PAUL SCHERRER INSTITUT

PSI

Photonics Spring Workshop

SwissFEL ATHOS and SLS-2

10–12 April 2017

Abstract Book

Monday, 10.04.2017

Keynote session
09h00 – 12h30

Keynote 1: Storage Rings and FELs: Different horses for different courses
HASTINGS Jerome (SLAC)

The age of Free Electron Lasers is upon us. It is the time of discovery and the need to look for opportunities beyond a lot of x-rays in a short time. Thoughts on the use of multiple beams and multiple colors will be presented. The storage ring is not to be forgotten. The photon energy range between 2-5 keV with SLS 2.0 will now have a diffraction-limited source and opportunities to study quantum materials with unprecedented resolution will be possible. The 'whys' and 'hows' will be discussed. The concepts for studying disordered systems using both SWISSFEL and SLS 2.0 will also be touched upon.

Keynote 2: The emergence of metastable order outside equilibrium: time-evolution through electronic phase transitions in di-chalcogenides
MIHAILOVIC Dragan (Josef Stefan Institute)

The study of phase transitions in real time under nonequilibrium conditions is of fundamental interest in many areas of physics. A special category of recent fundamental and practical interest are transitions to metastable hidden states which occur under conditions of particle-hole asymmetry. While such behavior has been invoked in cosmology to explain Baryogenesis, it is not commonly observed elsewhere. In the quasi-two-dimensional dichalcogenide, 1T-TaS_2, conditions for the formation of an electronically textured hidden "false vacuum" state are created by femtosecond laser photoexcitation and the resulting state is distinct from others states of the system in the equilibrium phase diagram. Femtosecond photoexcited low temperature scanning tunneling microscopy reveals long range order and a remarkable quantum duality of polaron behavior with a vivid real-space illustration of the interplay of Mott physics, Anderson disorder localization, orbital stacking order and collective polaron behaviour. The current system – and the concept of metastable states created by charge injection - are of practical interest for ultrafast low-energy low-temperature non-volatile

memory devices with immediate applications in cryogenic computing.

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Keynote 3: Fast and ultrafast magnetic Phenomena
EISEBITT Stefan (Max-Born-Institut Berlin)

Dynamic magnetic phenomena occur over many orders of magnitude in time and length scale, in particular including the spatial scale from nanometers to atomic distances and temporal scales down to a few femtoseconds. X-rays do not only provide exquisite sensitivity to magnetic moments in an element specific way, but due to the increased coherence approaching the diffraction limit and the possibility to create ultrashort pulses allow to access in particular fast dynamics on small lengthscales.

I will discuss how these improved source properties can be put to good use to study fundamental questions in magnetism, e.g. via time pump-probe resonant scattering and imaging approaches.

Machine PSI session
13h30 – 14h30

PSI 1: Design and operation modes of Athos, the soft X-ray beamline of SwissFEL
PRAT Eduard (Paul Scherrer Institut)

Athos, the soft X-ray beamline of SwissFEL, is expected to provide FEL light to scientific users by 2021 for radiation wavelengths between 0.65 and 5 nm. Athos will employ short undulator modules based on APPLE technology with the capacity to generate special configurations such as transverse gradients and continuous taper. A unique feature of Athos is the installation of integrated chicanes between the undulator modules, which will allow novel operating modes besides the standard SASE operation. For instance, Athos will significantly reduce the spectral bandwidth of the FEL signal without the need of any seeding technique, and will generate high-power and ultra-

short FEL pulses in the terawatt-attosecond level. This talk will give an overview of the Athos design and its distinctive operation modes.

PSI 2: SLS-2 storage ring upgrade
STREUN Andreas (Paul Scherrer Institut)

The upgrade scenario for the Swiss Light Source is based on a complete exchange of the existing storage ring by a new one providing forty times lower emittance. The new lattice is a 12-periodic structure composed from 7-bend achromatic arcs and 5½ m long straight sections. Bending magnets with longitudinal field variation up to 6 Tesla peak field and anti-bends (i.e. dipoles with reversed field) form a novel type of lattice cell in order to realize an equilibrium emittance of only 138 pm rad at 2.4 GeV beam energy within a comparatively small circumference of 290.4 m.
A conceptual design report (CDR) is in preparation and will be issued in summer 2017. Its main contents are a proof of feasibility with regard to beam physics and technology, and a detailed cost estimate and time schedule for the upgrade, which is planned for the years 2021-24. An overview of the CDR status will be given, covering design of the lattice and of critical components, and the required modifications of the storage ring tunnel and the beam lines.
Finally, the recent concept for an extended upgrade may be discussed, which targets a diffraction limited hard X-ray source. It would be realized as a new ring of about 450 m circumference and 20 pm emittance, which is filled from the existing storage ring.

