**Scientific Opportunities with SwissFEL**

*Wednesday, 23.08.2017, CICG: Room 14*

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<tr>
<th>Time</th>
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<tbody>
<tr>
<td>14:00</td>
<td>701</td>
<td><strong>SwissFEL: The New Femto Second X-ray Laser Source at PSI</strong></td>
<td>Luc Patthey, Paul Scherrer Institut, Villigen</td>
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<td>The new X-Ray Free Electron Laser (SwissFEL) facility at PSI has produced its first FEL light at 4.1 nm and will deliver 20 fsec pulses of coherent x-rays in the wavelength range 0.1 to 7 nm, with extremely high peak brightness. These characteristics will provide opportunities for new experiments in chemistry, solid state physics, biology and materials science. The Aramis hard x-ray FEL branch will begin normal user operation in 2018 with two dedicated end-stations. The Alvra end-station is focused on using time resolved x-ray spectroscopy (XAS/XES) to investigate femtosecond chemical processes and time-resolved x-ray diffraction for serial femtosecond crystallography (SFX) experiments on proteins. The Bernina end-station is designed for femtosecond time-resolved pump-probe hard x-ray diffraction and scattering experiments in condensed matter systems. The Athos soft x-ray FEL branch is in the early phase of construction and should provide its first FEL light for experiments in 2020. After a brief status report, the presentation will focus on novel applications, the description of the fundamental aspects of the planned facility with an emphasis on the photonics part of the project.</td>
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<td>14:30</td>
<td>702</td>
<td><strong>Using X-ray Techniques to Investigate Ultrafast Chemical Dynamics</strong></td>
<td>Chris Milne, Jakub Szlachetko, Tom Penfold, Majed Chergui</td>
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<td>Time-resolved X-ray spectroscopy is a versatile tool for investigating both electronic and structural dynamics in functional chemical systems. By measuring both the X-ray absorption and X-ray emission signals simultaneously we obtain information on both the occupied and unoccupied electronic states of the sample, as well as structural information from both the near-edge and Extended X-ray Absorption Fine Structure (EXAFS) regions of the absorption spectrum. When combined with X-ray scattering techniques, which provide structural information on the system and its interaction with the environment, we can obtain unparalleled details on the ultrafast dynamics of both energy flow and structural changes. In this presentation, I will show how we have developed these techniques at the Swiss Light Source and other X-ray facilities, and applied them to investigate ultrafast dynamics in photo-excited systems. I will present several examples of the kind of information that can be obtained on a large variety of samples, ranging from photoactive proteins in solution through to colloidal suspensions of semiconductor nanoparticles. I will conclude with a brief overview of the types of experiments we anticipate being able to perform at SwissFEL in the coming years.</td>
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<td>15:00</td>
<td>703</td>
<td><strong>New opportunities for molecular physics using high-harmonic and FEL light sources</strong></td>
<td>Hans-Jakob Wörner (i)</td>
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### 15:30 704

**Serial femtosecond crystallography of two-dimensional protein crystals on solid supports: state of the art and perspectives**

Cecilia Casadei 1, Anton Barty 2, Bill Pedrini 1, Celestino Padeste 1, Guido Capitani 1, Karol Nass 1, Leonardo Sala 1, Mark Hunter 3, Matt Coleman 4, Matthias Frank 4, Xiao-Dan Li 1  
1 Paul Scherrer Institut, 2 DESY / CFEL, 3 LCLS, 4 LLNL / UC Davis

Ultra-short, ultra-bright X-ray pulses from Free Electron Lasers are a viable tool for observing diffraction from two-dimensional (2D) crystals, unlike synchrotron-based data collection, extending the possibilities of structural determinations in membrane proteins. Using serial diffraction frames from bacteriorhodopsin 2D crystals we extended the resolution limit of zero-tilt data to 4 Å (detector-limited) by summing equivalent portions of images, and developed a method to reconstruct diffraction intensities along Bragg lines, from which structural information can be gained. Using these methods a data collection strategy (100000 -200000 images at high tilt angles) allowing to detect structural changes in the length-scale of a few Å in a pump-probe configuration can be envisaged.

