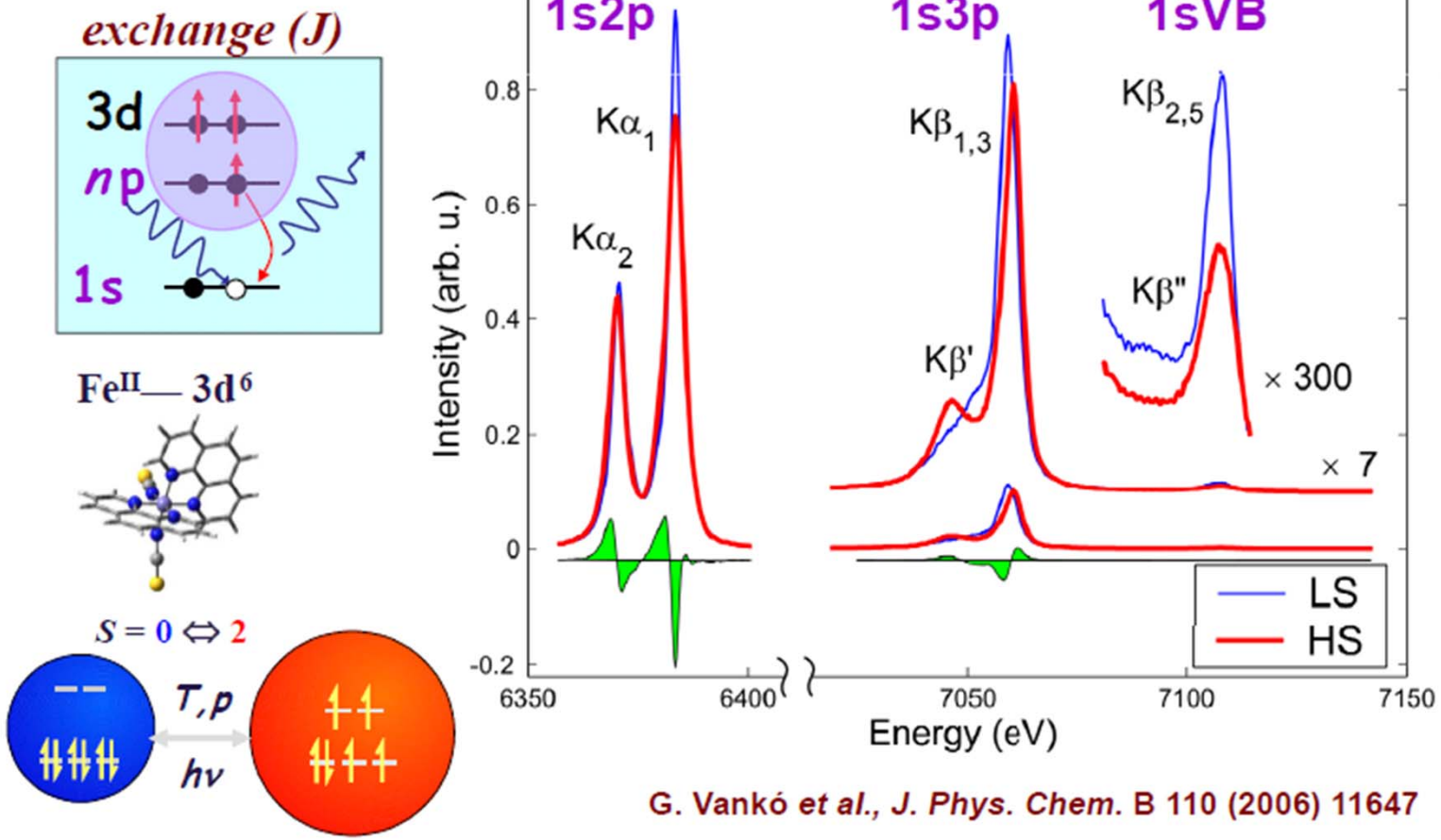
Combined optical and x-ray results





→ Need now a *Spin*-Sensitive Tool !!

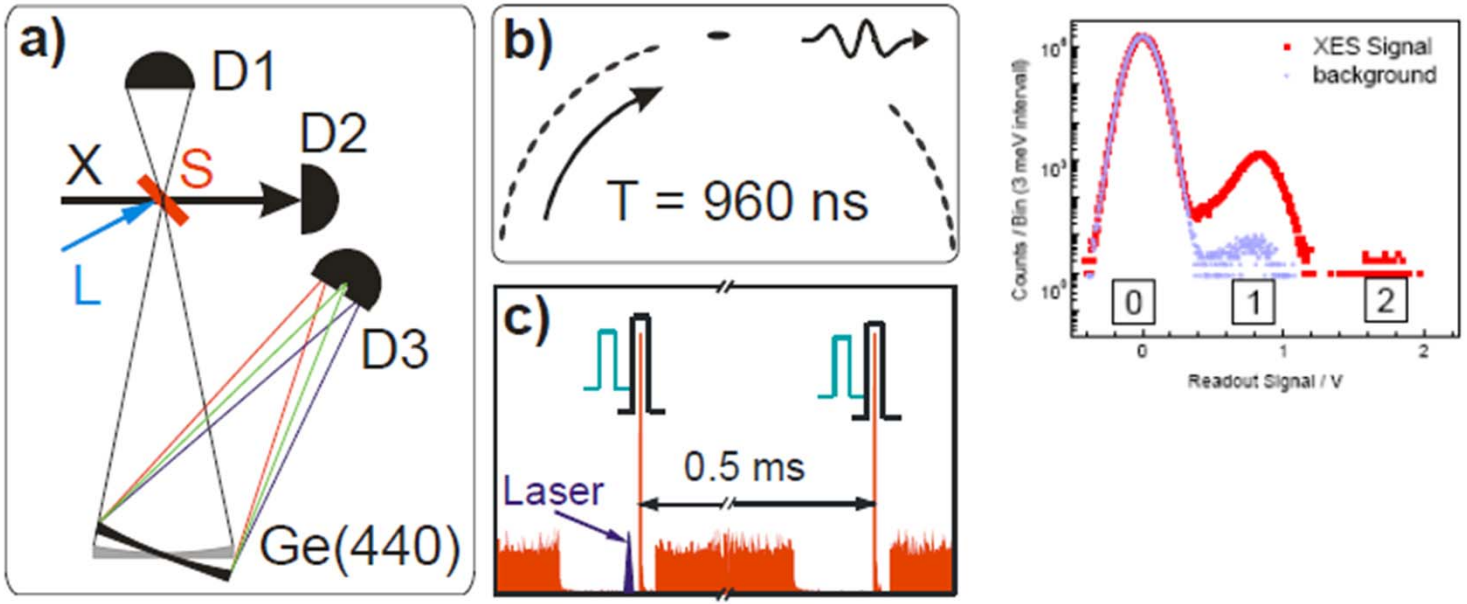
1s XES of a spin transition molecule



G. Vankó *et al.*, *J. Phys. Chem.* B 110 (2006) 11647

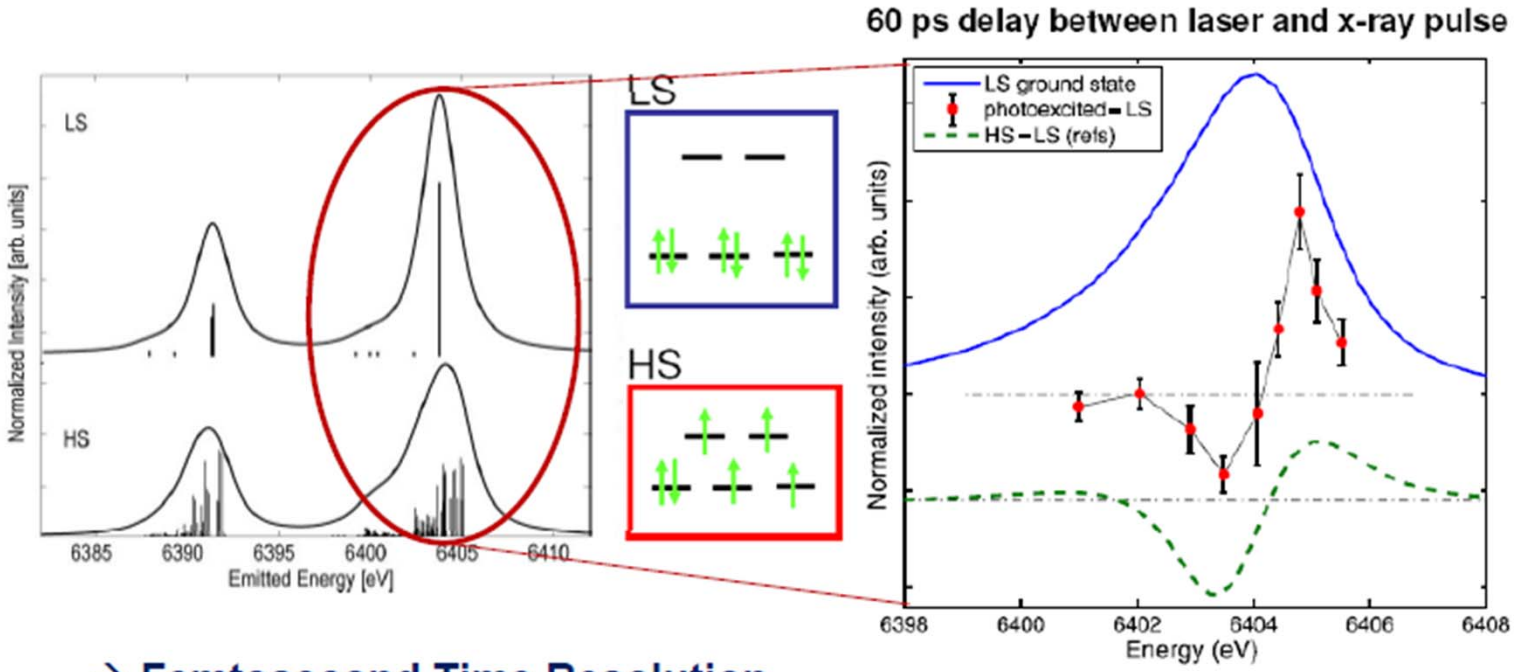
Towards ultrafast X-ray ***Emission*** Spectroscopy

10^3 – 10^6 ph/pulse (100 ps)
10-12 ph/pulse (200 fs)
10^{-3} ph/pulse (100 ps XES)



G. Vankó et al., *Angew. Chem. Int. Ed. (2010)*

Direct spin probing: first TR-XES (ps)



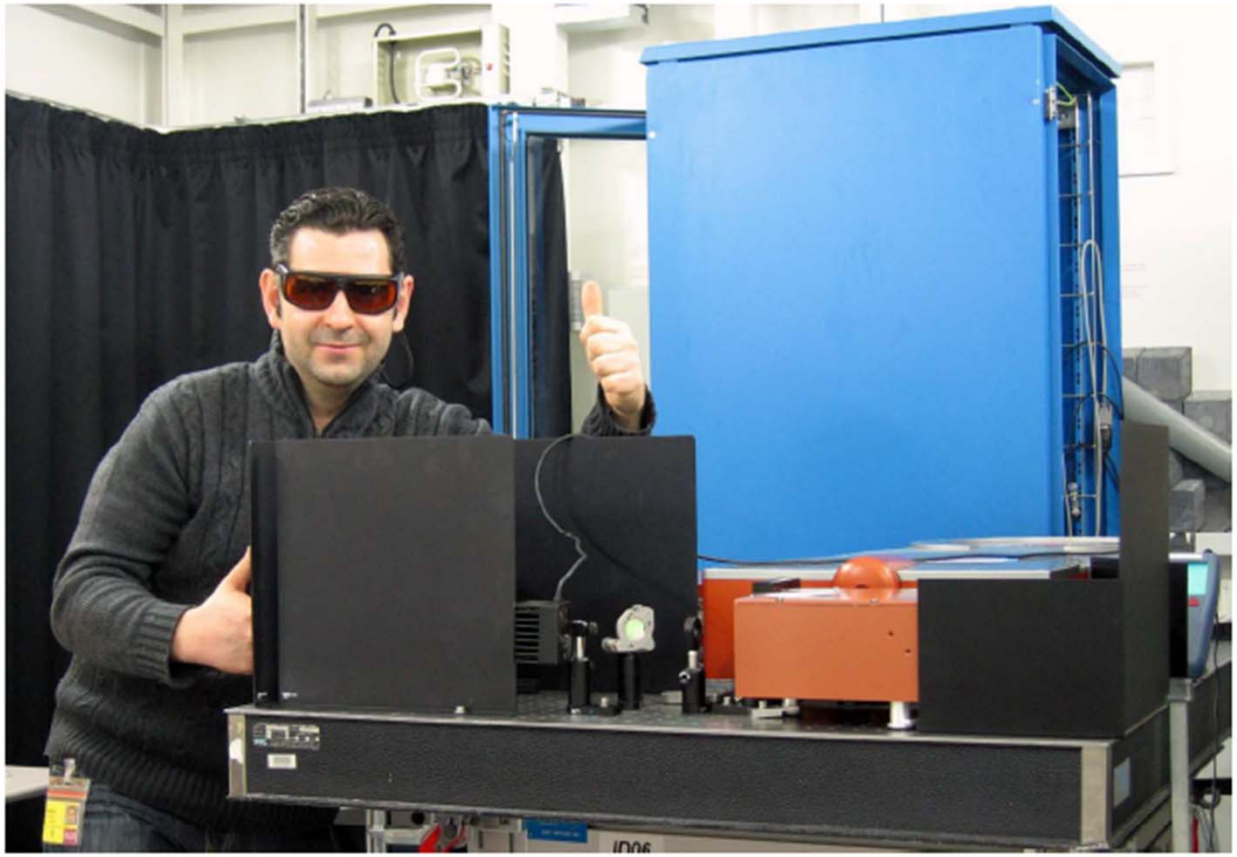
→ **Femtosecond Time Resolution**
→ **Ideally suited for single wavelength XFEL experiments**
→ **MHz repetition rates !!!!**

Direct measurement of change of Fe spin state.

