PAUL SCHERRER INSTITUT

PSI



Experimental station Bernina :: SwissFEL :: Paul Scherrer Institut

# Bernina status and objectives

SwissFEL Performance Workshop 2022

# Who we are - now

**Scientists**

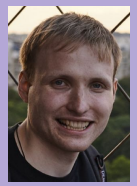
**Roman Mankowsky**

**Paul Beaud**

**Mathias Sander** **HL**

**Postdocs**

**Xin Liu**



**Danylo Babich**

*SNF/ANR project*

**Techs**

**Alex Oggenfuss**

**80%**

**Robert Kälin**

**20%**

**Aramis diagnostics**

**Christopher Arrell**

**Matrix**

**Yunpei Deng (LNO)**

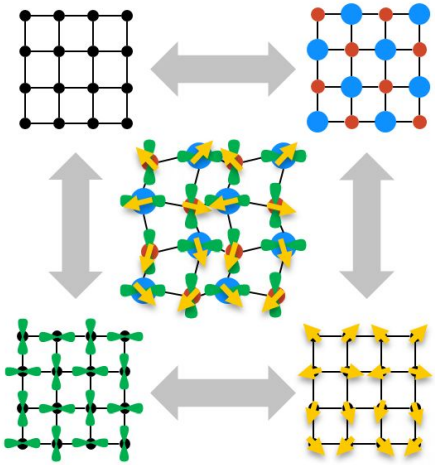
- Laser

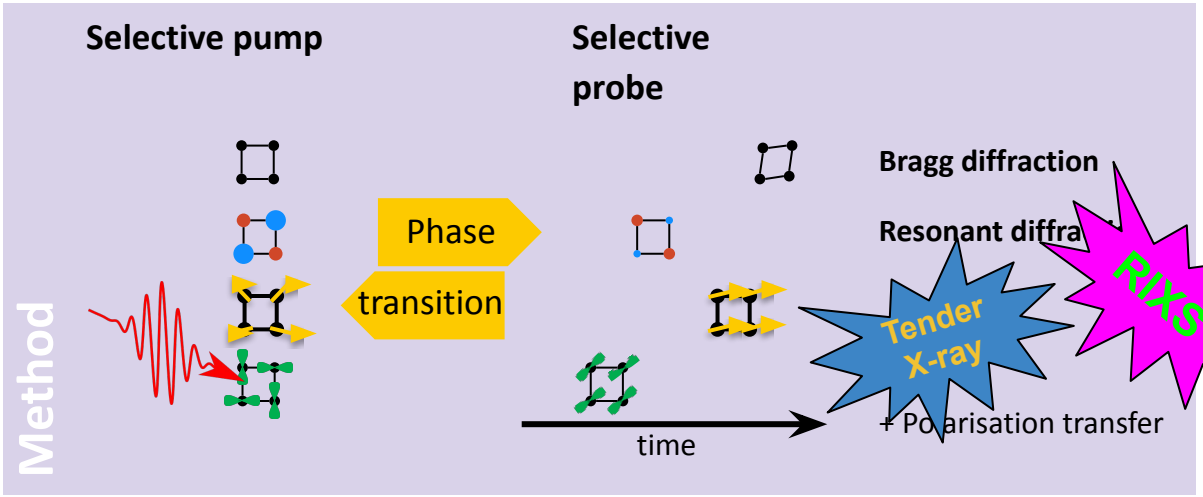
**Thierry Zamofing (Controls)**

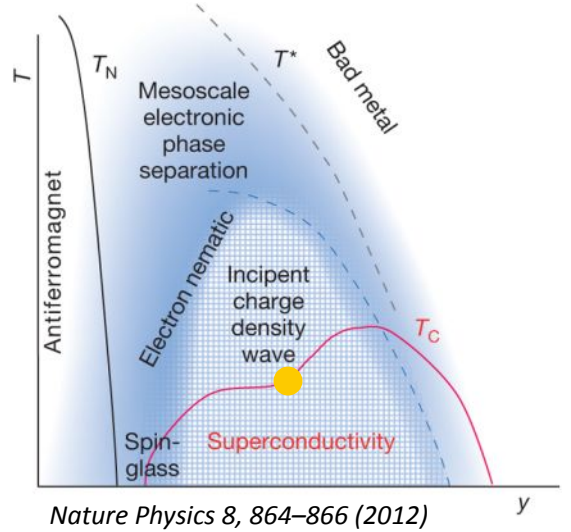
- Motion control

# What is our goal?

Understanding of complex interactions
creating functional materials
by unravelling their degrees of freedom on the time domain.

