SACLA Users' Meeting
August 28-29, 2019

Breakout Session 3
"Extension of Pump-probe Capabilities for Biology and Chemistry"

Shin-ichi Adachi (KEK) & Tetsuo Katayama (JASRI)

Session 3. Extension of Pump-probe Capabilities for Biology and Chemistry		
Presenter	**Affiliation**	**Title**
M. Chergui	EPFL	Pump-probe experiments on biological systems at XFEL's
W. Gawelda (absent)	European XFEL	Femtosecond X-ray experiments: combining local and global observables for chemical dynamics studies
Y. Umena	Okayama Univ.	Development of simultaneous analysis of XES and XRD in a pump-probe experiment for multi-metal protein crystal
K. Tono	JASRI	Progress in pump-probe setup for SFX experiments at SACLA

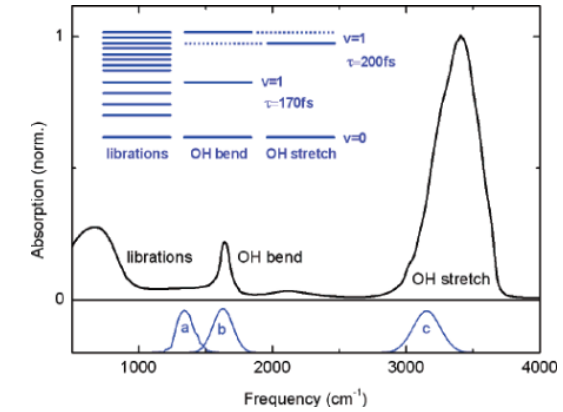
Topics given by M. Chergui

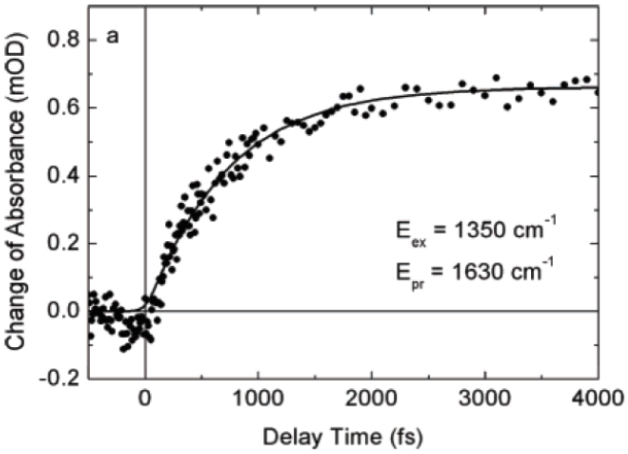
Extending capabilities for pump-probe experiments at XFELs

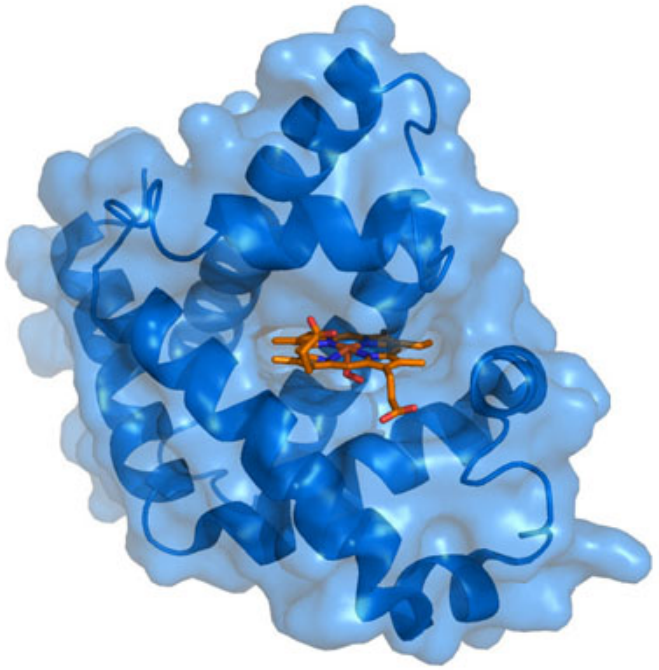
Excitation: extending into IR excitation

- Only a small fractions of (bio)chemical reaction can be triggered with light...
- T-jump experiments
- Vibrational excitation
- Mode-selective chemistry

Non-light driven reactions or functions: Laser T-jump







Ashihara *et al*, JPCA 2007 Ma *et al*, PNAS 2008

Repetition rate, flux, polarization

- Photon-in/photon-out spectroscopies (XES, X-ray Raman, RIXS, etc.)
- Helical dichroism (HD):

CD spectroscopy is weak due to the magnetic dipole interaction (spin angular momentum). HD relies on the orbital angular momentum (see Rouxel, Mukamel et al). First steady state tests at the SLS.