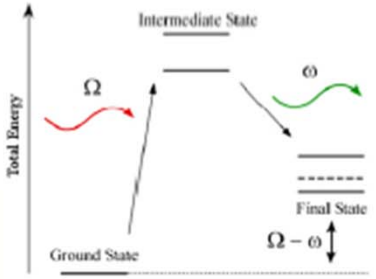
G. Vanko et al., Angew. Chem. Int. Ed., (2010)

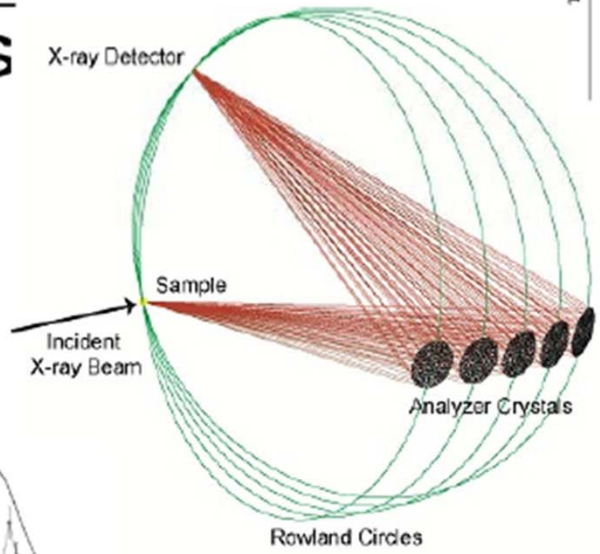
European XFEL

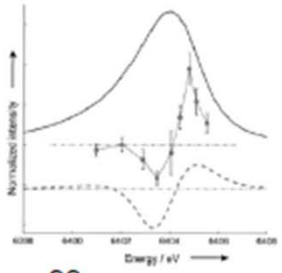
Ready to Pump-Probe at MHz rep-rates!!

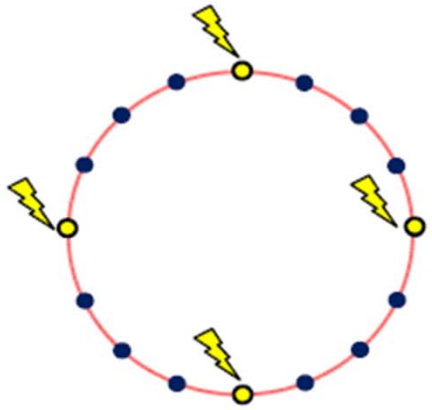


ID26 – X-ray Emission/Absorption Spectroscopy



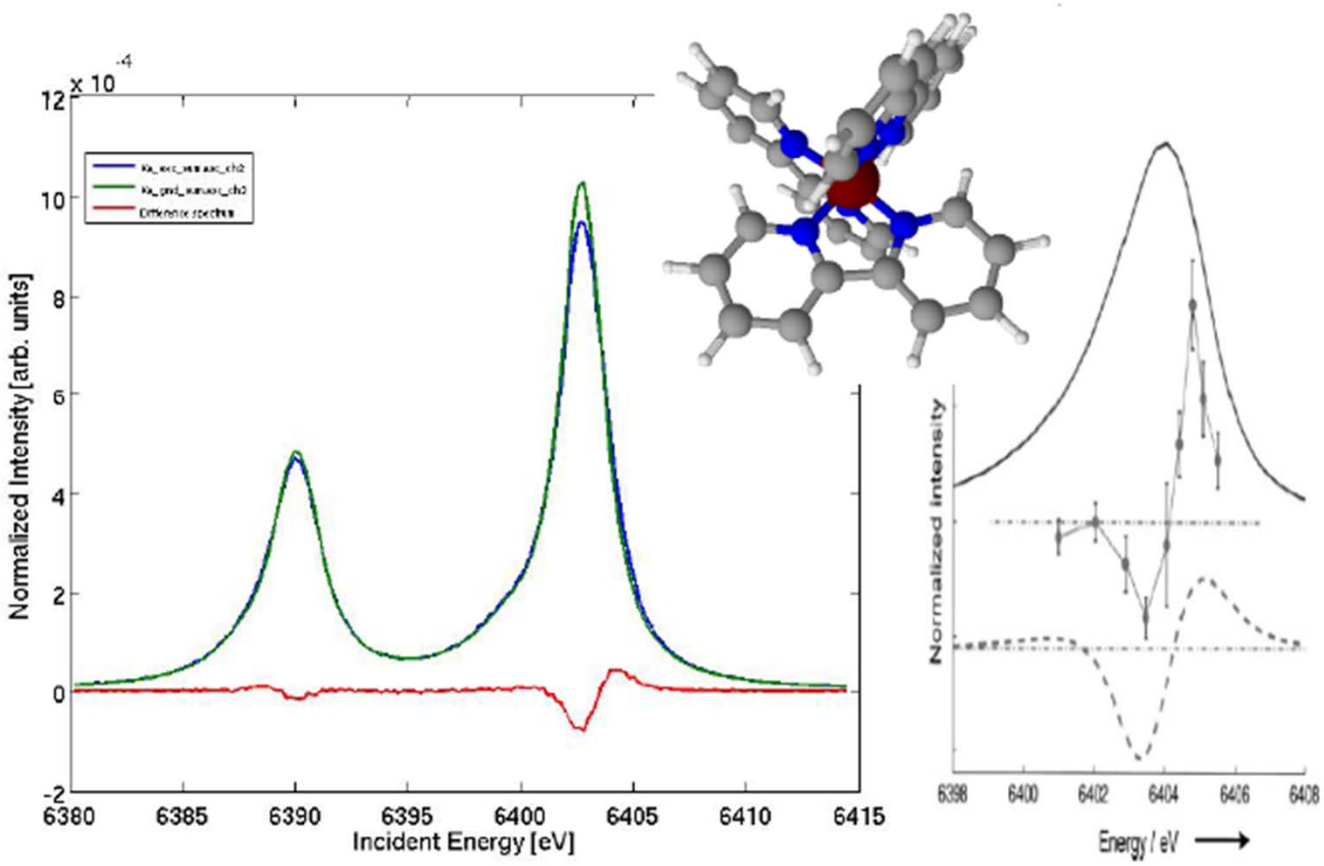






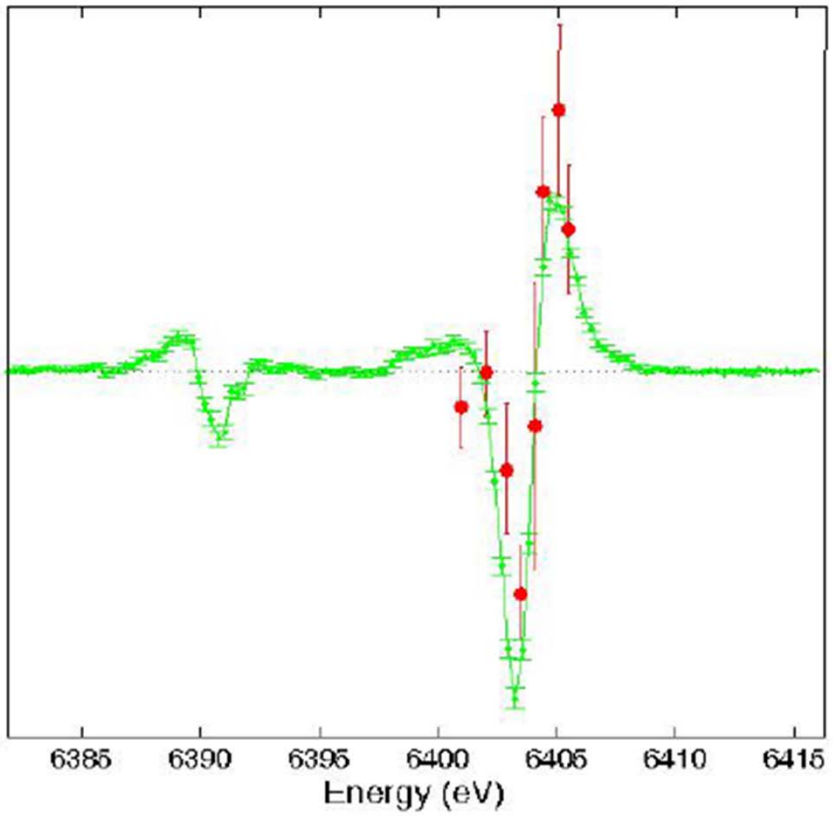
1.4 MHz

ID26/ESRF (March 2011)



APS, sector 7 (March 2011)

