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2 contributions at scientific conferences

Project acronym: Sylinda

Project full title: Synchrotron Light Industry Applications

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PU	Public	v
PP	Restricted to other programme participants (including the Commission Services)	
RE	Restricted to a group specified by the consortium (including Commission Services)	
CO	Confidential, only for members of the consortium (including Commission Services)	

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20.06.2023	1.0	Initial draft	Magdalena Zychowska
15.03.2024	1.1	Final version approval	Prof. Josef Hormes



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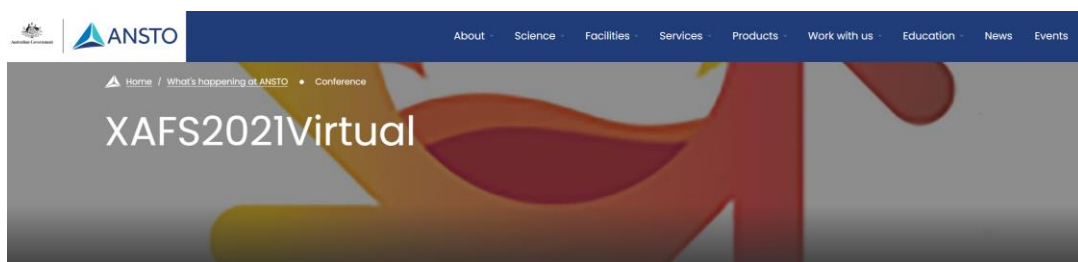
1. Introduction

This report constitutes description of actions which were undertaken to present capabilities of the SOLARIS XAS-beamline (ASTRA beamline) at scientific conferences.

Those conferences were conducted both remotely (at the beginning of the COVID-19 pandemic) and on-site. Selected meetings are highly recognized in the scientific community and draw a large number of participants. Therefore, the capabilities and potential of the XAS beamline improved under the Sylinda project were presented to the wide audience precisely during these events.

2. Description of the scientific conferences

The first conference organized by the **Australian Nuclear Science and Technology Organization** was conducted entirely remotely due to the COVID-19 pandemic.



Date	Sun 11 Jul at 9:00am - Tue 13 Jul at 5:00pm
Cost	Varies
Venue	Virtual
Register today	

Due to the ongoing COVID-19 pandemic, the Local and International Organising Committees have made the decision to postpone the in-person XAFS2021 conference to July 2022.

A virtual event is now scheduled for 11-13 July 2021, to prelude the in-person July 2022 conference. The aim of this virtual conference is to provide a platform for the international XAFS community to remain connected leading into 2022. Students and early career researchers are the focus of this event with a program of workshops, sessions on up-to-date developments in synchrotron radiation science and, above all, the opportunity for students and early career researchers to connect with the XAFS community and showcase their research.

A call for abstracts for the 2021 virtual conference, and its program, will be released shortly.

Further details and updates regarding the in-person 2022 XAFS conference will also appear on the XAFS website: <https://xafs2021.org/index.php> or email info@xafs2021.org

The XAFS2021Virtual conference took place on July 11-13, 2021. In this meeting two lectures showing abilities of SOLARIS XAS-beamline were performed.



Alexey Maximenko, PhD presented the design and measurement possibilities of the ASTRA beamline, and the second speaker, Piotr Ciochoń, PhD talked about the potential opportunities offered by SOLARIS XAS-beamline in industrial applications (link: <https://www.youtube.com/watch?v=xGaB6gep8Bg>).

Alexey Maximenko, PhD

Project partners: SOLARIS, TRIAS SYNCHROTRON, Hochschule Niederrhein, UNIVERSITÄT DUISBURG

Beamline SOLABS (ASTRA in the future)



XAS End Station



$\mu(E) \propto \ln(I_0/I_1)$ or F/I_0

Measurement modes

- **Transmission mode;**
- **Fluorescence mode (In process);**
- **Total Electron Yield mode (In process);**
- **Conversion Electron Yield mode (In process);**
- **Fluorescence spectrometer with high energy resolution (Summer 2022).**

JAGIELLONIAN UNIVERSITY IN KRAKOW, SOLARIS, TRIAS SYNCHROTRON, Hochschule Niederrhein, UNIVERSITÄT DUISBURG

Beamline availability

The first friendly Users – End of January 2022
The First Call for Proposals - in March 2022

Projects at SOLABS

EU Horizon2020 program SYLINDA

Project Partners: SOLARIS, ALBA, Hochschule Niederrhein, UNIVERSITÄT DUISBURG

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 952148.