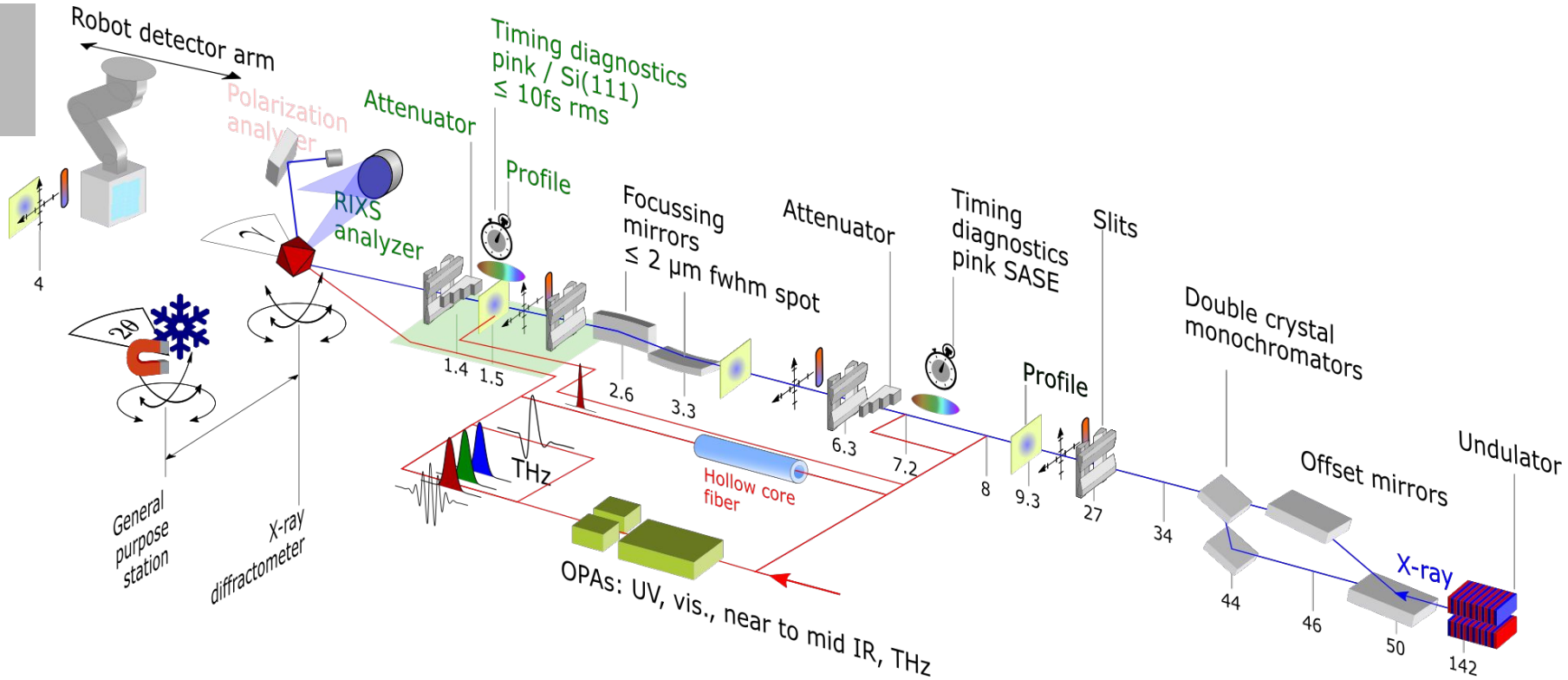





*Nature Physics 8, 864–866 (2012)*

# What do we have to do this?

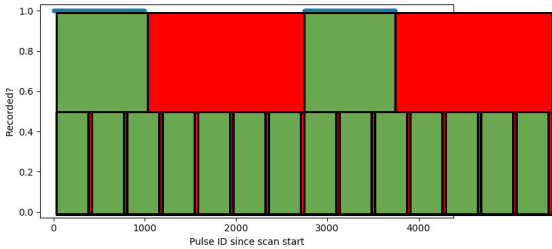


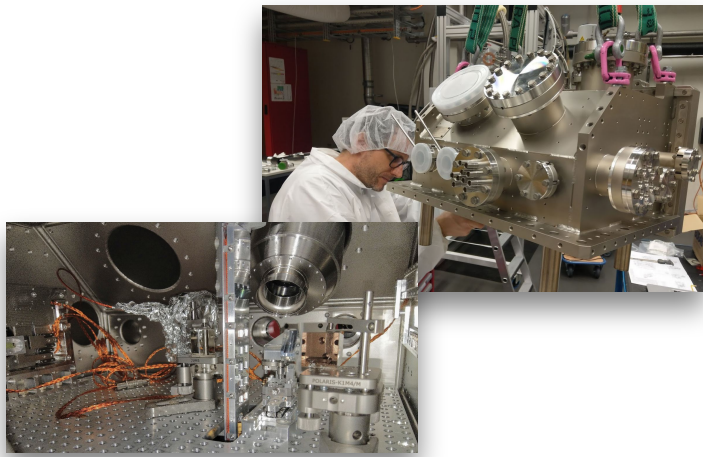
# Experience with recent upgrades

- Relatively stable operation and efficient data acquisition at 100 Hz.
  - *regular restart of subsystems required*

- Reproducible operation at narrow bandwidth (1.2-1.5 ‰).
  - *remaining spatial chirps*