Picosecond K alpha XES at APS

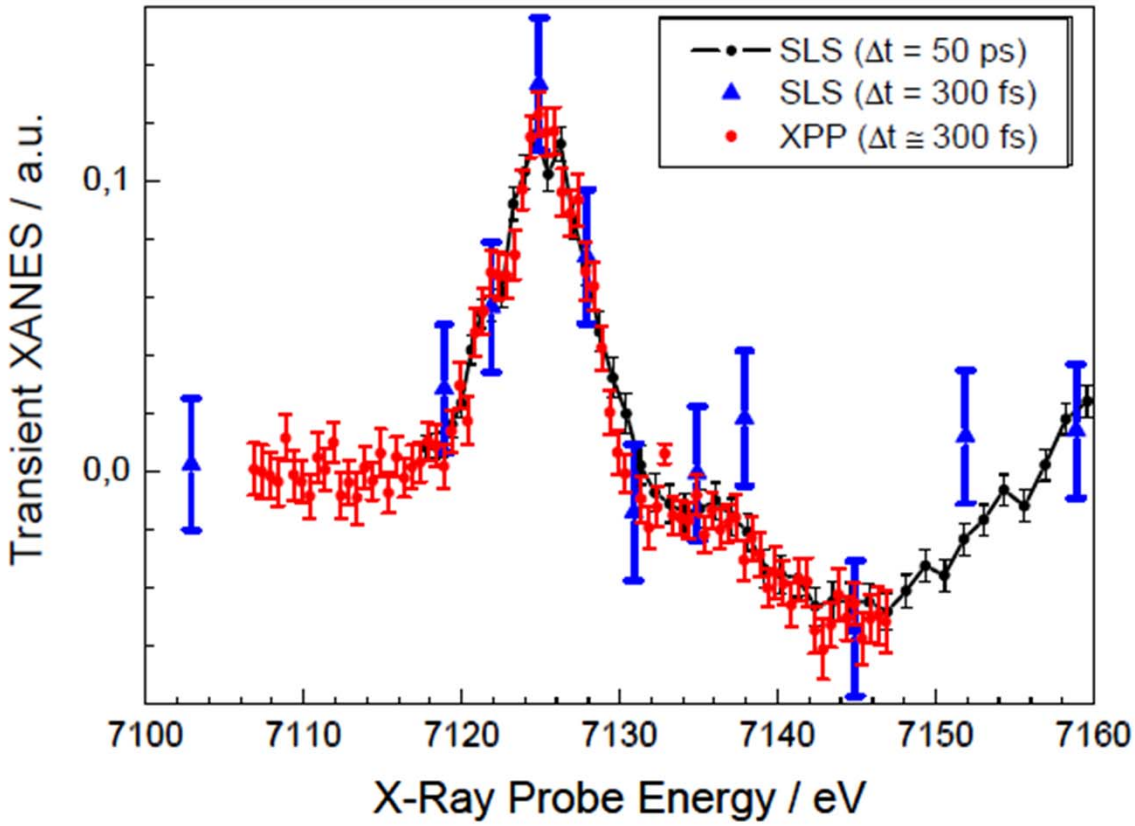


1 kHz pp studies at SLS

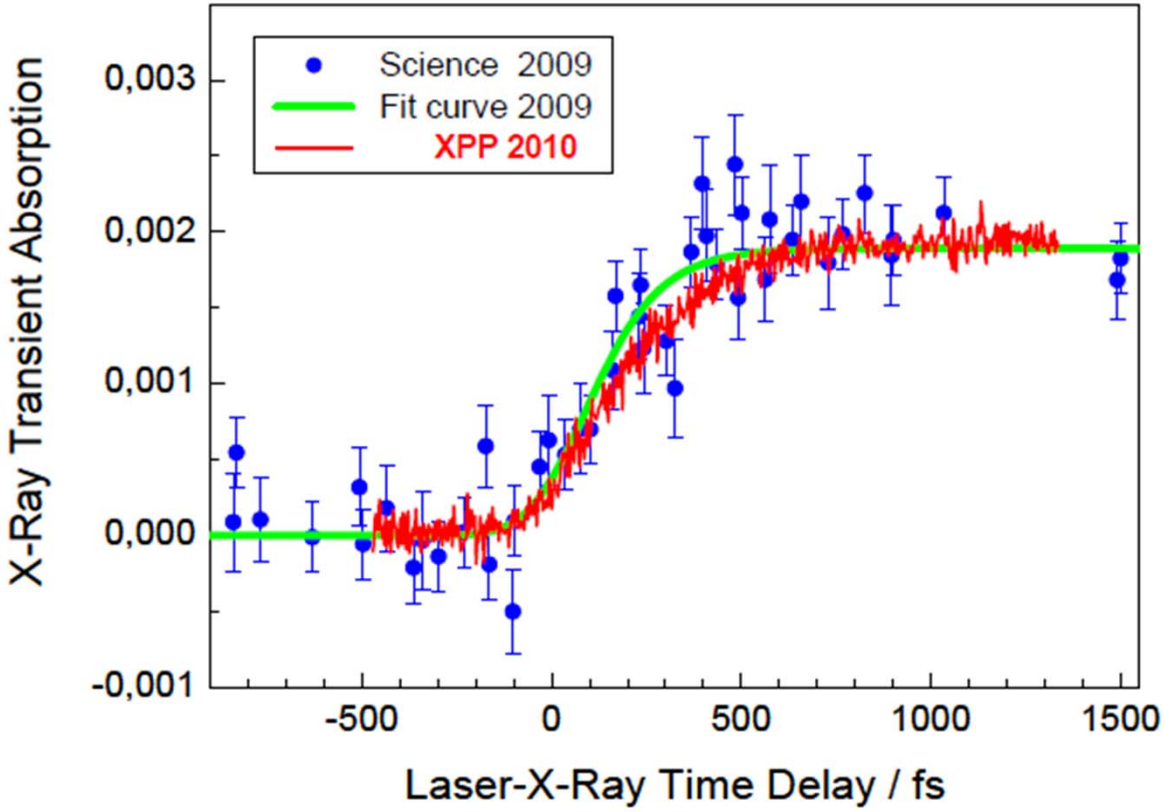
(Angew. Chem. 2010)

0.13 MHz at APS

Oct 2010: XPP commissioning



Real-Time Traces



High Energy Accelerator Research Organization (KEK)
Institute of Materials Structure Science (IMSS)
Photon Factory

XDL2011
RPCC, Cornell Univ.
June 20-21, 2011

Toward Fourier-limited X-ray Science

Photon Factory, KEK
& PREST, JST

Shin-ichi Adachi

outline

- Time-domain X-ray science
  - with Storage Ring (Photon Factory Advanced ring, KEK)
- Current status of Energy Recovery Linac (ERL) project at KEK
  - 35-245MeV ERL test facility (under construction)
  - 3.5GeV ERL + XFEL Oscillator (not approved)
- Towards Fourier-limited X-ray Science with XFEL-O and seeded XFEL
  - Inelastic X-ray scattering
  - Nonlinear X-ray Optics
  - Two-photon correlation spectroscopy
  - Transient grating
- Summary

outline

- Time-domain X-ray science
  - with Storage Ring (Photon Factory Advanced ring, KEK)
- Current status of Energy Recovery Linac (ERL) project at KEK
  - 35-245MeV ERL test facility (under construction)
  - 3.5GeV ERL + XFEL Oscillator (not approved)
- Towards Fourier-limited X-ray Science with XFEL-O and seeded XFEL
  - Inelastic X-ray scattering
  - Nonlinear X-ray Optics
  - Two-photon correlation spectroscopy
  - Transient grating
- Summary

TR x-ray applications at KEK

Picosecond photoresponse of perovskite manganite (NSMO) thin film (τ~ 50ps ~ 2ns)

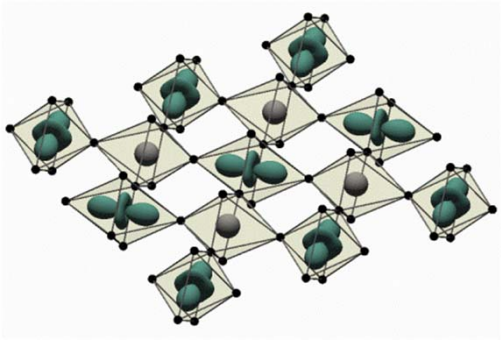
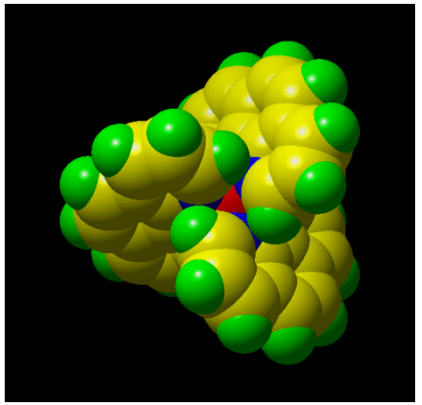
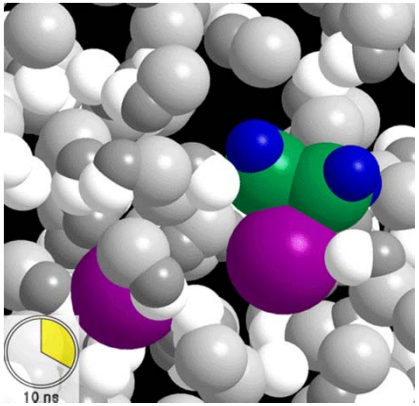


Photo-induced spin-crossover transition of metal complex in solution

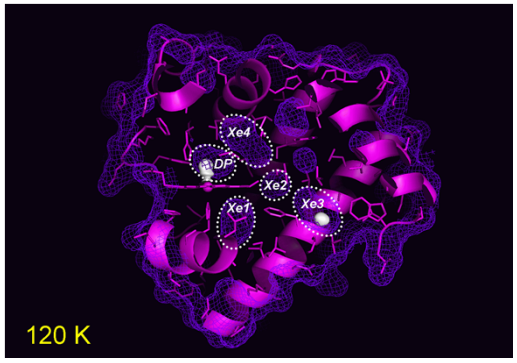
(TR-XAFS: τ ~700ps)



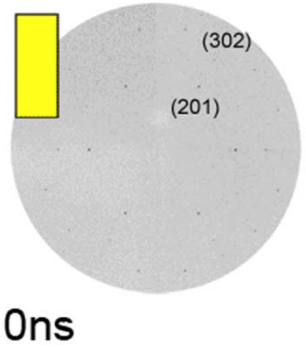
Photochemical reaction in liquid (TR-liquidography: τ~100ps~1μs)



Ligand migration dynamics in protein crystal (τ~800 min)



Laser shock-induced lattice deformation of CdS single crystal (TR single-shot Laue diffraction: τ~1ns~10ns)



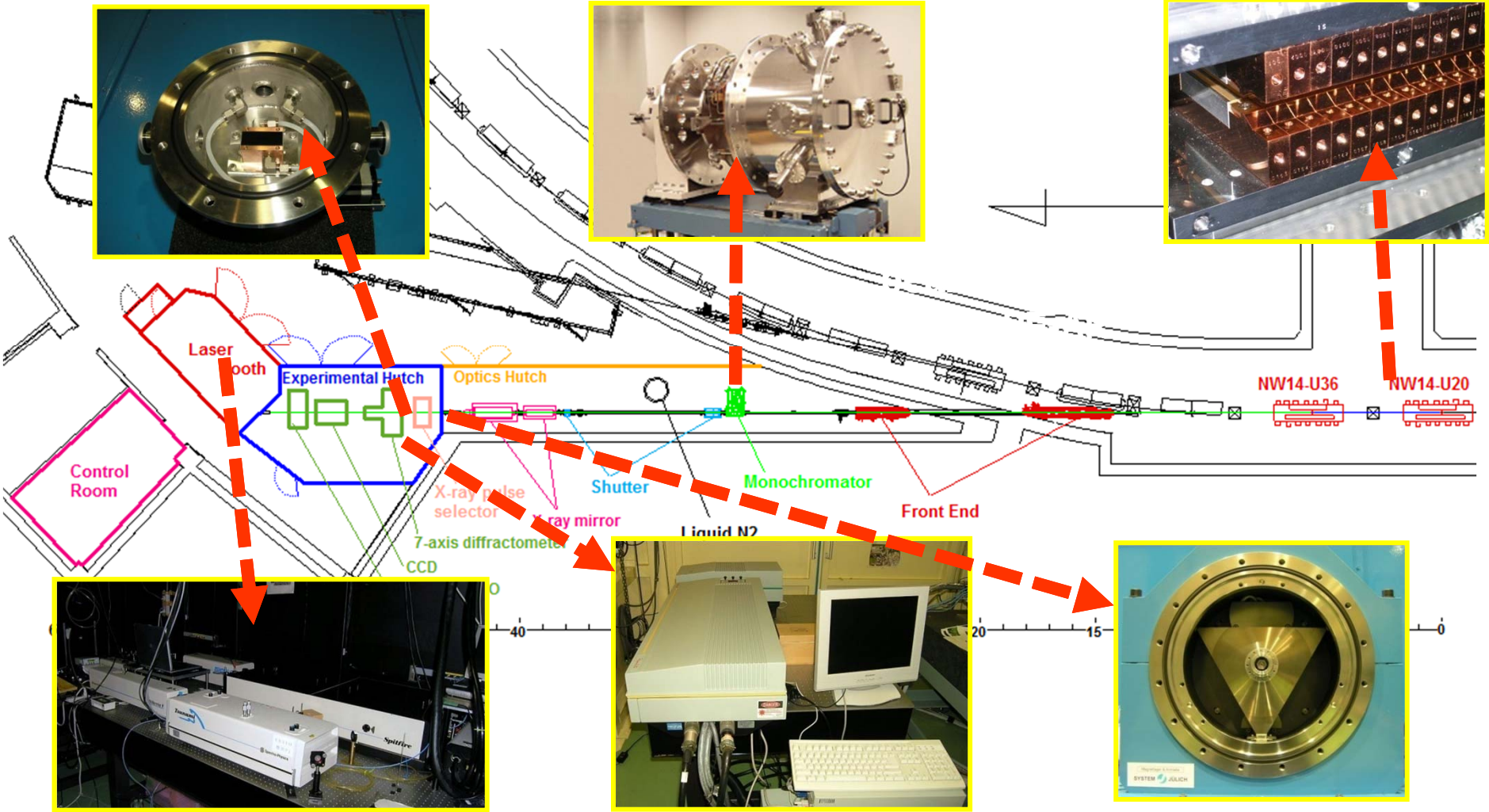
PF-AR (6.5GeV) Full-Time Single-Bunch Operation