Piotr Ciochoń, PhD

X-ray absorption spectroscopy at SOLARIS for industrial applications

SYLINDA

X-ray absorption spectroscopy at SOLARIS for industrial applications

Piotr Ciochoń, Marta Avila, Josef Hormes, Henning Lichtenberg, Alexey Maximenko, Alexander Prange, Alejandro Sanchez

Project partners: **Good morning everyone, my name is Piotr Ciochoń, I'm from SOLARIS National Sychrotron Radiation**

X-ray absorption spectroscopy at SOLARIS for industrial applications

Technique of choice: XAS

- **Versatility** (possibility to study most elements, liquids/gases allowed)
- **Chemical sensitivity** (oxidation state, bonding type, local structure)
- Possibility of performing **in-situ measurements**
- **Minimal sample preparation** required

SOLABS beamline at SOLAIRS synchrotron, dedicated to industrial research, especially concerning low-Z elements (S, P, Si, Al, Mg...)

At SOLARIS we are currently commissioning a SOLABS beamline, which will be dedicated to

Project coordinator:
 SOLARIS National Synchrotron Radiation Centre
 ul. Czerwone Maki 98
 30-392 Kraków, Poland
www.sylinda.eu

Project partners:

- ALBA Synchrotron
Carrer de la Llum 2-26
08290 Cerdanyola del Vallès,
Barcelona, Spain
- Hochschule Niederrhein
University of Applied Sciences
Reinartzstraße 49
47805 Krefeld, Germany
- Rheinische Friedrichs-Wilhelms-Universität Bonn
Regina-Pacis-Weg 3
53113 Bonn, Germany

SOLARIS, ALBA, Hochschule Niederrhein, UNIVERSITÄT DUISBURG

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 952148.

Another conference, the **Joint Meeting of the Polish Synchrotron Radiation Society and SOLARIS Centre Users** was organized in September 2022. During the four-day meeting lecturers had the opportunity to present scientific achievements and experiences in conducting research using synchrotron radiation. Professor Josef Hormes highlighted the capabilities of the SOLARIS XAS-beamline and further prospects for its use. In addition, Alexey Maximenko, PhD presented measurement capabilities on the SOLARIS XAS-beamline in soft, hard and sensitive X-ray energies.

JOINT MEETING OF PSRS MEMBERS
AND SOLARIS CENTRE USERS

20th-23rd
SEPTEMBER 2022
Krakow



JOINT MEETING OF POLISH SYNCHROTRON RADIATION SOCIETY
MEMBERS AND SOLARIS CENTRE USERS
KRAKÓW, POLAND, SEPTEMBER 20 – 23, 2022

SOLARIS National Synchrotron Radiation Centre, Czerwone Maki 98, 30-392 Kraków, Poland
Polish Synchrotron Radiation Society, ul. Radzikowskiego 152, 31-342 Kraków, Poland



ASTRA beamline: 'work horse' for absorption spectroscopy at tender and higher X-ray energies

The abstracts should be submitted via conference e-mail: users.conference@uj.edu.pl

Oral Presentation A.Maximenko¹, G.Gazdowicz², J.Hormes^{2,3}, H. Lichtenberg⁴, M.Piszak¹, A.Prange^{1,4}

ASTRA (Absorption Spectroscopy beamline for Tender energy Range and Above) is a bending magnet beamline at the SOLARIS synchrotron. The beamline is built as an international collaboration of SOLARIS with Hochschule Niederrhein University of Applied Sciences (leader of the project), the Institute of Physics at Bonn University and the Synchrotron Light Research Institute (Thailand). It was specifically designed as a 'work horse' beamline for X-ray absorption spectroscopy (XAS) and related techniques at low photon energies (range ~1-15 keV) [1]. The beamline has no additional optical components such as lenses or mirrors and does not require radiation safety hatches. In SOLARIS' experimental hall the following four main beamline components are installed: a diagnostic module, a differential ion pump, a double-crystal monochromator and an end station (Figure 1a). The diagnostic module is used to visualize and determine the position and profile of the white beam. A compact differential ion pump maintains a pressure difference of 4-5 orders of magnitude between the diagnostic module operating in ultra-high vacuum (1.0×10^{-10} mbar) and the fixed exit beam Lemmonier type double crystal monochromator operating in high vacuum (1.0×10^{-8} mbar). It allows to operate the beamline without any windows between the source point and the monochromator in order to minimize absorption of low energy photons. Thus, XAS data at the Na, Mg, Al and Si K-edges can be measured at ASTRA. There is only one thin Kapton or PP foil window to isolate the monochromator vacuum from the pressure in

Acknowledgements: The ASTRA beamline was partly funded within the project „Innovative Hochschule – Leuchtturm NR – Aus der Höhe in die Breite“ (03-IHS-084) by the German Federal Ministry of Education and Research, and its further development for measuring at low photon energies and with high energy resolution fluorescence detection is supported within the EU Horizon2020 program (952148-Sylinda).



