

# EBS workshop on X-ray Emission Spectroscopy

ESRF, Grenoble, France

ESRF auditorium

## PROGRAMME

Tuesday 3<sup>rd</sup> December 2019

11:00 - 12:00	Registration in the ESRF Central Building entrance hall	
12:00 - 13:30	Lunch at the EPN campus restaurant	
13:45 - 14:00	Welcome/Introduction	<b>H. Reichert</b> <i>ESRF Director of Research</i>
14:00 - 15:50	<b>Session 1: Instrumentation</b> Chair: <b>P. Glatzel</b>	
14:00 - 14:30	Current and future possibilities of XES and XAFS in the laboratory	<b>B. Kanngießner</b> <i>TU Berlin, Germany</i>
14:30 - 15:00	Status of XES spectrometer at Balder beamline at MAX IV	<b>K. Klementiev</b> <i>Lund University, Sweden</i>
15:00 - 15:30	High resolution X-ray spectroscopy at SLAC	<b>D. Sokaras</b> <i>SLAC NAL Stanford, USA</i>
15:30 - 15:50	FAME-UHD: High-Energy Resolution Fluorescence Detected X-Ray Absorption Spectroscopy on ultra-trace elements	<b>O. Proux</b> <i>CNRS St Martin d'Hères, France</i>
15:50 - 16:20	Coffee break	
16:20 - 18:30	<b>Session 2: Instrumentation</b> Chair: <b>M. Rovezzi</b>	
16:20 - 16:50	What to do with a portable von Hámos spectrometer?	<b>C. Sternemann</b> <i>TU Dortmund, Germany</i>
16:50 - 17:20	X-ray emission spectroscopy in the tender and hard X-ray regime at the Swiss Light Source and SwissFEL	<b>M. Nachttegaal</b> <i>PSI Villigen, Switzerland</i>
17:20 - 17:40	High-resolution hard X-ray spectroscopy at PETRA III beamline P64: present and future	<b>A. Kalinko</b> <i>Paderborn University, Germany</i>
17:40 - 18:00	PINK: tender X-ray beamline for an X-ray emission spectroscopy at BESSY II. First results	<b>S. Peredkov</b> <i>MPI Mülheim/Ruhr, Germany</i>
18:00 - 18:30	Sponsors: XRStech, easyXAFS, SAINT GOBAIN	
18:30 - 21:00	Poster session + Buffet dinner on the ESRF mezzanine	

# Wednesday 4<sup>th</sup> December 2019

## 09:00 - 10:40 Session 3: Materials Science and Coordination Chemistry Chair: S. Lafuerza

- 09:00 - 09:30 Spectroscopic studies of Intermediates in biological dinitrogen reduction **S. DeBeer**  
*MPI Mülheim/Ruhr, Germany*
- 09:30 - 10:00 X-ray emission spectroscopy to understand photochemical reactions and mechanisms **M. Bauer**  
*Paderborn University, Germany*
- 10:00 - 10:20 What can we learn about nanoparticle synthesis in solution from photon-in photon-out spectroscopy? **D. Koziej**  
*Hamburg University, Germany*
- 10:20 - 10:40 Monitoring structural changes in molybdenum sulfide phase within the confinement of Zeolite-Y under sulfidation/hydrogenation conditions via HERFD-XAS and VtC-XES measured under *operando* conditions **R. Khare**  
*TU Munich, Germany*

## 10:40 - 11:10 Coffee break and group picture

## 11:10 - 12:40 Session 4: Materials Science and Coordination Chemistry Chair: S. Butorin

- 11:10 - 11:40 Selective redox catalysis over Cu-zeolites: insights by HERFD-XANES and vtc-XES **E. Borfecchia**  
*Turin University, Italy*
- 11:40 - 12:00 Lithium-sulfur batteries studied by tender X-ray emission spectroscopy **M. Kavcic**  
*Institute J. Stefan Ljubljana, Slovenia*
- 12:00 - 12:20 TEXS: in-vacuum tender X-ray emission spectrometer based on eleven Johansson crystal analysers **M. Rovezzi**  
*CNRS FAME Grenoble, France*
- 12:20 - 12:40 Local coordination of molybdenum in crystalline compounds from high-energy resolution L3-XANES: experiment and theory **A. Svyazhin**  
*ESRF Grenoble, France*

