July 22, 2018

***Workshop on Advances in XAFS Experimental Techniques: Bridging The Light Source Generations***

Organized by **Hiroyuki Oyanagi** (KEK)

Small hall (Aula Mala), 9:00-16:20, on-site registration from 8:00

*09:00* *XAFS Opportunities at the 4th GEN Light Sources*
**Konstantin Klementiev** (MAXIV)

*09:35* *XAFS for real-time chemical speciation at SLS 2*
**Maarten Nachtegaa**l (SLS)

*10:10* *Coffee*

*10:40* *Advanced XAS Opportunities at ESRF-EBS*
**Sacura Pascarelli** (ESRF)

*11:15* *Future of RIXS at ESRF-EBS*
**Pieter Glatzel** (ESRF)

*11:50* *Lunch*

*12:50* *Opportunities in polarization-dependent spectroscopy at APS-U*
**Daniel Haskel** (ANL)

*13:25* *Opportunities & Challenges in Nanoprobe Spectroscopy at SIRIUS*
**Narcizo Marques Souza Neto** (LNLS)

*14:00* *Recent progress in XAS and XMCD at SPring-8 towards the ultra-low emittance light source*
**Motohiro Suzuki** (JASRI)

*14:35* *Status & Future opportunities of European XFEL*
**Christian Bressler** (European XFEL)

*15:15* *Panel Discussion on Scientific Opportunities in XAFS Research at the 4th GEN LSs*

*16:20* *Closing*

About the workshop

*The advent and privileges of the 4th GEN light sources are high brilliance and transverse coherence that allows scientific opportunities made possible use of (1) focused beam (nanobeam), (2) uniform phase wavefronts and (3) ultra short pulses (100 fs). These superior capabilities are utilized individually or in combination allowing going beyond the current limitations toward new x-ray spectroscopy science such as spectro-imaging and photon-correlation spectroscopy for studies of slow dynamics in disordered materials. Although the power density is similar to the previous low emittance rings, beamline optics is going to face various challenges, energy scan of nanobeam and versatility in focus size to avoid soft sample damages. We anticipate that advances in time-resolved XAFS experiments utilizing short pulses will be another focus of this workshop, ranging from energy-dispersive setup to timing experiments at XFEL facilities represented by European XFEL.*

*As challenging issues are strongly dependent on the facility and/or beamline, it is important to overview different cases and intensive discussion by experts. The aim of the workshop is to discuss scientific opportunities in XAFS research at the 4$^{th}$ GEN light sources with different views and perspectives. In order to fully make use of superior specifications of the new light sources some challenging issues are to be recognized and solved. It is truly amazing that the 4$^{th}$ GEN light sources are rapidly increasing their family members following MAX IV; Sirius, Diamond II, SOLEIL II, SLS II, ALS-U, APS-U, Spring-8 II, PETRA IV… It is the organizer's pleasure if this workshop will be a wonderful opportunity for bridging the generations of light sources. Lastly, but not least, it could be a nice opportunity to pay respect to the Mikael Eriksson (Maxlab) and MAX IV lattice design team for inventing a new lattice based on multibend achromat strategy.*

About the panel discussion

*Invited speakers represent different facilities with different specifications and thus may have different scientific contexts expecting the future of the 4$^{th}$ GEN light sources differently. Therefore these views would be quite topical and interesting to explore with a limited number of slides. The participants (invited speakers who are willing to participate) could be asked for two slides: one about the presently available methods/instruments evolved towards the 4$^{th}$ generation – how these techniques are expected to become better and the second one about presently impossible experiments (related to XAS/XES) enabled at the 4$^{th}$ generation – for which one's imagination is welcome. Secondly, as PETRA IV is soon going to join the DLSR family, Dr. Edmund Welter (DESY) was invited to join the panel discussion.*

July 22, 2018

***An Introduction to XAFS Data Analysis with Athena and Artemis (and Larch)***

Organized by **Matt Newville** (U Chicago) and **Mauro Rovezzi** (CNRS/ESRF)