  - *Difficult control/characterisation of pulse length → ATHOS x-talk*

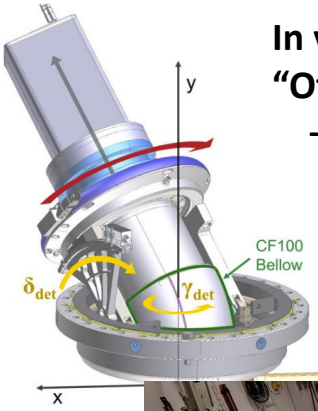
- Robust timing tool operation in new upstream diagnostics vacuum chamber.
  - *further streamlining of alignment*



# New upgrades in 202

just works!

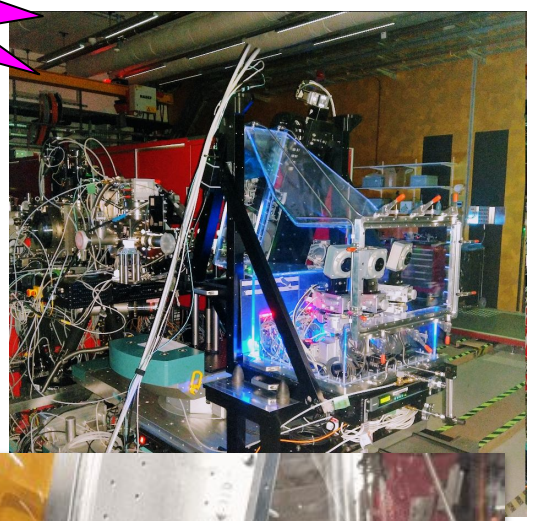


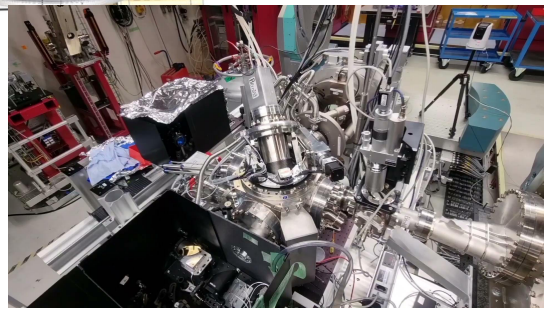

**In vacuum detector arm "Ottifant"**

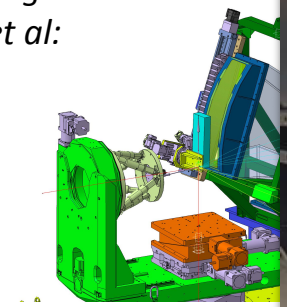
- **Allows in-HV detector distance > sample chamber.**