Detection: higher efficiency

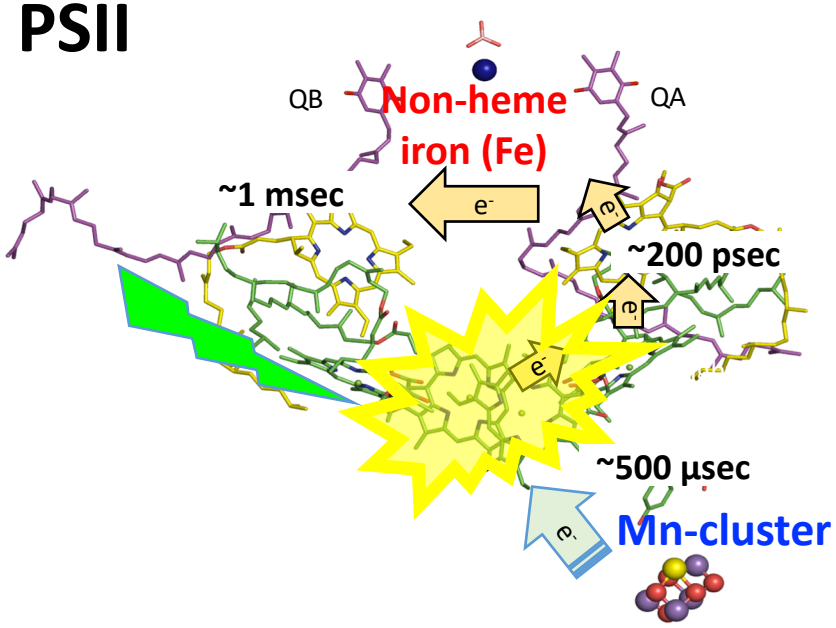
- Increase collection efficiency of von Hamos spectrometer (or a Johann spectrometer) to allow for weak signals such as valence-to-core XES and inelastic scattering experiments (X-ray Raman) in a pump-probe scheme.
- Allow for simultaneous XES and XDS recordings.

Topics given by Y. Umena

XES & XRD

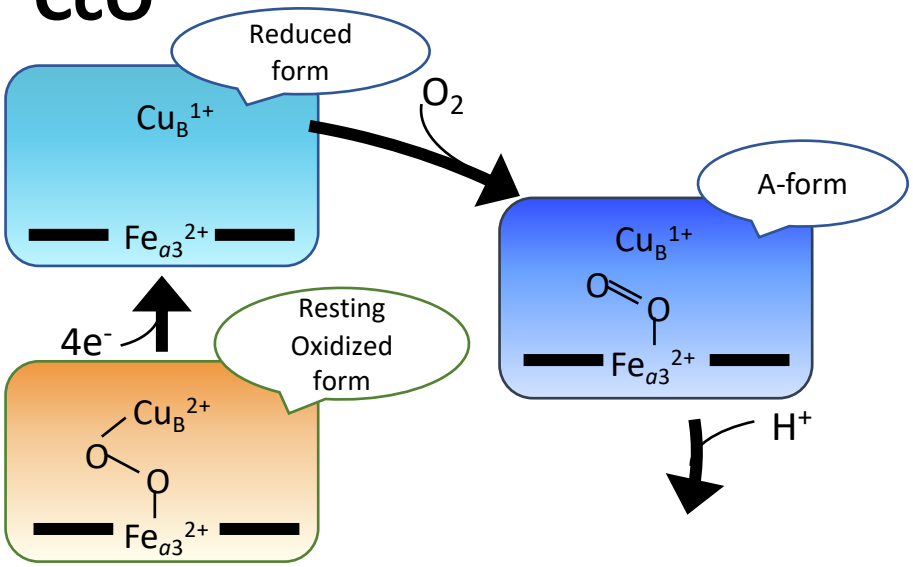
Research plans of PSII and CcO

PSII



1. Confirm the electron transfer from Mn-cluster to non-heme iron (NHI) by photoexcitation.
2. Time resolved XES analysis using chemical oxidized NHI.
3. Investigate how the natural ferric NHI works by ultra-time resolved XES.