Exhibition room A (Sala Wystawowa A), 9:00-16:00, on-site registration from 8:00

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| *09:00* | *Introduction, Overview of XAFS* |
| *09:45* | *XAFS Data Processing Steps* |
| *10:15* | *Coffee* |
| *10:30* | *Modelling EXAFS with Feff, Path expansion and Feff-fitting* |
| *11:15* | *EXAFS Analysis demonstration* |
| *12:00* | *Lunch* |
| *13:00* | *EXAFS Analysis demonstration, Hands-on analysis* |
| *14:00* | *Larch scripting, plugins, Python programming with Larch*<br>presented by **Yohei Uemura** (UVSOR), **Konstantin Klementiev** (MAX IV), **Marius Retegan** (ESRF), and **Christoph Sahle** (ESRF) |
| *15:00* | *Discussion: Python and Larch application developments for XAFS and beyond.* |
| *16:00* | *Closing* |

About the workshop

*This one-day session will provide an overview of XAFS data processing and EXAFS analysis using Larch. The session will begin with lectures on analysis methods, but students should have some familiarity with X-ray absorption spectroscopy. The course will emphasize interactive demonstrations of data processing and analysis of EXAFS spectra with practical tips for real analysis strategies for students to learn how to apply these methods to their own research. The session will include a discussion of using the scripting capabilities of Larch and Python. The last two hours of the session will feature presentations and discussions of current and future developments with Larch and Python.*

Requirements

*Each participant is expected to have own laptop. The Larch software is available at https://xraypy.github.io/xraylarch/ for Windows, MacOS, and Linux, and can be installed before the course, or during the first hour of the course.*

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***Hands-on workshop on spectroscopy with FEFF and DFT***

Organized by **Joshua J. Kas** (University of Washington)

Exhibition room B (Sala Wystawowa B), 9:00-14:00, on-site registration from 8:00

*09:00 Introduction to FEFF9 and JFEFF GUI*

*10:30 Coffee*

*11:00 DFT supported FEFF calculations*

*14:00 Lunch*

About the workshop

*This hands on workshop will focus on using FEFF9 to simulate XANES and related spectroscopies. We will begin by instructing participants on the use of FEFF9 with the JFEFF GUI, from installation, to simple examples and tips. Participants will follow along on their own laptop. We will also talk about the combined use of DFT and FEFF to obtain more accurate calculated results and improved physical interpretation of data. Finally, if time permits, we will help participants in simulating XAS of some physical system of interest to them.*

Requirements

1. *Laptop: Most reasonably modern laptops will work.*
2. *WINDOWS and LINUX users: Current version of Java JRE installed. You can download at https://java.com/en/download/*
3. *MAC OSX users: Current version of Java JDK installed. You can download at http://www.oracle.com/technetwork/java/javase/downloads/jdk8-downloads-2133151.html*
4. *Please bring a system from your own research, for which you would like to simulate a spectrum.*

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***Hands-on workshop on spectroscopy with GNXAS/RMC/GUI***

Organized by **Andrea Di Cicco** (University of Camerino)

Seminar room (Sala Seminaryjna), 9:00-14:00, on-site registration from 8:00

*09:00 Theoretical background, methodology for GNXAS*

*10:30 Coffee*

*11:00 The basic GNXAS package and its advanced usage (GUI, RMC-GNXAS)*

*12:30 Tutorials: examples of GNXAS data-analysis*

*14:00 Lunch*

About the workshop

*The workshop will focus on using GNXAS package for EXAFS data analysis. GNXAS is an advanced software based on multiple-scattering (MS) calculations and a rigorous fitting procedure of the raw experimental data. Its main characteristics are: atomic phase shifts calculations in the muffin-tin approximation based on atom self-consistent relativistic calculations, inclusion of inelastic losses through complex Hedin-Lundqvist potential, calculation of MS signals associated with two, three, and four atom configurations using advanced algorithms.*

Requirements

*Attendants are expected to carry their own laptop and can possibly have already downloaded the GNXAS software. They may carry their own data, and possibly try to use GNXAS before the workshop. Software is freely available after registration. The page for downloading is: http://gnxas.unicam.it/pag_gnxas/gnxas_download.html.*