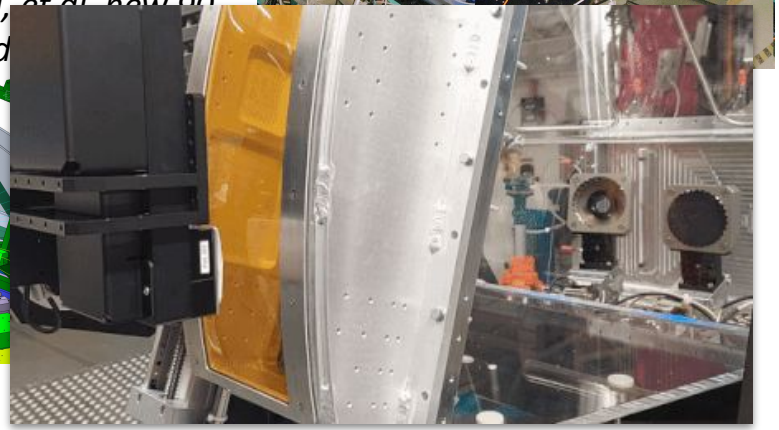
**RIXS analyzer**

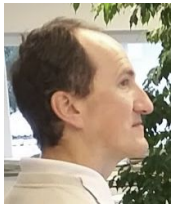
*Collaboration with Giulia Mancini, Rolf Versteeg, Majed Chergui, EPFL*
*Assembly, control, electronics: Alex Oggenfuss, Robert Kälin, Lukas Schmid, Thierry Zamofing, Claude Pradervand, et al. new 90 deg JF detector: Ald et al:*











**Design and Construction: AIK**
*Pirmin Böhler, Achim Ammon, Renzo Rotundo, Stefan Maag*

# Experiments in 2021 – January to June

**User run 5**

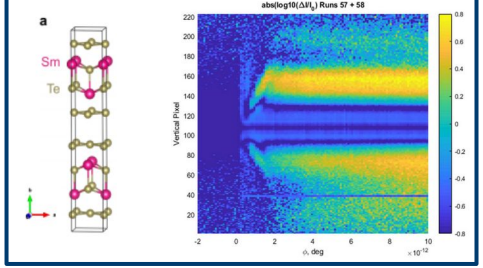
Jan Feb Mar Apr May Jun

100% remote

**Effect of topological defects in the light-Induced Charge Density Wave of LaTe3**

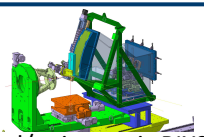
***M. Trigo et al. , SLAC***

Charge density wave control observed as function of crystal direction in diffuse ordering signals. Extended study of excitation conditions at high rec space resolution. Experiment was performed ***fully remotely.***

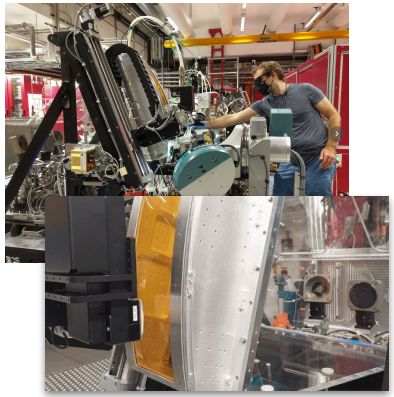


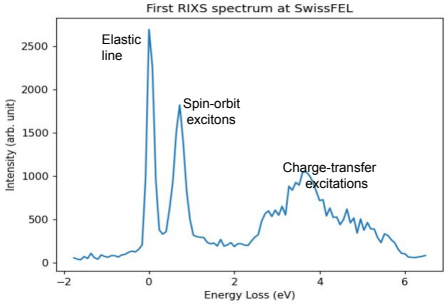

**Ultrafast formation of quasimolecular dimer orbitals in the honeycomb Mott insulator α-Li2IrO3**

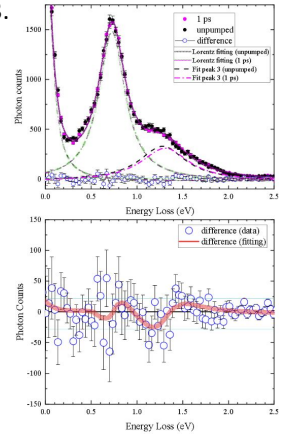
***M. Chergui et al., EPFL***



First commissioning of Bernina/EPFL hard X-ray RIXS analyzer, measured good signal/noise static RIXS spectrum, Dir. disc. experiment on exciton control in the iridate honeycomb Mott insulator α-Li2IrO3.





