PAUL SCHERRER INSTITUT

PSI

Camila Bacellar on behalf of Alvra :: SwissFEL :: Paul Scherrer Institute

Alvra Status and Future Plans

4th SwissFEL Performance Workshop – Jan 26th 2022

LVR

Alvra Group

Group Leader

Camila Bacellar

Scientists

Claudio Cirelli

New Position Opening soon

Technicians

Dardan Gashi

Jörg Schneider

Postdocs

Abdullah Kahraman

Victoria Kabanova

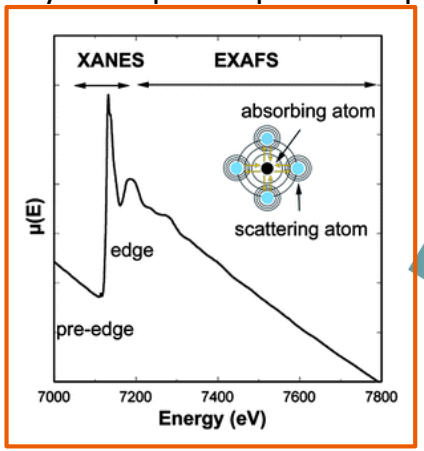
Emma Beale

Laser (NLO)

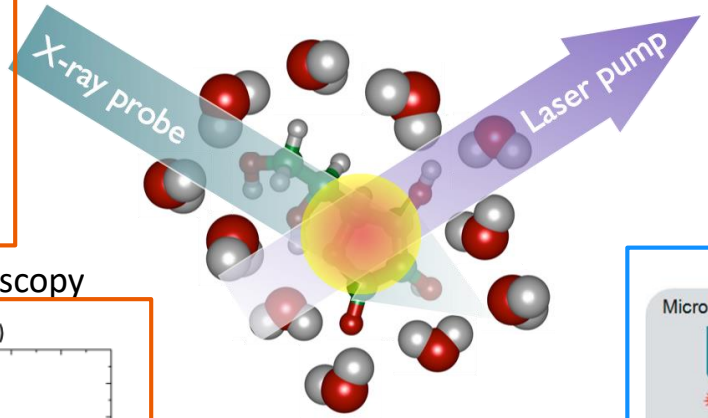
Philip Johnson

Alvra Core Capabilities

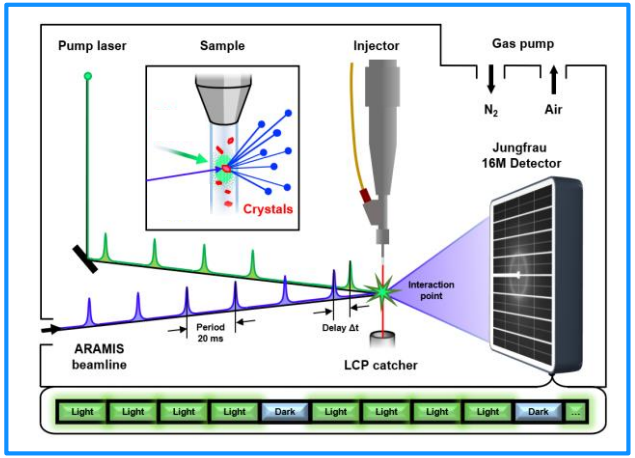
X-ray absorption spectroscopy



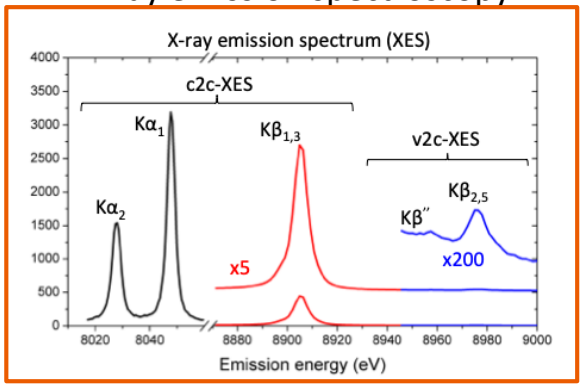
State-of-the-art techniques to explore **ultrafast dynamics** in chemical and biological systems