~200days/year

multilayer mirror

Si(111) monochromator

undulator



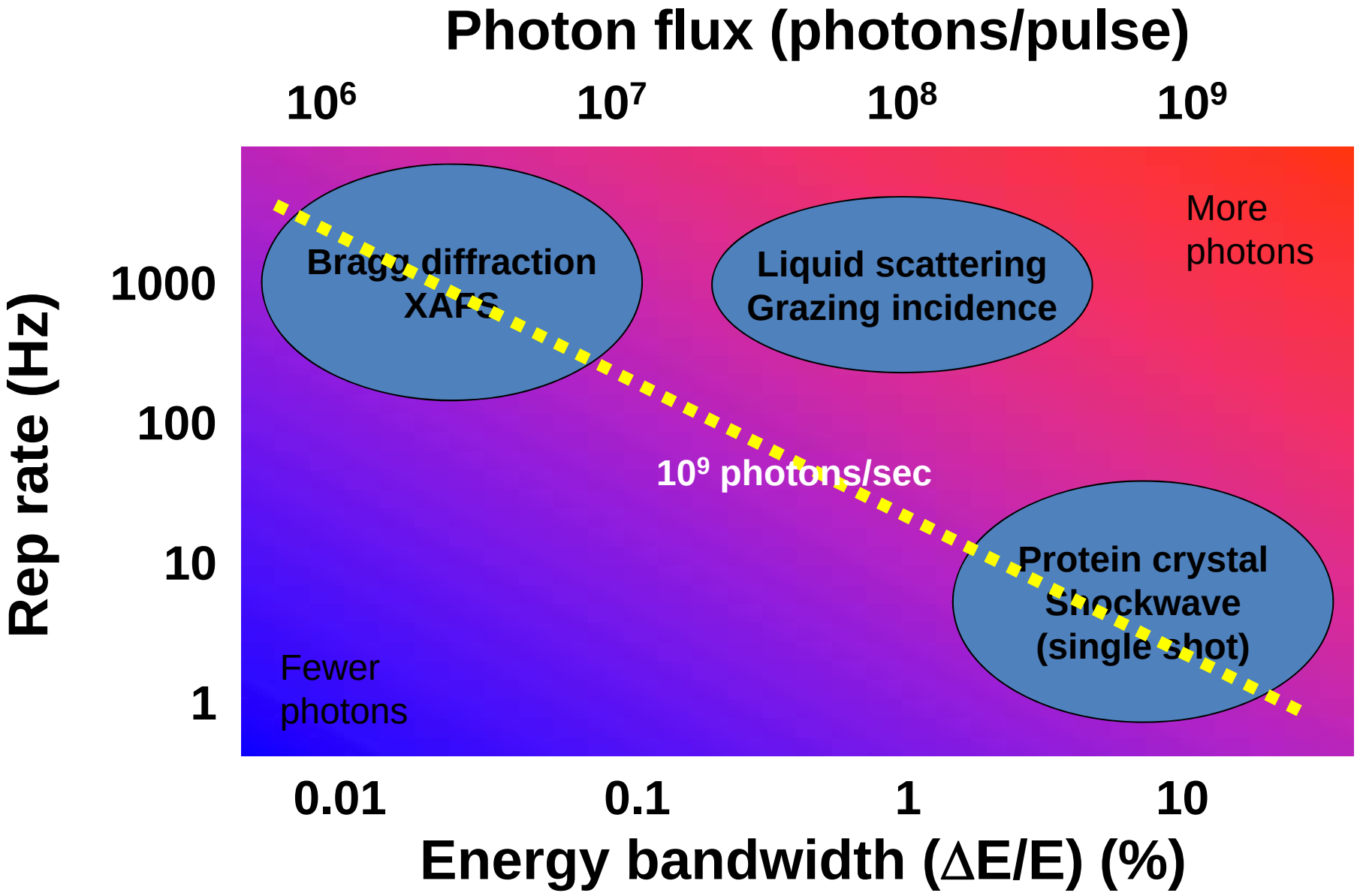
femtosecond laser system

nanosecond laser system

Jülich x-ray chopper

What is the key issue in TR X-ray Experiments?

Energy bandwidth vs. Rep rate



#1 TR-Diffraction

Picosecond photoresponse of perovskite manganite (NSMO) thin film

1 kHz rep rate

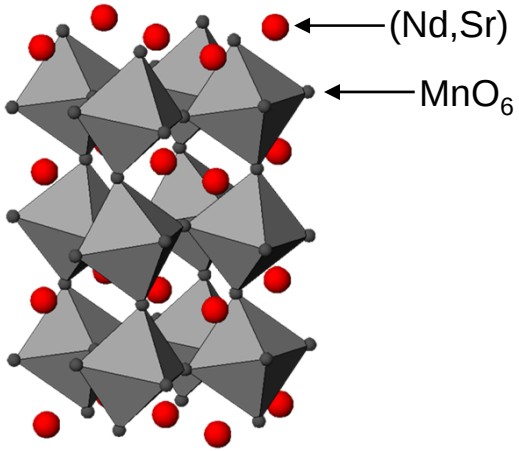
with mono X-ray ($\Delta E/E$ ~ 0.01%)

~10^9 photons/sec

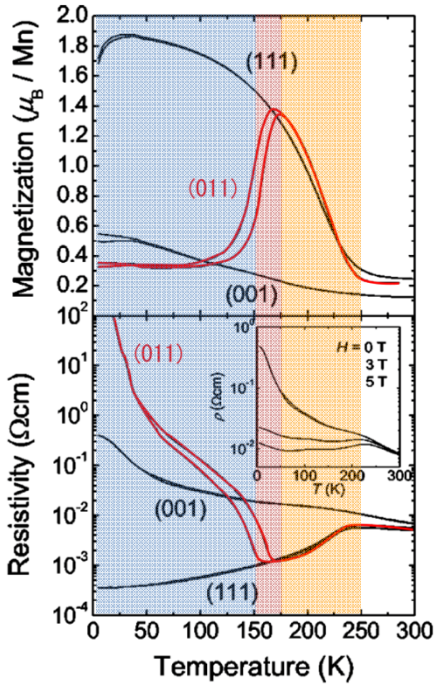
Phase Transition in Manganite Thin Film

Ichikawa *et al.*
Nature Materials,
10, 101-105 (2011)

$Nd_{0.5}Sr_{0.5}MnO_3/SrTiO_3(011)$
(NSMO/STO(011))

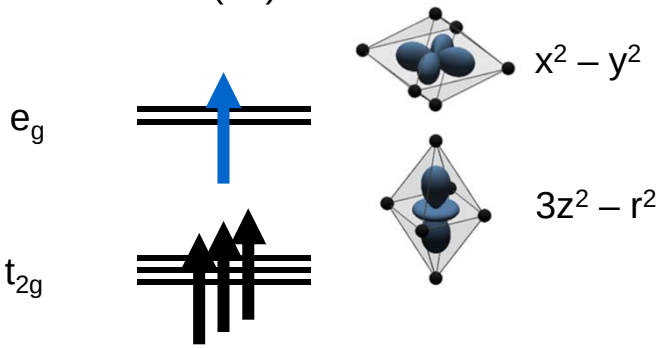


thickness: 80 nm

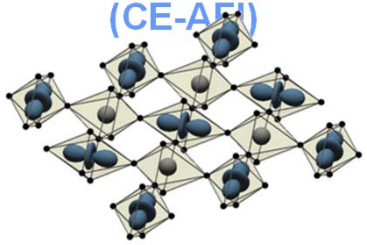


Nakamura *et al*. APL **86** 182504 (2005)

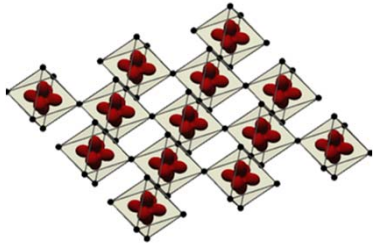
Mn^{3+}: $(3d)^4$



CE-type Antiferromagnetic insulator (CE-AFI)



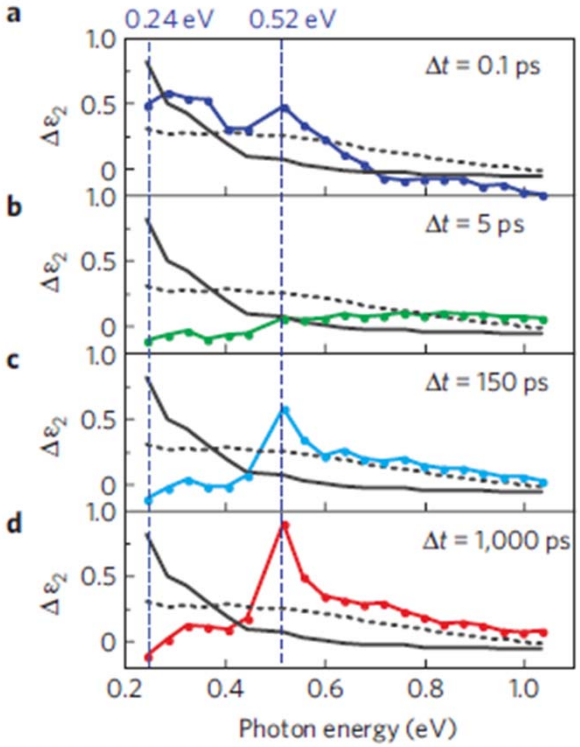
Ferrometal (FM)



Optical pump-probe results

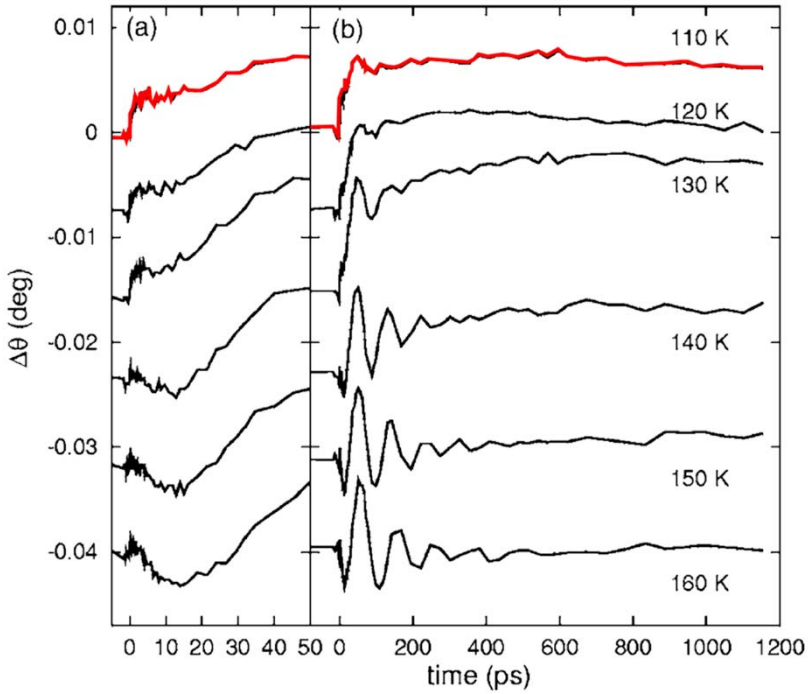
Collaboration with K. Miyano Group (Univ. of Tokyo)

TR-Reflectivity (100K)



Ichikawa *et al.*
Nature Materials, 10, 101-105 (2011)