### 15:45 705

**Spectrometers for Photon Diagnostics at SwissFEL**

Jens Rehanek 1, Mikako Makita 1, Christian David 1, Gediminas Seniutinas 1, Jakub Szlachetko 2, Joanna Czapla-Masztafiak 3, Christopher Milne 1, Luc Patthey 1, Pavle Juranić 1  
1 Paul-Scherrer Institute, 2 Institute of Physics, Jan Kochanowski University, 3 The Henryk Niewodniczanski Institute of Nuclear Physics

SwissFEL, like other SASE-based x-ray FEL facilities, requires the monitoring of the photon spectrum (photon energy and intensity) on a shot-to-shot basis for machine optimization and for experiments. In order to cover the Hard X-ray range variations (4 - 15 keV) for the Aramis beamline, the Photon Single Shot Spectrometer has been designed to measure the spectrum with high resolution over the bandwidth of the SASE FEL beams. Additionally, a new idea and first results of a proof of-principle experiment for an online device in Tender X-ray regime (2 - 4 keV) will be shown and discussed. The concept is based on dispersive von-Hamos geometry composed with a scattering sample to look at the elastic scattering spectrum.

### 16:00 706

**Design of the interaction chamber for ACHIP at PSI**

Nicole Hiller, Rasmus Ischebeck, Lenny Rivkin, Eugenio Ferrari, Franziska Frei, Micha Dehler, Eduard Prat Costa, Simona Bettoni, Sven Reiche, Marco Calvi, Paul Scherrer Institut

ACHIP is an international collaboration, funded by the Gordon and Betty Moore Foundation, whose goal is to demonstrate that laser-driven accelerator on a chip can be integrated to fully build an accelerator based on dielectric structures. PSI will provide access to the high brightness electron beam of SwissFEL to test structures, approaches and methods towards achieving the final goal of the project. In this contribution we describe the design of the interaction chamber, in collaboration with EPFL, to perform the proof-of-principle experiments. We will present the positioning system for the samples, the magnets focussing the beam to sub-micrometer dimensions and the diagnostics to measure beam properties at the interaction point.

### 16:15 707

**Superconducting Undulators for Porthos**

Marco Calvi, Thomas Schmidt, Sven Reiche, Eduard Prat Costa, Romain Ganter  
Paul Scherrer Institut

The next hard X-ray line (2025-2029) at SwissFEL, Porthos, is planned to further extend the photon energy of Aramis, reaching wavelength down to 0.03 nm. Harmonic lasing and inter-undulator chicanes will be implemented to meet this target. Nevertheless the undulator period length must decrease to 10 mm while the K value has to increase to 2.4 with a vacuum gap above 4 mm. These parameters cannot be achieved with conventional technology, neither with advanced permanent magnet cryogenic undulators: it requires the use of superconductors. An overview of this technology will be given, focused on recent Nb₃Sn experimental results but alternative approach, like bulk HTS superconductor, will also be discussed.

### 16:30

**Coffee Break**

### 19:00

**Transfer to Dinner**
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<tr>
<td>14:30</td>
<td>711</td>
<td><strong>Athos: The Soft X-ray Line of SwissFEL</strong></td>
<td>Marco Calvi, Thomas Schmidt, Sven Reiche, Eduard Prat Costa, Romain Ganter</td>
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<td>Paul Scherrer Institut</td>
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<td>15:00</td>
<td>712</td>
<td><strong>Femtosecond x-ray techniques: a window towards material control</strong></td>
<td>Steven Johnson, ETH Zürich</td>
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<td>15:30</td>
<td>713</td>
<td><strong>Time and spin resolved photoemission: A new look at ultrafast magnetism</strong></td>
<td>Yves Marc Acremann, Rafael Gort, Kevin Bühlmann, Andreas Vaterlaus, ETH Zürich</td>
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<td>16:00</td>
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<td><strong>Coffee Break</strong></td>
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<td>16:30</td>
<td>714</td>
<td><strong>Nonlinear electron-phonon coupling in doped manganites</strong></td>
<td>Vincent Esposito ¹, Michael Fechner ², Michael Foerst ², Paul Beaud ¹, Roman Mankowsky ², Urs Staub ¹</td>
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<td>² Max Planck Institute for the Structure and Dynamics of Matter, CFEL, Hamburg</td>
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## 16:45 715

**Investigating ultrafast magnetization dynamics with circularly polarized soft x-ray FEL radiation**

*Christian Stamm, ETH Zürich*

The planned SwissFEL ATHOS beamline features all necessary parameters for femtosecond time-resolved experiments in magnetism using x-ray absorption spectroscopy and circular dichroism: intense fs soft x-ray pulses with linear and circular polarization. An exemplary measurement investigates spin currents between two magnetic films separated by a spacer layer: the upper, fs laser pulse excited film launches a spin current which is detected in the lower layer. Such a structure did surprisingly show fs magnetization enhancement in the lower film. X-ray spectroscopy can be used in a unique way to quantitatively probe the spin and orbital moments separately for each layer with femtosecond resolution.