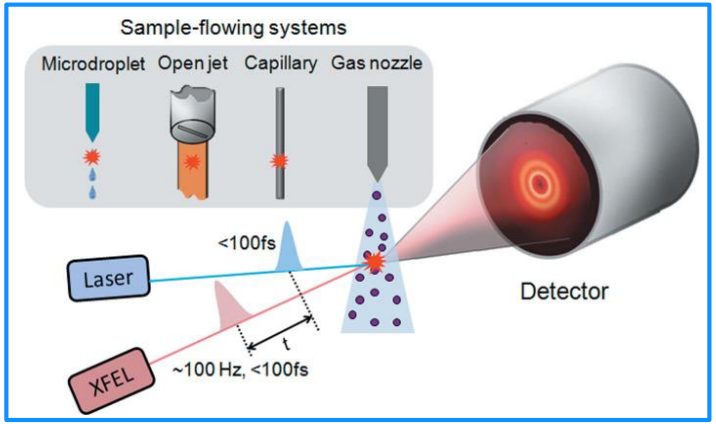
Serial Femtosecond Crystallography



X-ray emission spectroscopy



X-ray Scattering



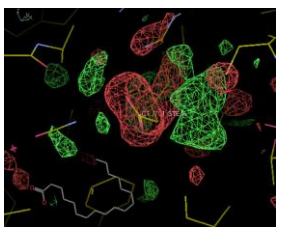
SwissFEL – Alvra Users 2021

User run 5: Jan Feb Mar Apr May Jun

User run 6: Jun Jul Ago Sept Oct Nov Dec

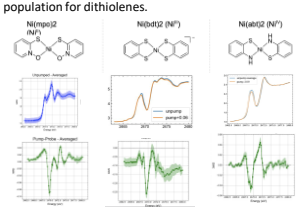
Deciphering the catalytic mechanism of fatty acid photodecarboxylase by time-resolved SFX
M. Weik, IBS

Newly discovered photoenzyme from microalgae transforms lipids to hydrocarbons in one step. 3D Structure and reaction intermediates were observed, in order to understand the photocatalysis at a molecular level



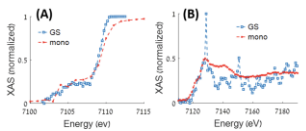
Identifying photocatalyst excited state character and relaxation mechanism using S and Ni K-edge absorption spectroscopy
A. Cordones-Hahn, SLAC

Fully remote experiment!
Identified the excited state character and relaxation mechanism of 3 photocatalysts. Distinguished populations of CT and MC excited states in real-time. S K-edge XAS very sensitive to valence electronic population for dithiolenes.



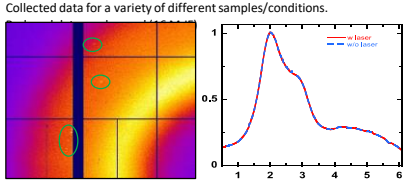
Ghost spectroscopy with XFEL
S. Shwartz, SLAC

Successfully demonstrated ghost spectroscopy (GS) at hard X-ray wavelengths for the first time, in solid targets and dilute solutions



How chemical tuning of the surface charge density affects electron-phonon coupling in colloidal nanoparticles
Kl. Sokolowski-Tinten, Univ. Duisburg-Essen

First liquid scattering experiment in Alvra.
Collected data for a variety of different samples/conditions.



Heme spin-crossover-induced coherent oscillations in photolyzed myogobin.CO probed by ultrafast time-resolved SFX
I. Schlichting, MPI. for Medical Research Heidelberg

Highest time resolution experiment in Alvra

SFX Block

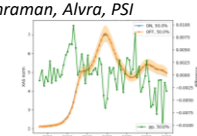
Time Resolved Serial Femtosecond Crystallography Studies of Light-Driven DNA repair by DNA photolyase
M. Maestre-Reyna, Academia Sinica

11 Time delays, 75K images per time point!
Dark and Oxygen free samples

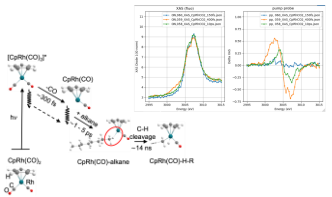
Time-resolved serial femtosecond crystallographic study of an eukaryotic photolyase
S. Westenhoff, Univ. of Gothenburg

+ In-house Multi Reservoir Commissioning
With J. Standfuss, PSI

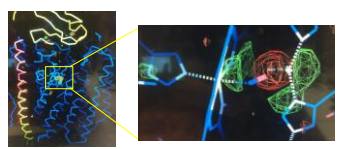
Probing the Ultrafast Charge Carrier Dynamics of Mn doped ZnO nanoparticles
A. Kahraman, Alvra, PSI



Revealing the electronic structure of the decisive intermediates in C-H activation reactions on femtosecond timescales using Rh L-edge spectroscopy
R. Jay, Univ. Uppsala