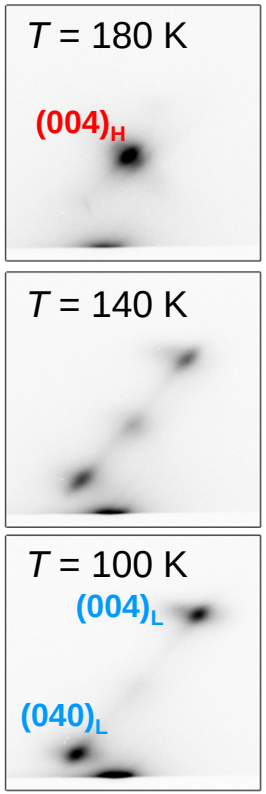
Kerr Rotation



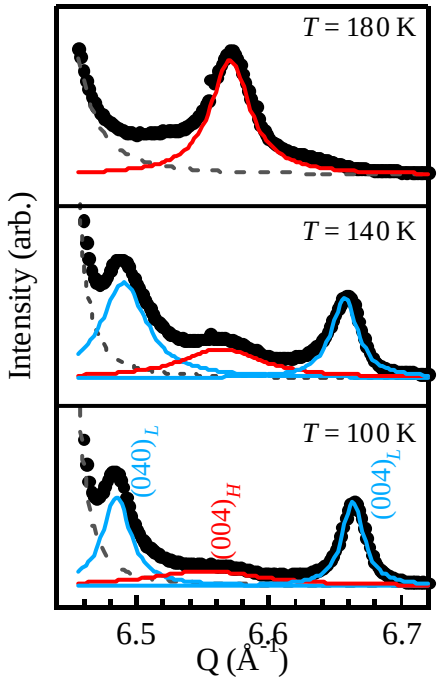
Miyasaka *et al*. PRB **74** 012401 (2006)

Temperature dependence of X-ray Diffraction

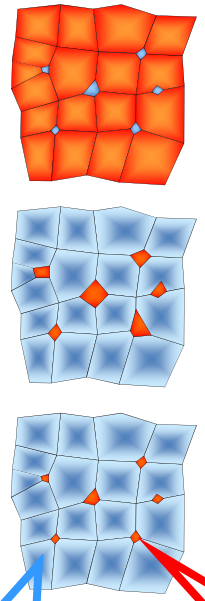
CCD Image

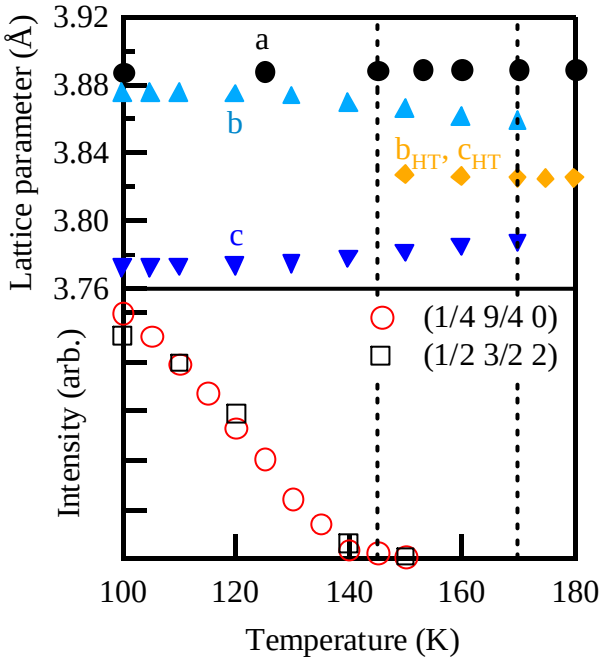


$Nd_{0.5}Sr_{0.5}MnO_3/SrTiO_3(011)$

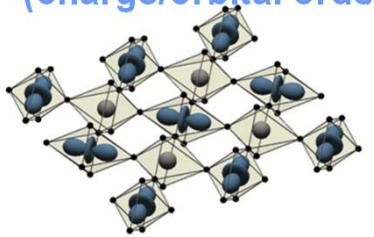


Heating

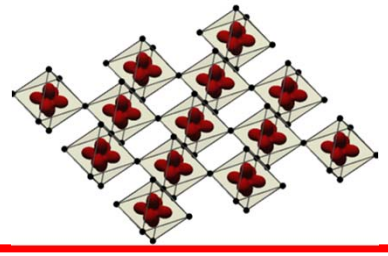




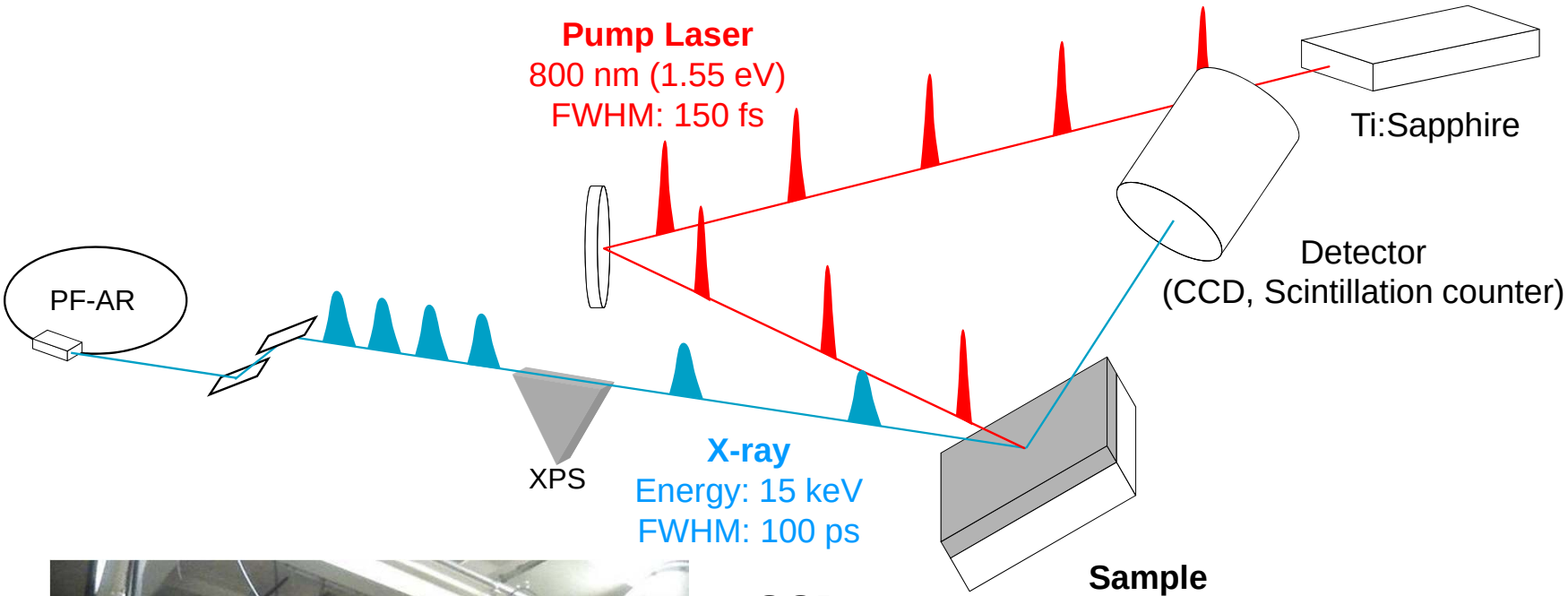
CE-AFI
(charge/orbital order)

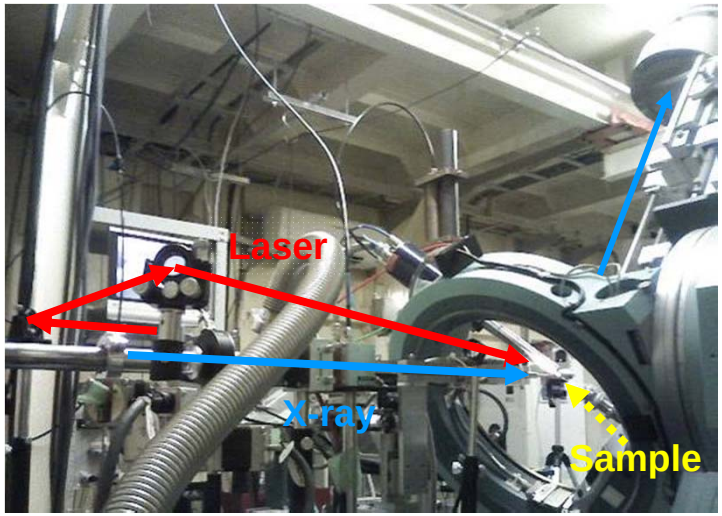


FM cluster
(charge/orbital disorder)



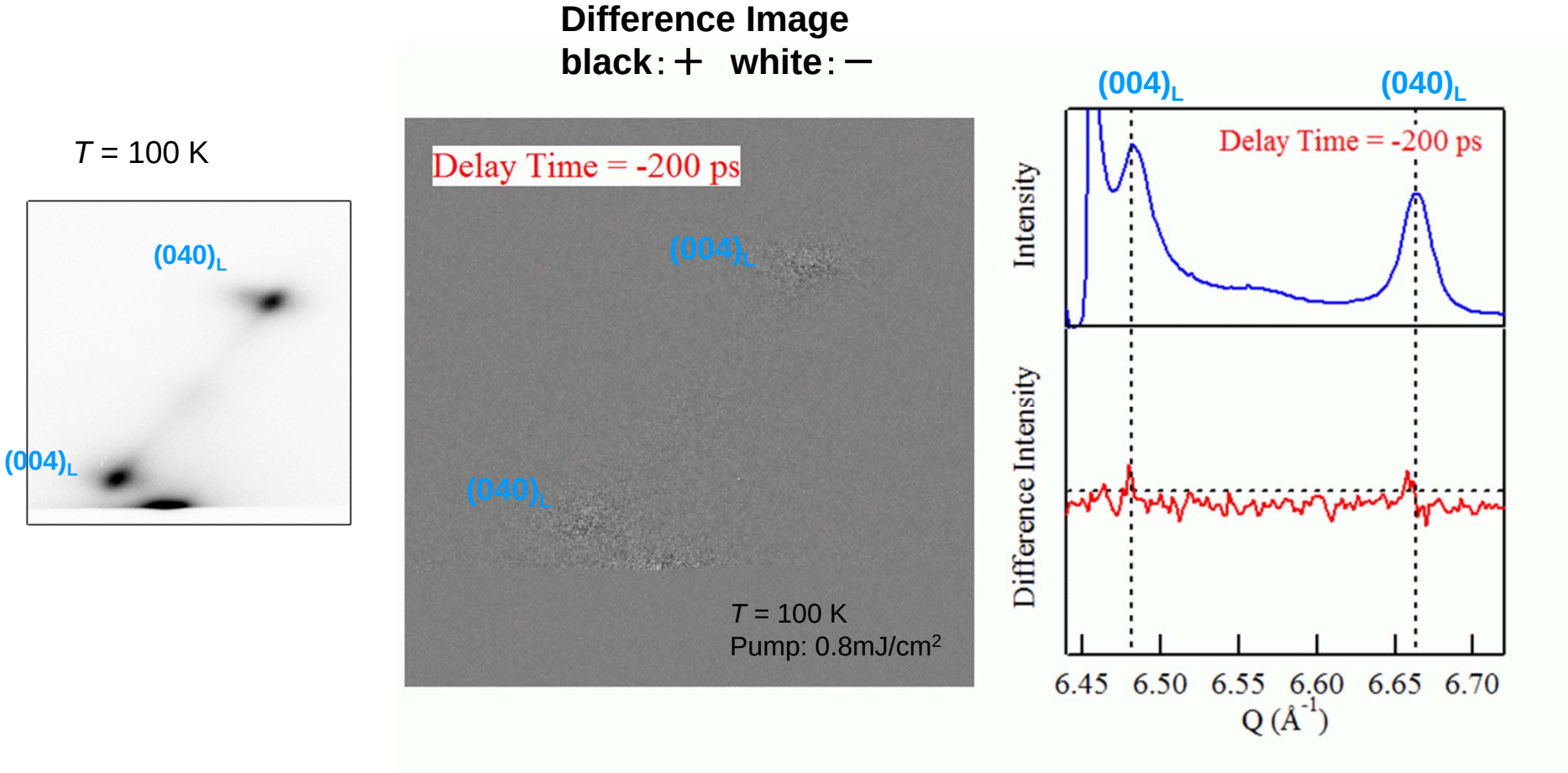
Layout of the laser-pump X-ray-probe experiment