SCES/CM PSI session
15h00 – 16h30

PSI 3: Condensed Matter Spectroscopy on Emerging Materials @ SLS-2
SCHMITT Thorsten (Paul Scherrer Institut)

The Swiss Light Source (SLS) is currently offering several synchrotron based condensed matter spectroscopy techniques that are powerful tools for understanding the basic materials properties of correlated and other emerging materials. Besides several beamlines for X-ray Absorption Spectroscopy (XAS) the SLS features also specialized beamlines for Resonant Inelastic X-ray Scattering (RIXS) and Resonant Soft X-ray Diffraction (RSXD) as well as Angle Resolved Photoemission Spectroscopy (ARPES) with and without spin

resolution in the VUV and soft X-ray energy range.
The diffraction limited storage ring upgrade of the SLS to SLS-2 will allow significantly improving and extending this set of advanced synchrotron radiation based spectroscopy instruments in terms of their energy and spatial resolution. Such improved and new tools will not only further the understanding but also enable the control of emerging materials for future devices. We will illustrate the science opportunities at SLS-2 on examples of interface phenomena in semiconductor and oxides materials, different classes of topological materials, unconventional superconductors as well as correlated materials with intermediate or strong spin-orbit coupling containing 4d and 5d transition metals, respectively.

PSI 4: Time-resolved soft x-ray techniques for condensed matter at SwissFEL

GERBER Simon (Paul Scherrer Institut)

The SwissFEL x-ray free-electron laser will feature two undulator branches ARAMIS and ATHOS, which will cover the tender/hard (2 – 12.4 keV) and soft (240 – 1'930 eV) x-ray regime, respectively. Commissioning of ARAMIS is under way, first pilot experiment will be conducted by the end of 2017 and regular user operation will begin in autumn 2018. In parallel, the ATHOS project has started at the beginning of this year and first accelerator components are being already installed. Now, one of the most urgent tasks is to settle on the techniques and respective experimental stations that will be available when ATHOS becomes operational. Related is also the question what requirements these instruments will have in terms of beamline/diagnostic parameters.
We will present an overview of the capabilities of ATHOS in combination with the unique CHIC operating modes, including some details on the expected beamline layout and specifications, as well as pump laser and detector performance. Secondly, the talk is also meant to provide a starting point for discussions in the break-out sessions by presenting several examples of approaches that may uniquely address open questions in condensed matter physics. These will cover a range of techniques, such as time-resolved resonant elastic and inelastic soft x-ray scattering (trRSXS/trRIXS), time-resolved x-ray magnetic circular dichroism (trXMCD) or employing nonlinear x-ray optics. We will conclude with a list of open questions that will be resolved during the break-out sessions.

PSI 5: Opportunities for magnetism research with SLS-2 and ATHOS

PIEMONTEZE Cinthia (Paul Scherrer Institut)

In this talk I will present examples from current magnetism research carried out at Swiss Light Source. The topics range from static and dynamic investigations on magnetic nanoparticles, molecular magnets, multiferroics, transition metal oxides heterostructures, artificial spin ice systems, skyrmions and spin waves, which are studied by a variety of X-ray-based techniques such as X-ray microscopy, X-ray absorption spectroscopy, X-ray scattering and angular resolved X-ray photo-emission. We will address the current status and important open scientific questions which we may attempt to answer with the new opportunities arising with SLS-2 and/or ATHOS. The aim of the talk is to stimulate discussions that will be further developed during the break-out section on magnetism.