CcO



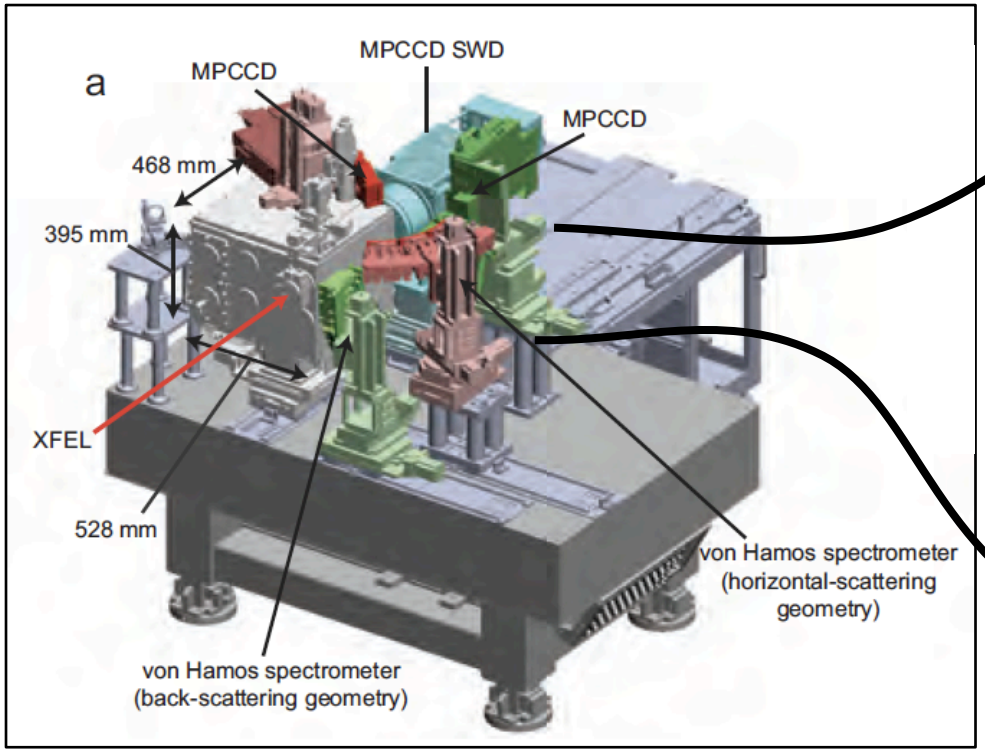
1. Distinguish whether resting oxidation and reduction
2. Determine the mixing ratio.
3. Advance the reaction using caged O_2 compound by Pump-probe experiment.

Schematics of experimental system

Person in charge : Dr. Tetsuo Katayama (JASRI, Riken)

SPINETT

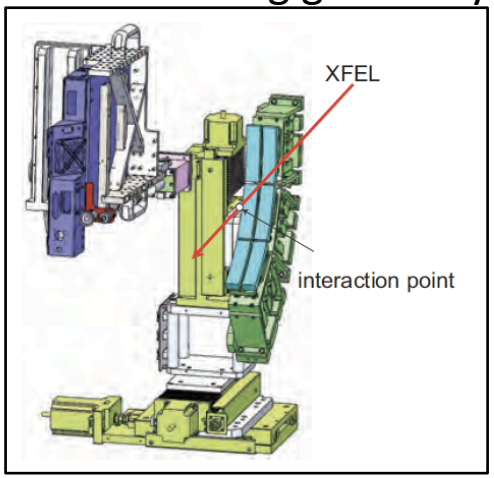
(SACLA Pump-probe INstrumEnt for Tracking Transient dynamics)