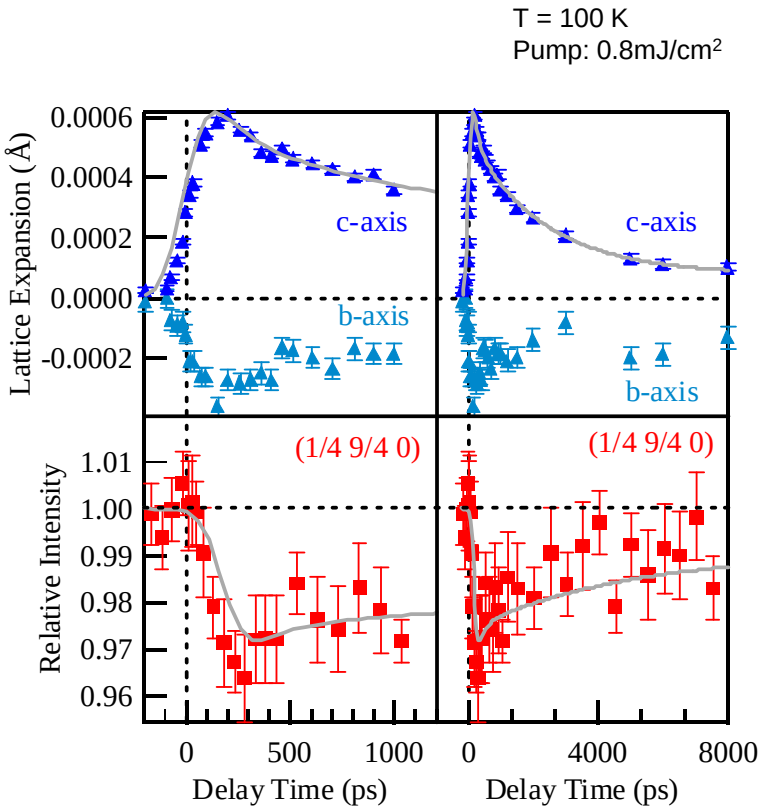
Time dependence of (004) reflection

$Nd_{0.5}Sr_{0.5}MnO_3/SrTiO_3(011)$



Time dependence of the (004) and (1/4 9/4 0) reflections

$Nd_{0.5}Sr_{0.5}MnO_3/SrTiO_3(011)$



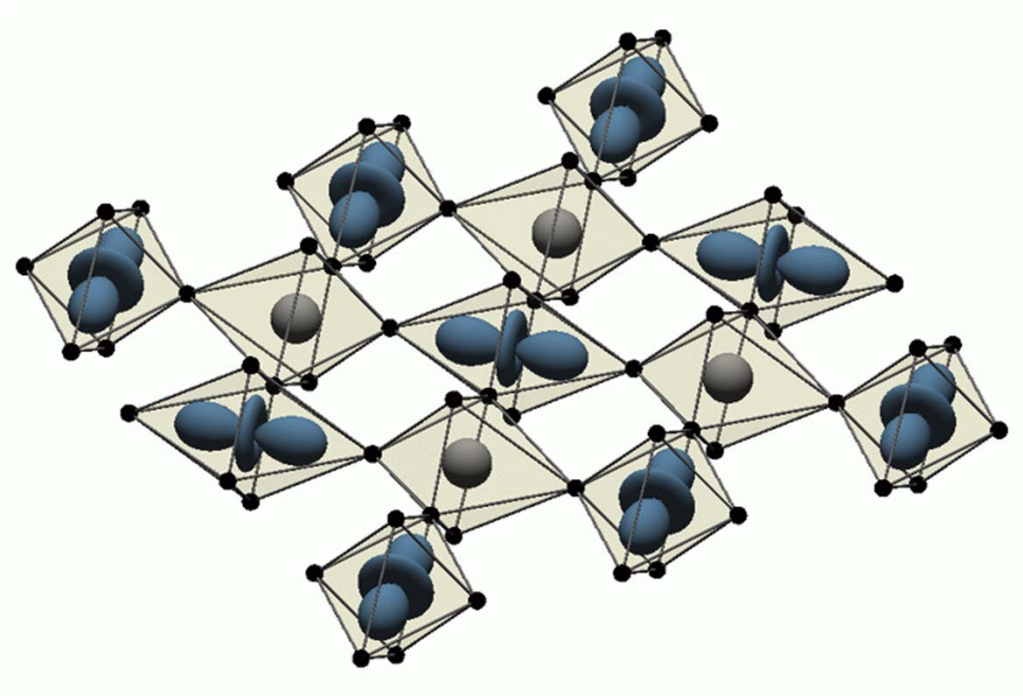


Photo-induced “hidden” state?

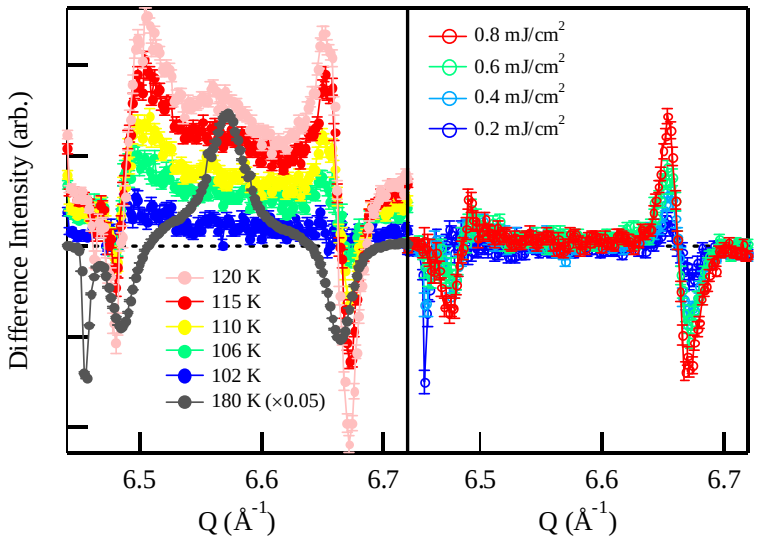
Temperature Dependence

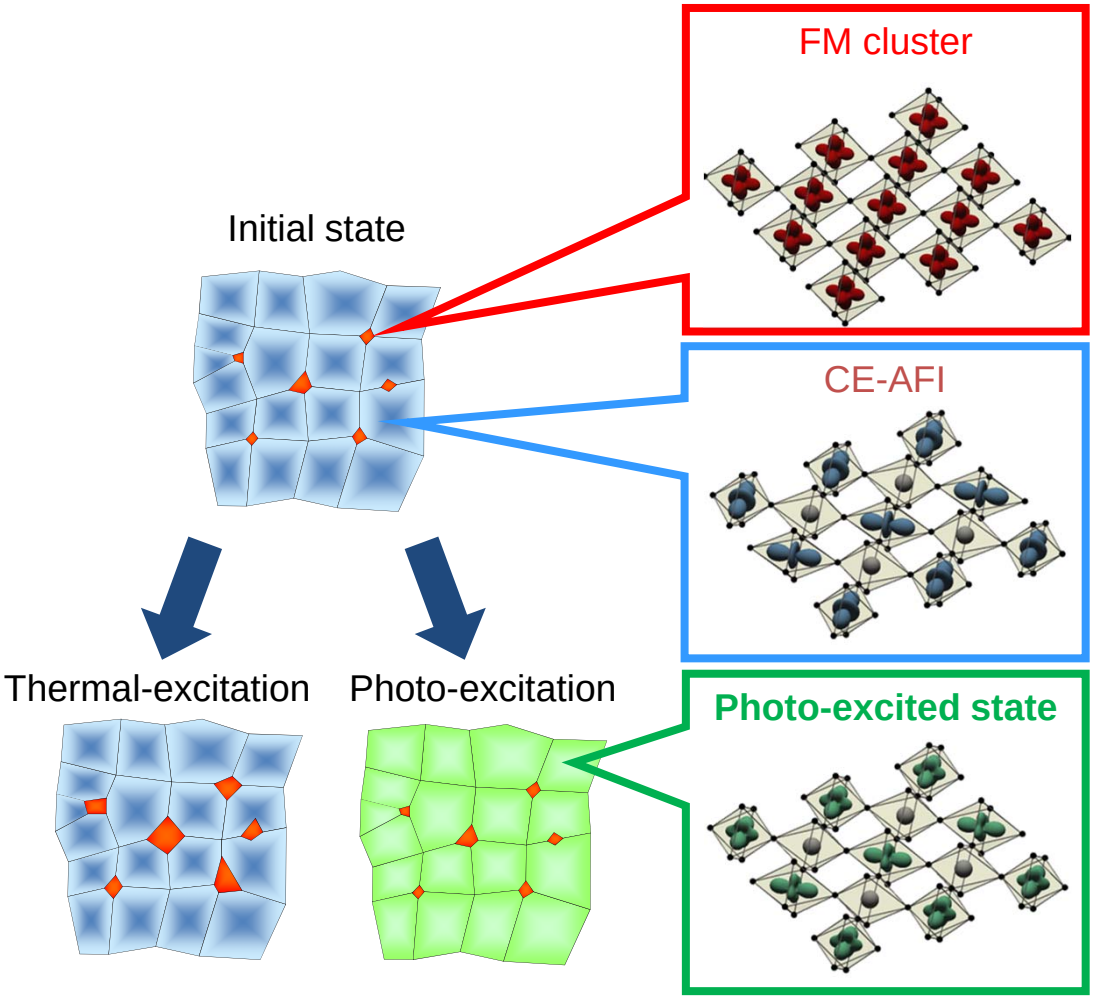
(Without laser irradiation)

Pump Power Dependence

T = 100 K

(Delay-time: +150 ps)





Ichikawa et al.

“Transient photoinduced ‘hidden’ phase in a manganite”

Nature Materials, 10, 101–105 (2011)

#2. TR-XAFS

Photo-induced spin-crossover transition of metal complex in solution

1 kHz rep rate
with mono X-ray ($\Delta E/E \sim 0.01\%$)
10^9 photons/sec

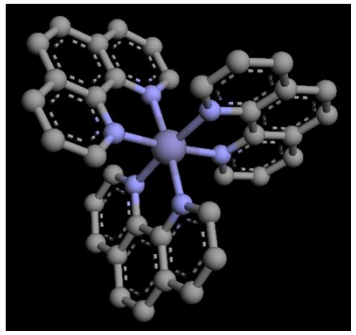
Nozawa *et al.* **J. Am. Chem. Soc., 132**, 61-63 (2010).

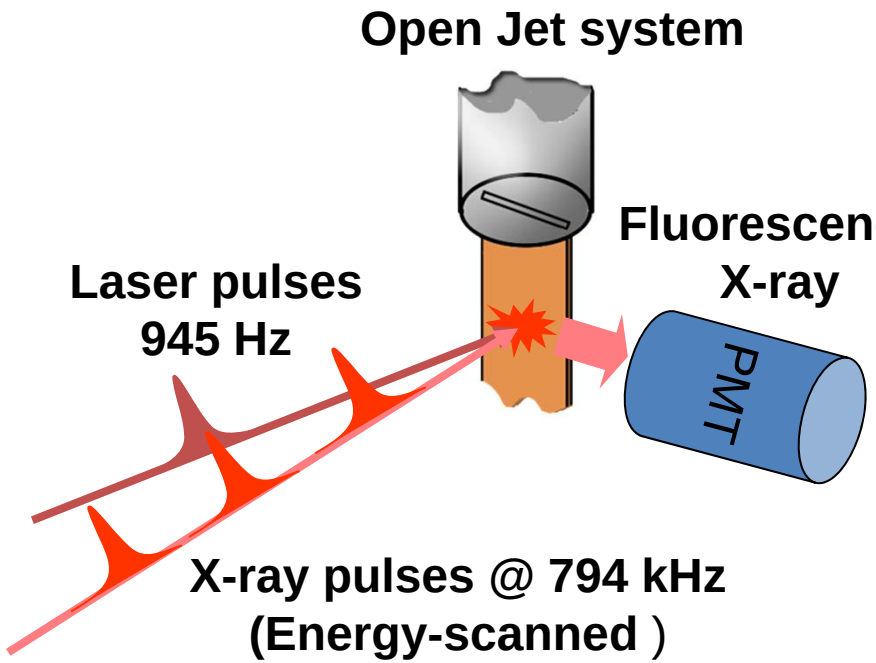
photo-induced spin-state transition by TR-XAFS

Shunsuke Nozawa (KEK)