Tuesday, 11.04.2017

Keynote session
09h00 – 12h30

Keynote 1: Recent strides in the characterization of solid catalysts with synchrotron radiation
WECKHUYSEN Bert (Utrecht University)

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Keynote 2: Probing Catalysis in Real Time
NILSSON Anders (Stockholm University)

In heterogeneous catalysis, reactants adsorbed on surfaces are converted to products, which eventually desorb via various intermediates. The transition state separates reactants and intermediates from products and the free energy required to reach it determines the kinetics of an elementary chemical reaction. Many surface reaction intermediates are, however, transient species with a short residence time and the population of species in the transition state region is near-zero making their observation a challenge during steady state conditions. Ultrafast pump-probe techniques have, however, opened up opportunities by promoting a sufficient population of molecules in transient states to allow detection on short time scales. Here recent results on probing chemical reactions on surfaces using X-ray free-electron lasers LCLS (Linac Coherent Light Source) at SLAC National Accelerator Laboratory) will be presented. Four examples will be shown CO desorption, Oxygen activation, CO oxidation and CO hydrogenation on Ru(0001). We demonstrate that both transient intermediates and the transition state region can be detected in surface chemical reactions. I will describe my vision of the future development of this field where Swiss FEL can play an important role.

Keynote 3: X-ray microscopy: transformational opportunities with the next generation of light sources

JACOBSEN Chris (Argonne National Laboratory)

We are in an era of fantastic new opportunities in x-ray science using both quasi-time-continuous and pulsed x-ray sources. These opportunities are particularly exciting for imaging, since many imaging methods require coherence and are presently flux limited. With today's sources, one can image cells and integrated circuits at sub-20 nm resolution, adding chemical imaging in 3D, or image objects as large as whole mouse brains. What might we as a community be able to achieve in the future? And what imaging methods and sources are matched to which scientific goal? Some challenges and opportunities are put forward, knowing well that predicting the future is difficult but inventing the future is our privilege!

Keynote 4: Directions for Synchrotron Macromolecular Crystallography

STUART David (University of Oxford)

Macromolecular crystallography (MX) has been a major success story for synchrotron radiation. Biology has been transformed by a comprehensive atlas of structural information and structure lies at the heart of much of the quest for new therapies for human and animal disease. Conversely MX has acted as an exemplar and driver of what can be achieved by careful optimisation of workflows and automation, providing lessons that are being exported to other types of beamlines. Advances have come across the board form X-ray optics and detectors to software and data management.
As of today the method is an order of magnitude more productive (in terms of structures deposited) than either NMR or electron microscopy, the other big beasts delivering atom level structural detail. Nonetheless the times are changing. I will look at where we are, how things have changed over recent years, what the opportunities and threats seem to be and where we might be in a few years.

Machine PSI session
14h10 – 15h10

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Chemistry/spectroscopy PSI session
14h10 – 15h10

PSI 1: Time-resolved soft x-ray techniques for chemistry and biology at SwissFEL

MILNE Christopher (Paul Scherrer Institut)

The SwissFEL X-ray free electron laser consists of two undulator branches: the Aramis branch covering the tender and hard X-ray photon energies (2-12.4 keV) and the Athos branch covering the soft X-ray photon energies (240-1930 eV). Commissioning of Aramis has begun, with Pilot Experiments planned for 2017 and User Operation in 2018. Installation of the first Athos accelerator components has started and an extensive scientific case has been established. One of the remaining tasks ahead is to establish the experimental stations that will be available at Athos and what beamline/diagnostic parameters will these instruments require ? This talk will present an overview of the Athos capabilities, with emphasis on the flexible operation modes allowed by the innovative CHIC design. It will also include some details on the expected beamline layout and specifications, pump laser source, and detector performance. To provide a starting point for the discussions in the break-out sessions several examples of experiments and instruments from other FEL facilities will be presented, covering a range of research including photochemistry and biology, nonlinear X-ray techniques, and scattering/imaging. The talk will conclude with a list of open questions to be resolved during the breakout sessions.