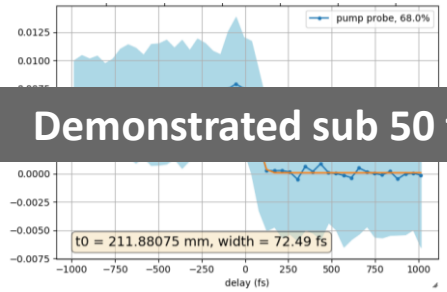
Time-resolved serial femtosecond crystallography studies of the reduction of oxygen to water by cytochrome c oxidase
R. Neutze, Univ. of Gothenburg



- **11 beamtimes** (9 user and 2 internal)
- ~50% “normal” machine parameters

Plans and Goals for 2021

Demonstrate sub 35 fs time resolution



Currently ~70 fs cross-correlation

Demonstrated sub 50 fs time resolution

X-rays <30 fs (??)

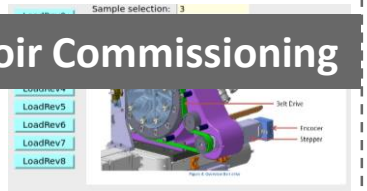
New timing-tool close to the sample

Increase SFX experiments throughput

Very successful line of research

Beamtime demand far exceeds

Multireservoir implementation



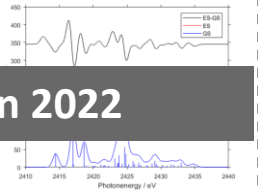
SFX Block + Multi Reservoir Commissioning

Ratio of prep to DAQ can be improved

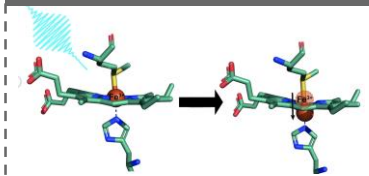
Emma Beale new postdoc for SFX improvements..

Strengthen in-house research and commissioning

Open new research avenues and technical developments



Room for improvement in 2022



And many interesting ideas!

Run successful cutting-edge user experiments even with COVID restrictions

We all (SwissFEL in general) did great!

Flexibly match setups for efficient beamtime, e.g. through reserve list

Longer user experiments

Alvra Updates – Time Resolution

Current state of art:

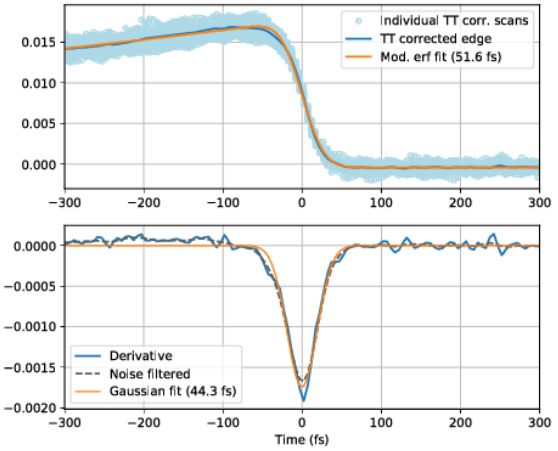
- < 50 fs instantaneous *Instrument Response Function* (NOPA + short pulse mode (x-rays))
- < 100 fs drift over 6h operation
- New Time Tool installed near interaction region

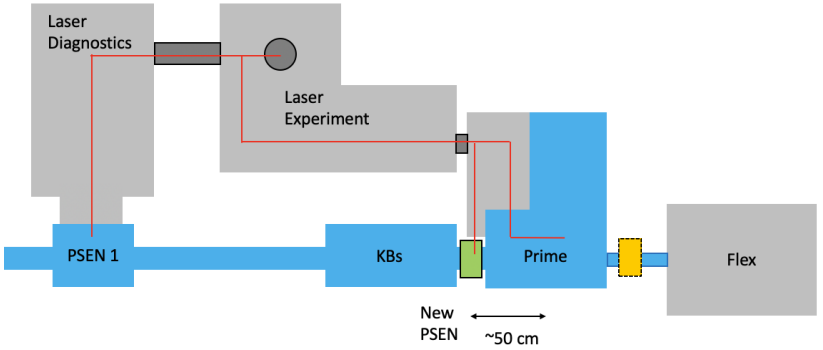
Improvements within next 6 months:

- Full commissioning of new Time Tool (ongoing)
- Installation of post-sample Time Tool (Tender X-rays)

Continous challenge:

- Long term drifts
- Note: heavy investment in AC, vibration, new hardware
- **Very challenging to go beyond current state of art**





Alvra Updates – Tender X-rays

Current state of art:

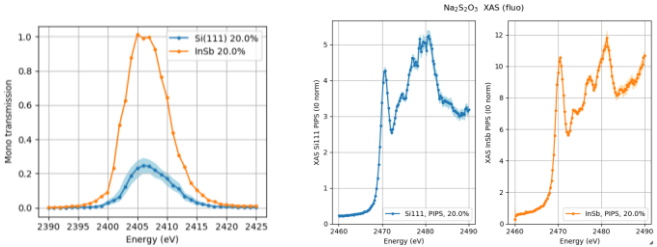
- 10x higher S/N compared to last year
- 1 mJ at 2.5 keV – Improvements from the machine side
- Commissioned InSb monochromator crystal
- Installed APD detectors
- PSSS working in third harmonic mode

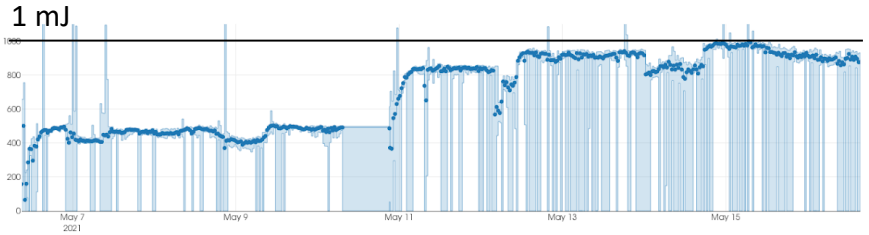
Improvements within next 6 months:

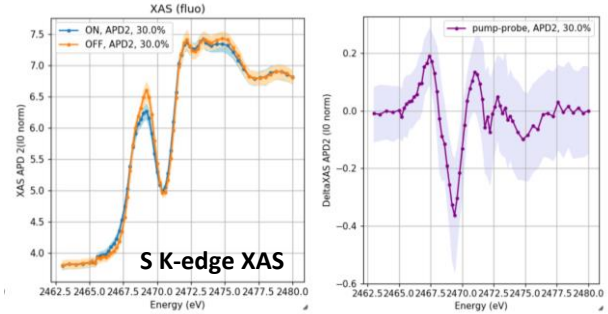
- Post-sample Time Tool for jitter correction

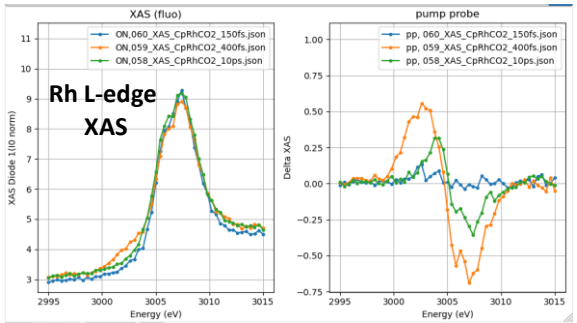
Continous challenge:

- Single-shot spectral characterization (TXS)



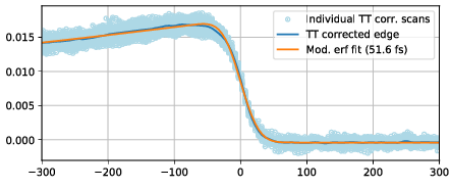






Plans and Goals for 2022

Demonstrate sub 35 fs time resolution



Currently ~**45 fs** cross-correlation

Laser < 20 fs

X-rays <30 fs (??)

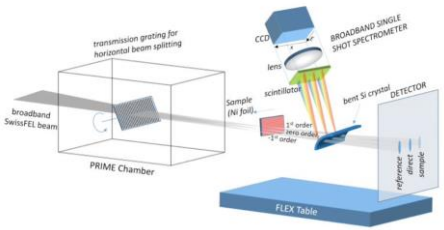
New timing-tools close to /after to the sample

Mature the use of “special” beam modes

Very successful use of “special” beam modes so far

Last Call (out of 16 proposals)

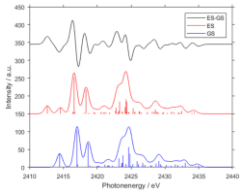
- 2x large BW
- 2x short pulses
- 3x tender x-rays

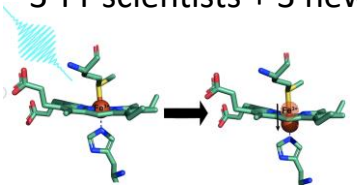


Strengthen in-house research and commissioning

Open new research avenues and technical developments

3 TT scientists + 3 new postdocs





And many interesting ideas!