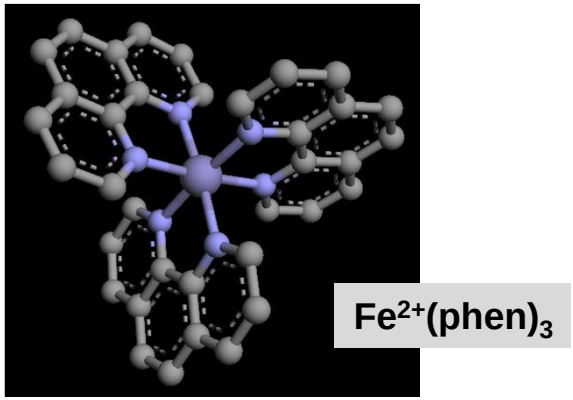
Tokushi Sato (KEK)

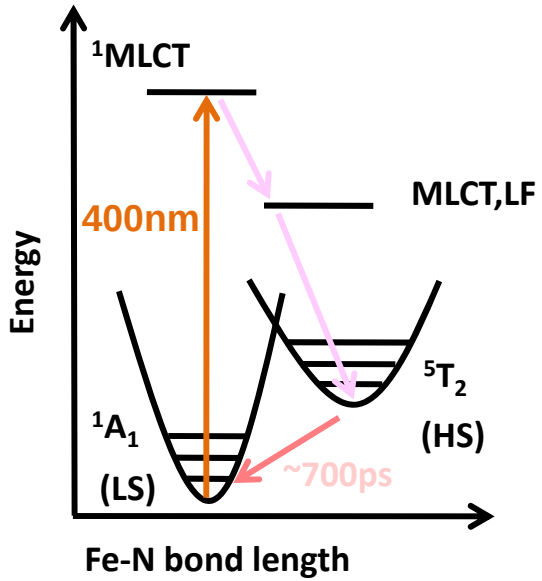
$Fe^{2+}(phen)_3$

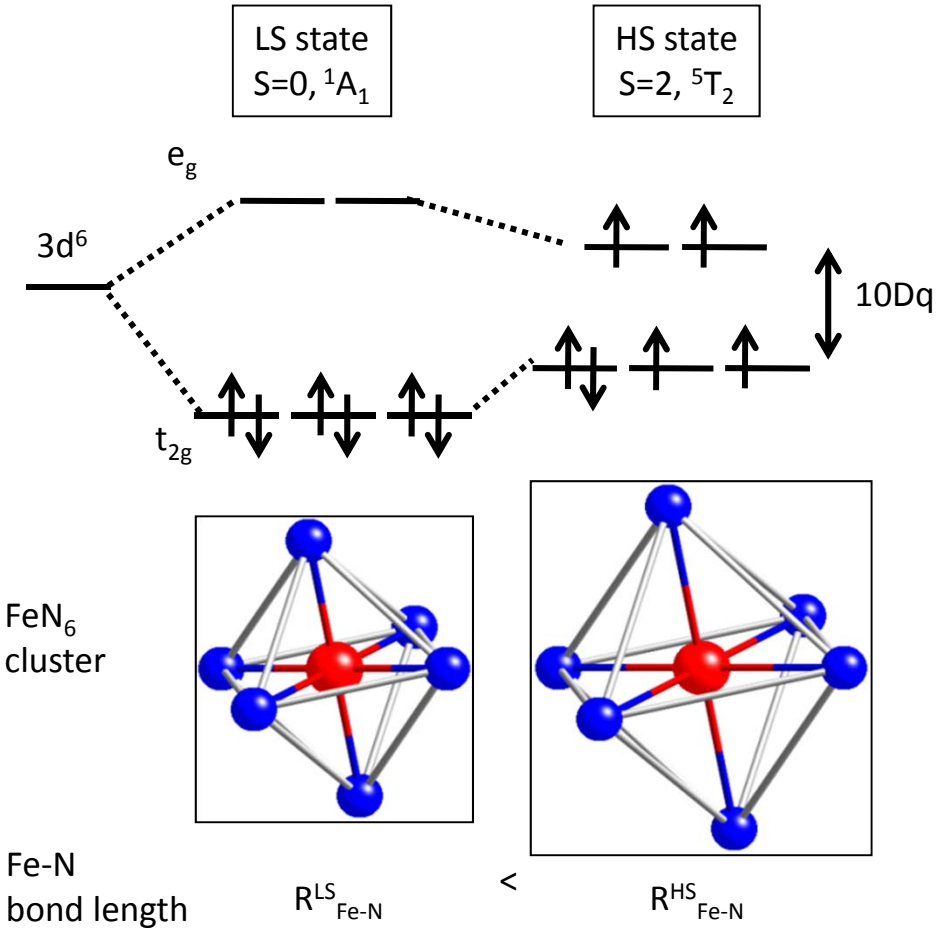




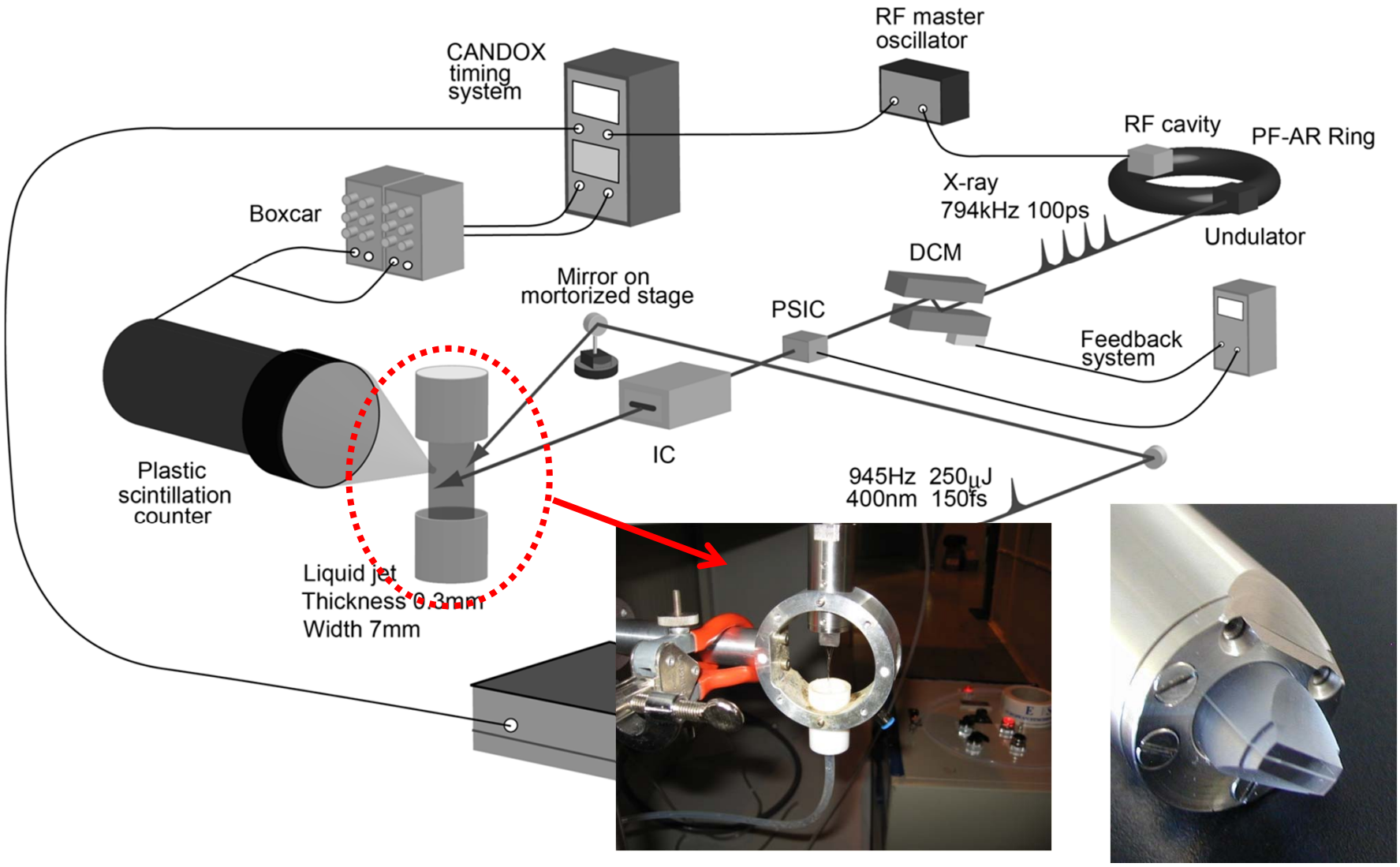
picosecond time-resolved spin-crossover transition of $Fe^{II}(phen)_3$