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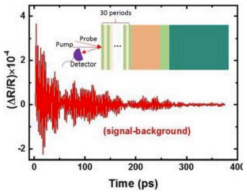
# Experiments in 2021 – July to December

## User run 6

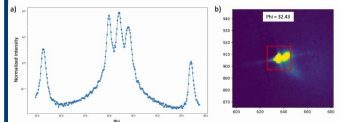
Jul | Aug | Sep | Oct | Nov | Dec

**Fourier-transform inelastic X-ray scattering of phonon quantum coherent coupling**

***Y. Cao et al. , Argonne***



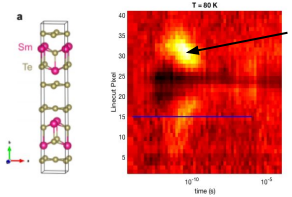

Study of transient coupling of laser excitation into superlative phonons, resembling Quantum coherent coupling

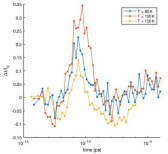


**Observing non-equilibrium domain dynamics of competing order with coherent x-rays**

***S. Teitelbaum et al. Arizona State Univ.***

Recovery of charge density waves in LaTe3 after quench was followed in low ΔQ intensity.

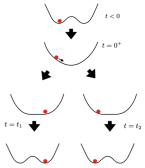


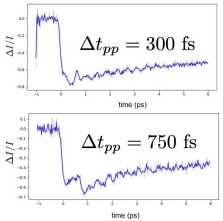
Thermal dependence of recovery observed.

**Directly observing the ultrafast coherent control of phase in a charge density wave**

***S. Johnson et al. Zurich local***

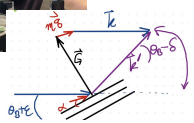


Controlling CDW recovery from soft mode by temporal separation of 2nd pump pulse. Repeated measurement showed different dynamics, interpretation in progress.

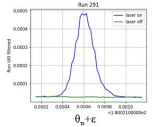



**Higher-order X-ray-Optical Sum-Frequency Generation**

***M. Fuchs, D. Reis et al. Univ. of Nebraska/SLAC National lab***



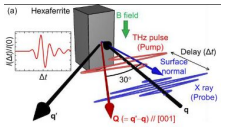
Investigation of higher-order X-ray-optical sum-frequency generation (XSFG). In XSFG an X-ray and an optical wave are mixed with the help of the crystal lattice.



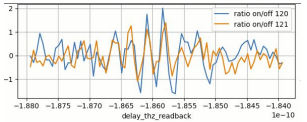
Phase matching ~0.2 mdeg

**Ultrafast structural dynamics of a strong electromagnon resonance in multiferroic hexaferrite**

***Ueda, Staub et al., PSI***




Studying lattice response due to excitation of an electromagnon in a cycloidic magnetic superstructure.



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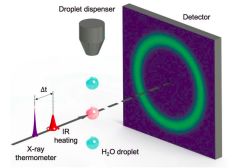
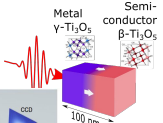
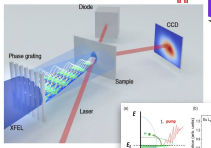
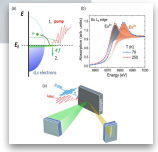
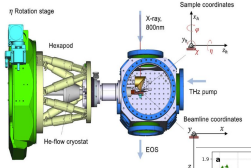
# First publications

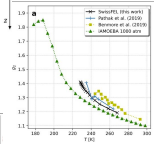


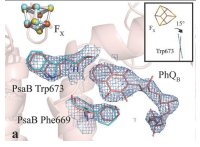








Pathak, Harshad, Alexander Späh, Niloofar Esmaeildoost, Jonas A. Sellberg, Kyung Hwan Kim, Fivos Perakis, Katrin Amann-Winkel, et al.
**“Enhancement and Maximum in the Isobaric Specific-Heat Capacity Measurements of Deeply Supercooled Water Using Ultrafast Calorimetry.”**
*Proceedings of the National Academy of Sciences* 118, no. 6 (February 9, 2021): e2018379118. https://doi.org/10.1073/pnas.2018379118.

Mariette, C., M. Lorenc, H. Cailleau, E. Collet, L. Guérin, A. Volte, E. Trzop, et al.
**“Strain Wave Pathway to Semiconductor-to-Metal Transition Revealed by Time-Resolved X-Ray Powder Diffraction.”**
*Nature Communications* 12, no. 1 (February 2021): 1239. https://doi.org/10.1038/s41467-021-21316-y.