PSI 2: Chemical spectroscopy of functional materials under operando conditions

NACHTEGAAL Maarten (Paul Scherrer Institut)

Chemical spectroscopy provides information about the electronic and geometric structure of an element of interest within materials used in catalysis, fuel cells, batteries, solar cells etc. as well as biological and geological samples. SLS beamlines currently provide a wide range of *ex situ* and *in situ* chemical spectroscopic techniques with a spatial resolution ranging from millimeters to nanometers and time resolution from minutes to picoseconds. The main scientific questions addressed with chemical spectroscopy are typically related to the structure-performance relationships, the nature of the active site, the identification of true intermediate species in the catalytic cycle and the reasons for material deactivation.

Relevant chemical processes happen on different length scales, ranging from the atomic scale to the nanometer and micrometer scales and might include particle growth, diffusion of elements at the interface, formation of new phases etc. Time scales of chemical processes typically range from the microsecond to hour scales, whereas photochemical processes can be faster. To look at these relevant length and time scales different SLS beamlines, including the superXAS, microXAS, PHOENIX, PolLux, VUV, SIM and Adress beamlines, continuously further develop chemical spectroscopic techniques.

The SLS-2 upgrade will result in an extension of the energy range, in higher flux density, and/or better spatial, spectral and time resolution for the chemical spectroscopy beamlines. This talk will give an overview of the current status and new possibilities of chemical spectroscopies at SLS-2 and provides an outlook on how these might contribute to relevant challenges in chemistry and energy research and development.

Wednesday, 12.04.2017

MX/imaging PSI session
09h20 – 10h20

PSI 3: Time-resolved Serial Crystallography using Synchrontrons and X-ray Lasers

STANDFUSS Joerg (Paul Scherrer Institut)

In 2017 the Swiss Free Electron Laser (SwissFEL) will start its operation at the Paul Scherrer Institute. Serial femtosecond crystallography (SFX) using such X-ray free-electron lasers (XFELs) is a powerful method to determine radiation damage free high-resolution structures and to study protein dynamics at room temperature.

One of the current bottlenecks in XFEL science is that many facilities are still under construction and, even when they will be finished, access will likely remain scarce. In this presentation I will describe how we have adapted high viscosity injector systems to carry out routine room-temperature serial millisecond crystallography (SMX) experiments at synchrotron sources (1, 2), where beamtime is more abundant. Based on these results we improved density and homogeneity of crystal preparations for efficient time-resolved data collection at the Spring-8 Angstrom Compact free electron Laser (SACLA) and Linac Coherent Light Source (LCLS), XFEL sources (3, 4). A series of 15 structural snapshots of the light-driven proton pump bacteriorhodopsin (bR) obtained with pump probe delays in the pico- to millisecond range demonstrate the feasibility of using sample efficient high viscosity injectors to determine three-dimensional molecular movies of membrane proteins in a native like environment.

References

1. Nogly P, et al. (2015) Lipidic cubic phase serial millisecond crystallography using synchrotron radiation. *IUCrJ* 2(Pt 2):168–176.
2. Weinert T, et al. Serial millisecond crystallography for routine room-temperature structure determination at synchrotrons. *under consideration*
3. Nango E, et al. (2016) A three-dimensional movie of structural changes in bacteriorhodopsin. *Science* 354(6319):1552–1557.
4. Nogly P, et al. (2016) Lipidic cubic phase injector is a viable crystal delivery system for time-resolved serial crystallography. *Nature Communications* 7:12314.

PSI 4: Exploring new imaging frontiers with next generation light sources: smaller, faster, better, ... and multi-modal

SCHLEPUETZ Chris (Paul Scherrer Institut)

The promise of next generation light sources featuring diffraction limited storage rings is bright and clear: An increase in source brilliance by nearly two orders of magnitude. This directly translates into x-ray beams with a much larger coherent flux and strikingly better focusing capabilities. While the total x-ray flux from insertion devices or bending magnets remains essentially unchanged, the boost in the source brilliance means a drastic increase in the number of useful photons that can be delivered to the sample in most cases, especially when small beam spots and highly coherent radiation are required. In this talk, we will explore the consequences and opportunities that these new beam properties represent for imaging applications, both in terms of the natural extension and upgrades of existing imaging programs currently in operation at the Swiss Light Source, as well as the potential to explore new approaches and to combine techniques that are so far difficult to interface. We will present examples of the current state of the art in imaging activities at SLS, together with an outlook into what types of new and challenging science cases the SLS-2 machine upgrade will enable us to address.