## 12:40 - 14:00 Lunch at the EPN campus restaurant

## 14:00 - 15:50 Session 5: Actinides Chair: K. Kvashnina

- 14:00 - 14:30 HERFD in actinide research **S. Butorin**  
*Uppsala University, Sweden*
- 14:30 - 14:50 Structural studies of actinide materials applying high resolution X-ray absorption and emission spectroscopy **T. Vitova**  
*Karlsruhe Institute of Technology, Germany*
- 14:50 - 15:10 Uranium M-edge HERFD-XANES at MARS beamline **M. Hunault**  
*Synchrotron Soleil, France*
- 15:10 - 15:30 HERFD-XAS studies of actinide materials **L. Zhang**  
*Chinese Academy of Sciences Shanghai, China*
- 15:30 - 15:50 Uranium transport by Cl-bearing aqueous fluids: insights from HERFD-XAS **E. Bazarkina**  
*Institut Néel Grenoble, France*

## 15:50 - 16:20 Coffee break

<b>16:20 - 18:20</b>	<b>Session 6: Environmental Sciences</b> <b>Chair: O. Mathon</b>	
16:20 - 16:50	Structural biogeochemistry of mercury in wildlife	<b>A. Manceau</b> <i>CNRS Grenoble, France</i>
16:50 - 17:10	Revealing the chemical form of 'invisible' gold in natural sulfides with high energy-resolution X-ray absorption spectroscopy	<b>M. Merkulova</b> <i>ESRF Grenoble, France</i>
17:10 - 17:40	New scientific opportunities for high energy-resolution XAS/XES measurements at ambient and extreme conditions - the ID24-EBS project	<b>A. Rosa</b> <i>ESRF Grenoble, France</i>
17:40 - 18:00	Valence-to-core X-ray emission spectroscopy of germanate glasses: sensitivity with respect to coordination and network polymerization	<b>G. Spiekermann</b> <i>Potsdam University, Germany</i>
18:00 - 18:20	High Energy Resolution Fluorescence Detected XANES spectra of Cu complexes	<b>M. Soldatov</b> <i>Southern Federal University, Rostov-on-Don, Russia</i>
<b>19:30 - 22:00</b>	<b>Workshop dinner at the Restaurant L'Epicurien, 1 place aux Herbes, Grenoble</b>	

## Thursday 5<sup>th</sup> December 2019

<b>09:00 - 10:30</b>	<b>Session 7: Data Analysis and Theory</b> <b>Chair: M. Retegan</b>	
09:00 - 09:30	<i>Ab initio</i> simulations to study valence to core XES and HERFD-XANES	<b>Y. Joly</b> <i>CNRS Grenoble, France</i>
09:30 - 10:00	Wavefunction based approaches in X-ray spectroscopy	<b>D. Manganas</b> <i>MPI Mülheim/Ruhr, Germany</i>
10:00 - 10:30	Modeling Resonant Inelastic X-ray Scattering and Resonant X-ray Emission in the LDA+DMFT framework	<b>J. Kolorenc</b> <i>Czech Academy of Sciences Prague, Czech Republic</i>
<b>10:30 - 11:00</b>	<b>Coffee break</b>	
<b>11:00 - 12:30</b>	<b>Session 8: Data Analysis and Theory</b> <b>Chair: L. Amidani</b>	
11:00 - 11:30	Chemical sensitivity of K $\beta$ and K $\alpha$ X-ray emission spectroscopy: insights from a systematic investigation on iron compounds	<b>S. Lafuerza Bielsa</b> <i>ESRF Grenoble, France</i>
11:30 - 11:50	The transition metal K edge spectral shape	<b>F. de Groot</b> <i>Utrecht University, The Netherlands</i>
11:50 - 12:10	Development of X-ray absorption spectroscopic methodology for investigating relaxation processes in periodically driven systems	<b>H. Singh</b> <i>Oulu University, Finland</i>
<b>12:10 - 12:30</b>	<b>Conclusions</b>	
<b>12:30 - 13:30</b>	<b>Lunch at the EPN campus restaurant</b>	