Rouxel JR, Fainozzi D, Mankowsky R, Rösner B, Seniutinas G, Mincigrucci R, *et al.*
**“Hard X-ray transient grating spectroscopy on bismuth germanate”**
*Nature Photonics*. 2021; 15: 499-503. https://doi.org/10.1038/s41566-021-00797-9.

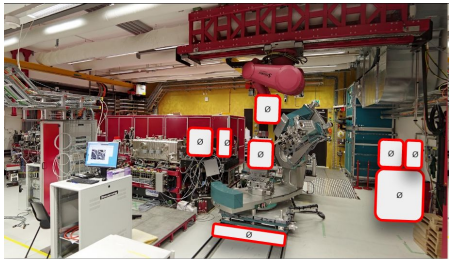
Mardegan JRL, Zerdane S, Mancini G, Esposito V, Rouxel JR, et al.
**“Ultrafast electron localization in the EuNi2(Si0.21Ge0.79)2 correlated metal”**
*Physical Review Research,* 2021; 3, 033211. https://doi.org/PhysRevResearch.3.033211

Mankowsky, R., Sander, M., Zerdane, S., Vonka, J., Bartkowiak, M., *et al.*
**“New insights into correlated materials in the time domain - combining far-infrared excitation with x-ray probes at cryogenic temperatures.”**
*Journal of Physics: Condensed Matter*, *33*(37), 374001 (16 pp.). https://doi.org/10.1088/1361-648X/ac08b5

Esmaeildoost, N., Pathak, H., Späh, A., Lane, T. J., Kim, K. H., Yang, C., … Sellberg, J. A. (2021).
**“Anomalous temperature dependence of the experimental x-ray structure factor of supercooled water.”**
*Journal of Chemical Physics*, *155*(21), 214501 (11 pp.). https://doi.org/10.1063/5.0075499

Keable, S. M., Kölsch, A., Simon, P. S., Dasgupta, M., Chatterjee, R., Subramanian, S. K., … Kern, J. (2021).
**“Room temperature XFEL crystallography reveals asymmetry in the vicinity of the two phylloquinones in photosystem I.”**
*Scientific Reports*, *11*, 21787 (14 pp.). https://doi.org/10.1038/s41598-021-00236-3

# Performance status Bernina



**Beamline HW**

- completion of baseline components
- remaining completions/implementations/fixes
- addition of smaller scale new components

**Pump laser source**

- Experiments performed over most designed wavelen range.
- ongoing developments
  - phase stable THz source
  - short-pulses tunable vis source

**Operation**

- Experimental techniques are approaching desired methods
- work intense, relies much on returning Users, repeate experiments

***continuing improvements and closing up to peer facilities***

***<u>requires</u>***

- ***completion of systems***
- ***sustainable routine solutions***
- ***efficiency in routine activities***

# Challenges for the coming year

**Data & controls**

- split of architecture for online data viewing
- long lag in configuration updates and removal of workarounds
- sustainable data storage and archiving
- versatile scalable online data processing framework
- data acquisition recording all relevant data
- finalisation of implementations for 100 Hz operation.
- **Robustness and support of centralized daq systems.**

**Da FEL**

- pointing stability often insufficient / spatial chirp
- systematic parameter changes at 50 Hz
- reproducibility and robustness of tuning results
- incorporation and standardisation of optimisation to more diagnostics and single pulse data
- better understanding of the FEL
- better understanding of pulse duration

**FEL/Laser timing**

- rediscussion of timing status and timing/sync. distribution systems
- Understanding and closing of a gap between expected and yet established time resolution

**All**

- grinding out long known issues with various devices and procedures
- **Work towards better collaboration and goal-orientation, solve ever lasting conflicts**

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# Outlook

**Towards sustainability and efficiency**

- online data analysis
  - bs streams/including JF data
  - bs pipeline
- motion control
  - fixing longstanding issues
  - pulse-synchronous - motion
- data management
  - data file format
  - data archive/retrieval
- documentation
  - user logbook
  - hardware/software documentation
- FEL reproducibility
  - 50 Hz issue
  - ATHOS Crosstalk

**Ongoing developments**

- general use low T grazing incidence sample environment
- pump laser sources (phase-stable, tunable short pulse)
- wavefront sensor

**Thanks everyone for continuos help and developments!**