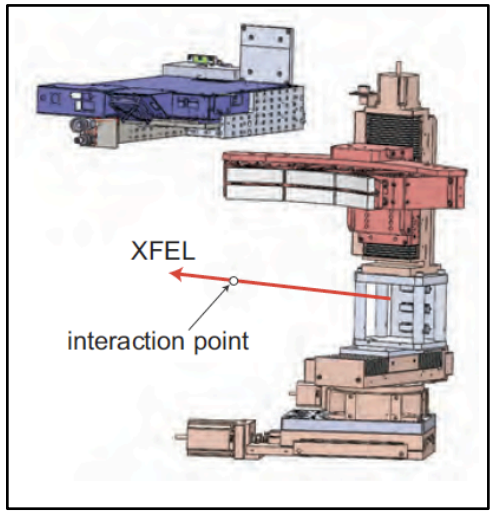
T.Katayama, In press

Von Hamos spectrometers

Back scattering geometry



Horizontal scattering geometry



Topics given by K. Tono & E. Nango

- Extended pump capability for protein dynamics studies
  - ✓Rapid mixing of liquids containing crystals and substrates.
  - ✓Temperature jump with IR laser.
  - ✓Photoexcitation of caged compounds ,

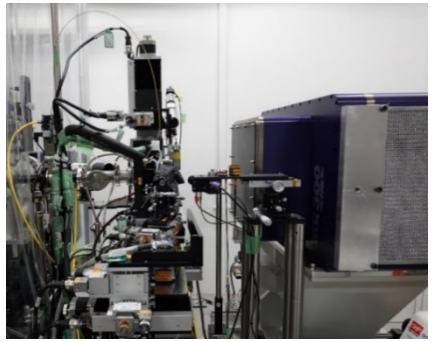
    => Tosha et al., Nat. Commun. **8**, 1585 (2017).
- New devices/methods useful for PX
  - ✓Large-area detectors
  - ✓Drop on tape sample delivery (under development)

Large area detector for PX, WAXS

MX300-HS (Rayonix, L.L.C.) is now operated *seamlessly* on the SACLA DAQ system.

Description	8 sensor MPCCD (Phase Ib)	MX300-HS*	
		2x2 binned	4x4 binned
Active area [mm^2]	110 x 110	300 x 300	
Max. frame rate [Hz]	60	10	33
Image format	2048 x 2048 50 um	3840 x 3840 78 um	1920 x 1920 156 um
Nominal Q.E. @12keV	0.2	0.8	0.8

* https://www.rayonix.com/product/mx300-hs/



DAPHNIS with MX300-HS

PX

For samples having large lattice constants (longer camera distance).

WAXS

For experiments targeting higher q.

CITIUS detector will be technically available for SACLA.

- Small system (0.3M-pixel single sensor) from 2021.
- Deployment plan of larger area detectors will be determined after hearing user needs.

requests to the facility

- Hardware
- Measurements (overall)
- Software, theory
- Accelerator
- others …

Hardware

- Alternative schemes for “pumping” of chemical reactions:
  - Going beyond the optical wavelengths! Only a small fractions of (bio)chemical reaction can be triggered with light...
  - Bio-sample, dilute systems, using exotic lasers will be good examples to promote science at SACLA, i.e. mid-IR pulses, THz pulses, etc.
  - Rapid mixing
- Detector
  - vacuum compatible CCD (@BL1)

Measurements (1/2)

- Existing methods to be improved:
  - X-ray scattering and diffraction, X-ray spectroscopies, i.e. XAS and XES, in particular EXAFS (!)
  - Particularly, EXAFS capability should be enhanced at SACLA.
- New methods to be considered:
  - Non-resonant valence-to-core XES, resonant XES, Inelastic X-ray Scattering, i.e. X-ray Raman…
  - Regarding new photon hungry methods, SACLA should not compete with high-rep-rate facilities (LCLS-II, European XFEL) directly.
  - photons/pulse might be the issue

Measurements (2/2)

- SACLA has realized the new scheme of self-seeding.
  - For application, stable operation and easy tuning will be key points.
  - What applications? Time-resolved RIXS, SFX with small molecule nanocrystals, …
  - Merit for SFX with protein crystal?

Software, theory

- Software improvements:
  - Many aspects of “user friendliness” have improved over past 5 years, thanks!
- Theory
  - for interpretation of TR-XES, XANES data

Accelerator

- New accelerator parameters:
  - two-color mode: transient grating, X-ray pump/X-ray probe experiments
  - Wavelength tunability in the hard X-ray range (>20 keV)

Others: Utility support

- On-site optical spectroscopy laboratories to carry out complementary optical measurements
- The environments in beam line hatch.
  - Temperature and Humidity

    → Condensation on sample holder
  - Light condition

    → Complete dark or non-excitation light
- Usability of large area detector (Rayonix)
- A place of sample preparation on site.