## 17:00 716

**Observing a phonon-driven structural phase transition in Sn$_2$P$_2$Se$_6$**

*Martin Kubli ¹, Matteo Savoini ¹, Vincent Esposito ², Lucas Huber ¹, Elisabeth Bothschafter ², Sergii Parchenko ², Gabriel Lantz ¹, Elsa Abreu ¹, Jochen Rittmann ², Makina Yabashi ³, Yoshikazu Tanaka ³, Tetsuo Katayama ³, Tadashi Togashi ³, Steven Lee Johnson ¹*

¹ Institute for Quantum Electronics, Physics Department, ETH Zürich ² Swiss Light Source, Paul Scherrer Institut ³ RIKEN SPring-8 Center

Sn$_2$P$_2$Se$_6$ is a ferroelectric semiconductor with interesting structural properties. In the temperature range between 193 and 221 K, just above the Curie-Temperature, an incommensurate phase emerges. This permanent structural modulation is believed to be the result of two coupled frozen phonon modes. In our experiment, we photoexcite the material and probe this structural modulation using ultrafast time-resolved x-ray diffraction and observe the dynamics of the two coupled modes across the phase transition. We found that the electronic excitation only couples indirectly via other phonon modes to these two coupled modes.

## 17:15 717

**Replicating the short-time recovery of a charge density wave state after photoexcitation**

*Martin Josef Neugebauer ¹, Tim Huber ¹, Matteo Savoini ¹, Sebastian Grübel ², Lucas Huber ¹, Teresa Kubacka ¹, Christian Dornes ¹, Elsa Abreu ¹, Martin Kubli ¹, Elisabeth Bothschafter ², Laurenz Rettig ², Jochen Rittmann ², Vincent Esposito ², Paul Beaud ², Gerhard Ingold ², Jure Demsar ³, Steven Lee Johnson ¹*

¹ Institute for Quantum Electronics, Physics Department, ETH Zürich ² Swiss Light Source, Paul Scherrer Institut ³ Physics Department, Universität Konstanz

We used ultrashort x-ray pulses to monitor the structural dynamics associated with the charge density wave (CDW)-state in K$_2$MoO$_3$ after photoexcitation. In a first experiment the response to different excitation fluences was investigated. Starting in a regime of coherent oscillations, increasing the excitation fluence leads to a complete melting of the ordered state. Remarkably, a further increase in fluence results in a short recovery of the CDW on a sub-picosecond time scale. In follow-up measurements, we could create a second recovery by applying another photoexcitation to the first one. An understanding of the microscopic mechanisms of this recovery may enhance our theoretical understanding of ultrafast CDW transitions in general.
Optically induced transient enhancement of a structural order parameter monitored via a FEL

Michael Porer ¹, Sergii Parchenko ¹, Martin Neugebauer ², Martin Kubli ², Milan Radovic ¹, Elisabeth Bothschafter ¹, Laurenz Rettig ¹, Sanghoon Song ³, Takahiro Sato ³, Awadesh Narayan ⁴, Nicola Spaldin ⁴, Michael Fechner ⁵, Steve Johnson ², Urs Staub ¹
¹ Paul-Scherrer Institut, ² Institute for Quantum Electronics, ETH Zürich
³ Linac Coherent Light Source, SLAC National Accelerator Laboratory,
⁴ Materials Theory, ETH Zürich,
⁵ Max Planck Institute for the Structure and Dynamics of Matter, CFEL, Hamburg

Ultrafast optical control of correlation-induced order parameters in complex materials is a key challenge en route to new functional materials. Here we employ above-bandgap femtosecond pulses with various wavelengths to excite EuTiO₃ out of its low-temperature antiferrodistortive equilibrium phase. Monitoring the subsequent transient intensity of distortion-induced superlattice reflections via 80-fs hard x-ray pulses at LCLS, we observe a transient increase of their intensities in a sub-ps time window. This represents an optically induced ultrafast increase of the structural order parameter, which stands in strong contrast to the reduction of the distortion with thermal heating in equilibrium. Preliminary DFT calculations identify 4f-hole-doping as possible driving force.