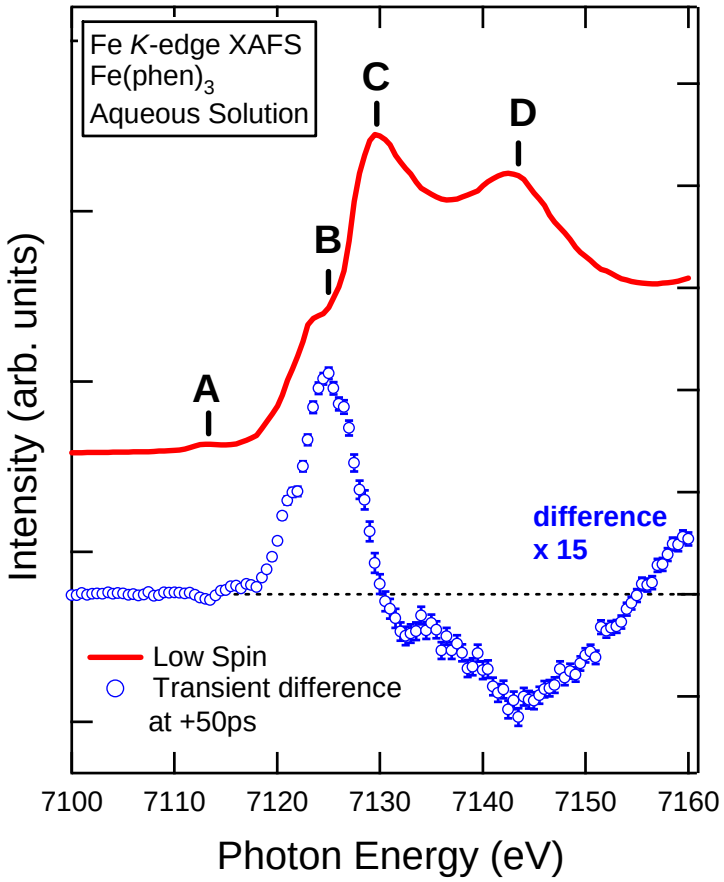


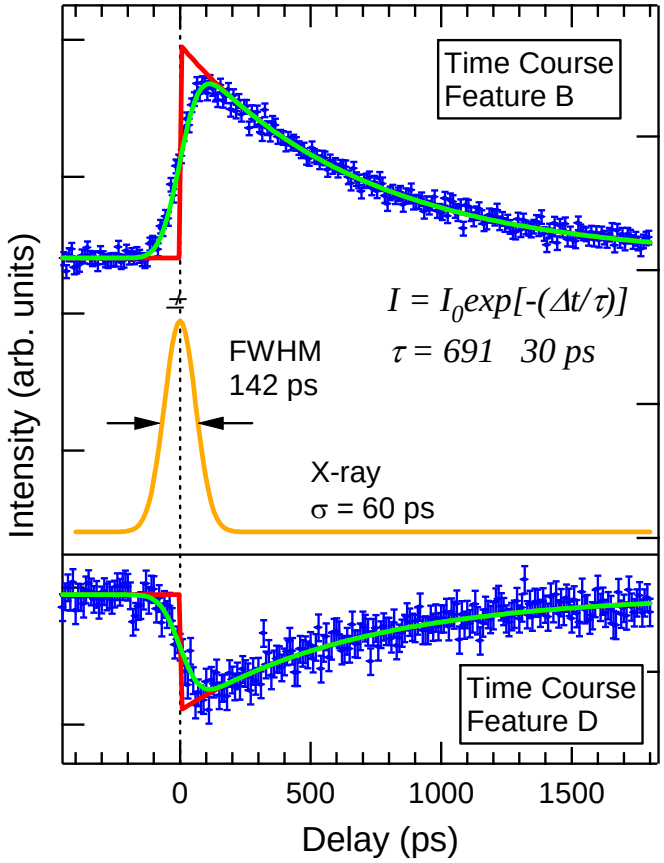


TR-XAFS: Experimental Setup

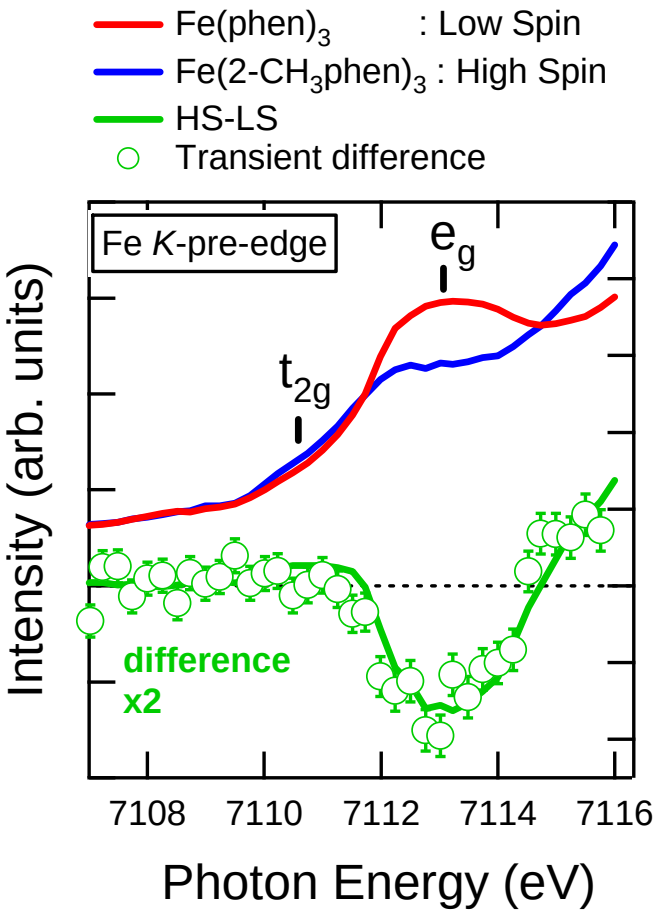


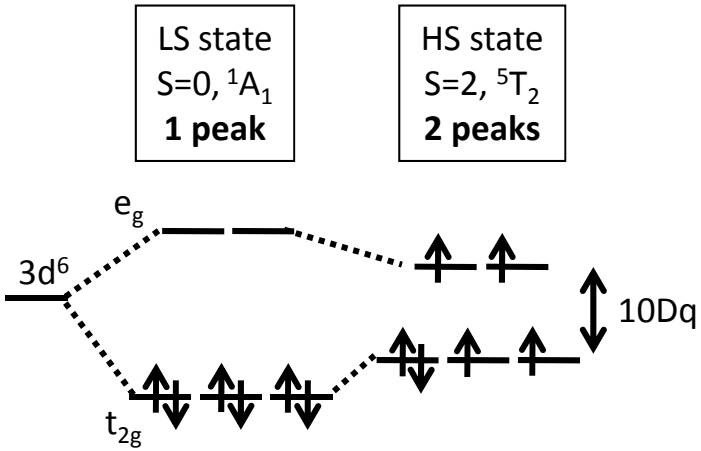
TR-Near Edge Structure

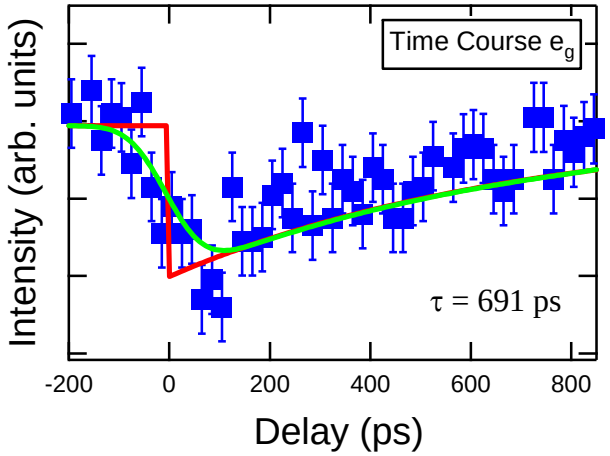




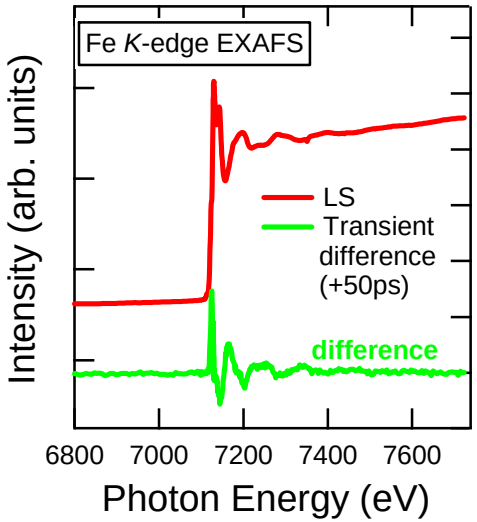
TR-XANES features in pre-edge region

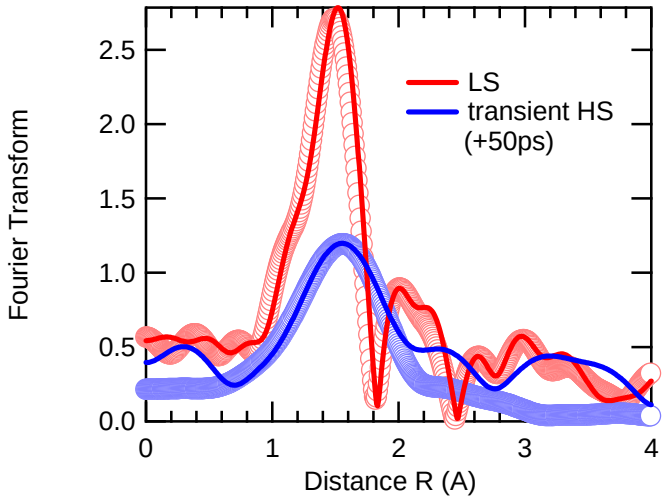






excited state EXAFS



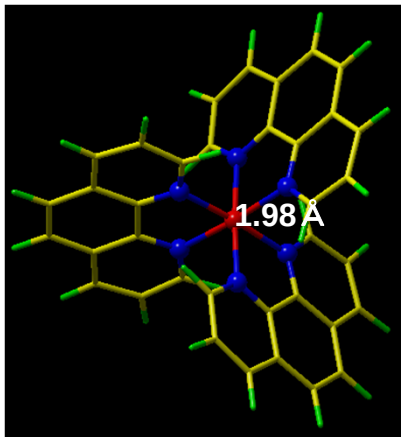


EXAFS analysis summary

Spectrum	$R_{Fe\text{-}N}$ (Å)	σ^2 (Å^2)
LS	1.98(1)	0.001(1)
Photo-excited HS	2.15(2)	0.011(3)

photoinduced structural change: a molecular movie!

Low Spin State



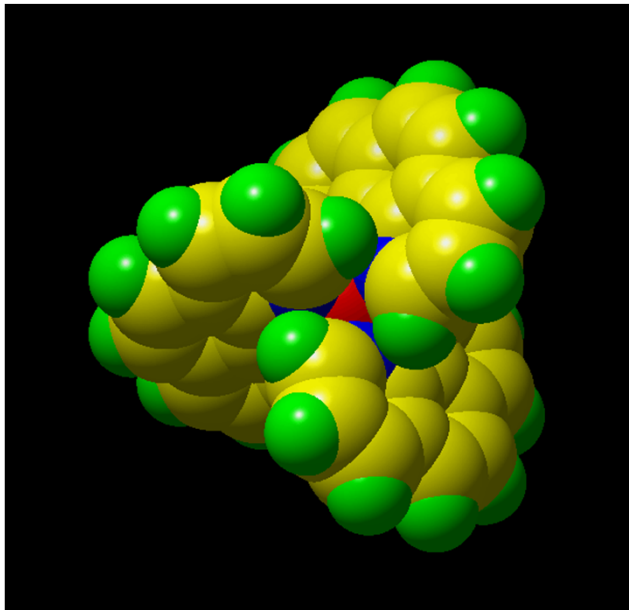
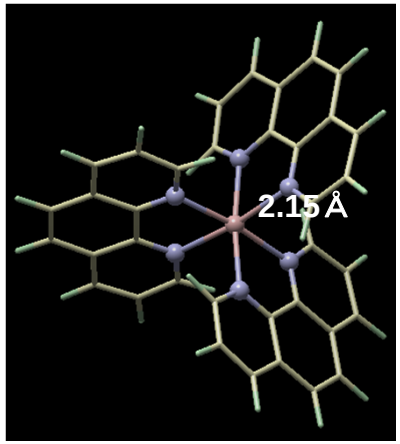
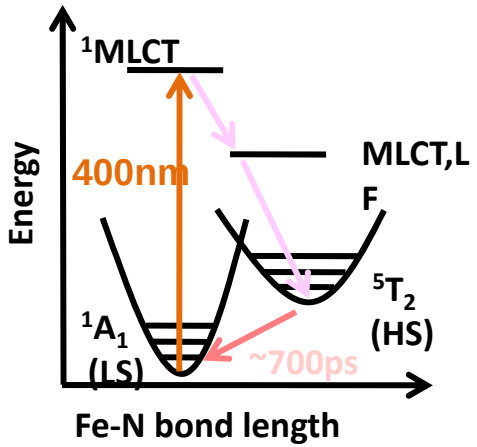


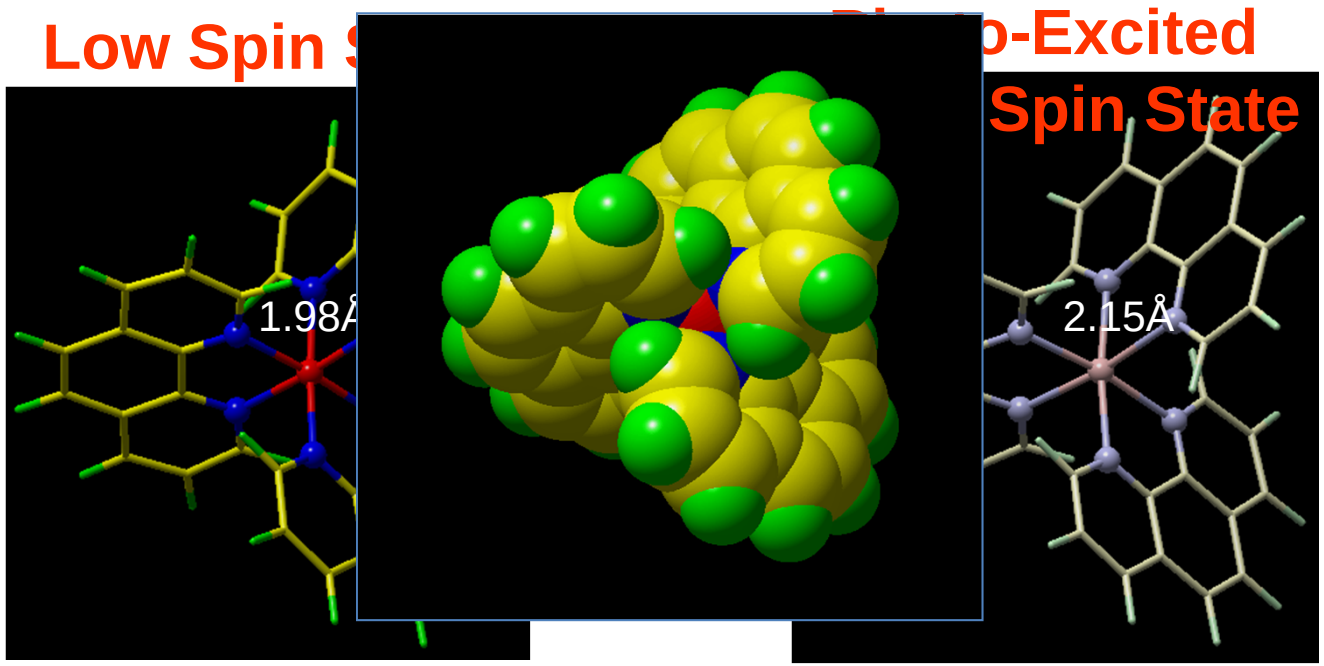
Photo-excited High Spin State





Nozawa *et al.* **J. Am. Chem. Soc., 132**, 61-63 (2010).

TR-XAFS - summary



- TR-XAFS provides spin, electronic and structural information of photo-induced states, which enables to produce molecular movies.