Optimize Beamtime Throughput

Optimize user shifts → how many are needed for a successful experiment?

Combine similar experiments close together for increased efficiency

Increase communication between SwissFEL Teams

Plans and Goals for 2021 – The Alvra Perspective

Goals	• Increase beamtime efficiency and throughput • Become leader in ultrafast experiments in chemical and biological systems
Requirements	• Beamline automation and instrumentation development • Parallel and Reliable Operation
Questions	• How do we strike balance of parallel and reliable and novel mode operations?

Wir schaffen Wissen – heute für morgen

Thanks to:

Everyone at PSI involved in the making Alvra a successful endstation!

SwissFEL – Alvra Users 2020

User run 3 | User run 4

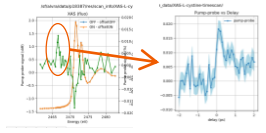
Jan | Feb | Mar | Apr | May | Jun | Jul | Aug | Sep | Oct | Nov | Dec

2020

Ultrafast geminate recombination of bio-organic disulfides upon UV excitation

N. Huse, U Hamburg

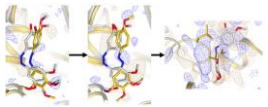
First sulfur measurements at SwissFEL with fs-XANES, XES and RIXS pump-probe data. Excellent signal-to-noise allows measuring tiny (1%) pump-probe signal.
Evidence of L-cystine radical formation in the pre-edge, estimated ps lifetime.



Monitoring ligand release using a photoswitchable anticancer drug

J. Standfuss, PSI

Demonstration of the use of synthetic photoswitches in SFX: visualization of the ligand release from tubulin and reorganization of the cholchicine binding pocket. Optimized jetting conditions with cellulose instead of LCP.

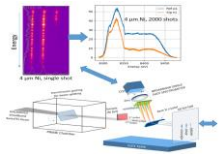


Towards single-shot XAS on transition metals at Aramis

C. David, PSI

First use of a new SwissFEL machine mode for Aramis: broad band and strongly chirped beam.
Used a diffraction grating to split the beam and record for each shot simultaneously a XAS from sample (Ni foil) and reference spectrum.

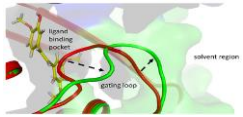
Proof of principle demonstrated; for application need to improve energy resolution



Monitoring ultrafast ligand release using a photoswitchable anticancer drug

J. Standfuss, PSI

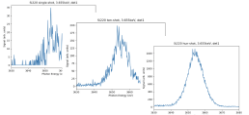
Continuation of the first beamtime (March 2020) now targeting ultrafast (sub-ps) dynamics. First SwissFEL SFX beamtime at 100 Hz. Covered 9 orders of magnitude in time delay points, from ultrafast chemical isomerization to biological structural changes.



Tender X-ray Spectrometer Comissioning

P. Juranic, PSI

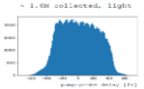
Goal was to commission a Tender X-ray Spectrometer (von hamos geometry) covering spectral information in 2-4 keV range for users and machine, complementing PSSS' 4-13 keV range.



The ultrafast time-resolved activation mechanism rhodopsin

V. Panneels, PSI

Study of the ultrafast isomerization of the chromophore retinal in rhodopsin, one of the fastest processes in biology.
Collected about 250k indexed images with a continuous scan over 1 ps.

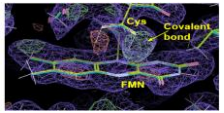


Exact arrival times retrieved by the Spectral Encoder timing tool with fs accuracy

Photocatalytic mechanism of covalent bond formation in LOV flavoprotein captured with SFX

P. Nogly, ETHZ

Resolved the structure for 11 timepoints of the photocycle of the LOV protein module that acts as translator of the incoming light into protein structural changes, with 1.5 Å resolution.

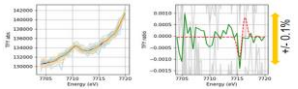


Found clear evidence of covalent thioether bond formation and deformation of FMN planar geometry.

Clarifying the microscopic mechanism of all optical magnetization switching

U. Staub, PSI

First spectroscopy experiment (XAS and XES) at FLEX, the second endstation of the Alvra instrument. First use of the Spectral Encoder timing tool for monochromatic beam



Reached an extremely high S/N ratio (0.1%) but did not observed pump-probe signal. Analysis ongoing, but this result can be explained with the absence of any electronic contribution to the magnetization dynamics.

- **8 beamtimes** (7 user and 1 internal)
- ~80% "normal" machine parameters