J. Hormes, A. Maximenko, H. Lichtenberg, A. Prange

SOLARIS + psrs, Krakow, September 23, 2022

Meeting agenda

Tuesday, 20th		Wednesday, 21st		Thursday, 22nd		Friday, 23rd	
17:30	Registration & Welcome	09:30	Conference opening	09:00	T4_FP1 - SOLARIS today & tomorrow - M. Stankiewicz - SOLARIS National Radiation Synchrotron Centre	09:00	F7_IS1 - Dust Surface Chemistry in the Inner Solar Nebula Simulated in the Lab and Investigated by Near Ambient Pressure X-ray Photoelectron Spectroscopy - P. Rudolf - University of Groningen
		10:00	W1_IS1 - A new setup for Auger Photoelectron Coincidence Spectroscopy (APECS) - N. Mårtensson - Uppsala University	09:20	T4_IS1 - Evolution of the electronic states at the Pb/NbP and Nb/NbP Interfaces - an ARPES study - B. Kowalski - Institute of Physics Polish Academy of Sciences	09:30	F7_IS2 - X-ray absorption spectroscopy at the SOLARIS ASTRA beamline: Present performance and expectations for the future - Prof. J. Hornes - Institute of Physics, Rheinische Friedrich-Wilhelms University
		10:30	W1_O1 - Effective Masses of Electrons in a 2D System with Nonparabolic Bands - J. Kołodziej - Faculty of Physics, Astronomy, and Applied Computer Science, Jagiellonian University	09:50	T4_O1 - Interactions of oxygen with MoS2 crystals Investigated on the macro- and microscopic length scales - R. Szożkiewicz - Faculty of Chemistry, Biological and Chemical Research Centre, University of Warsaw	10:00	F7_O1 - XPS analysis of Mn valence in phase-separated polycrystalline lanthanum manganite and its effect on magnetic refrigeration - M. Smarł - A. Chełkowski Institute of Physics, University of Silesia in Katowice
		10:50	W1_O2 - Unravelling the combination of the electronic structure with magnetism and microstructure for NZFO/f-MWCNTs nanocomposites - A. Bajorek - Institute of Physics, University of Silesia in Katowice	10:10	T4_O2 - Research capacity of the URANOS beamline - N. Olszowska - SOLARIS National Synchrotron Radiation Centre	10:20	F7_FP1 - DUO mini-workshop - A. Górkiewicz - SOLARIS National Synchrotron Radiation Centre
		11:10	W1_O3 - Analytical estimations of size polydispersity from small-angle X-ray scattering data based on unified exponential/power-law approximation - O. V. Tomchuk - The Henryk Niewodniczański Institute of Nuclear Physics, Polish Academy of Sciences	10:30	T4_O3 - The PIRX beamline performance presented on selected results - M. Zajac - SOLARIS National Synchrotron Radiation Centre	10:35	Conference closing & departures
		11:30	Lunch break	10:50	Coffee break	11:00	Transfer to SOLARIS Centre
		13:00	W2_IS1 - Seeing is believing - How we can understand the function of proteins under a cryo-EM microscope - S. Glatt - Malopolska Centre of Biotechnology Jagiellonian University	11:20	T5_IS1 - Millisecond - and micrometer - time and spatial resolutions at the Quick - EXAFS ROCK beamline: Applications in Heterogeneous Catalysis - V. Briais - Synchrotron SOLEIL	11:30	Beamlines "SOLARIS Centre tour"
		13:30	W2_IS2 - Structural characterisation of bacterial Tn7 transposase by cryo-EM - M. Czarnocki-Cieclura - The International Institute of Molecular and Cell Biology	11:50	T5_IS2 - X-ray spectroscopy of magnetic nanoparticles in liquid suspensions - M. Sikora - AGH University of Science and Technology		
		14:00	W2_O1 - Can we manipulate shape and size of virus-like particles on demand? - A. Biela - Malopolska Center of Biotechnology	12:20	T5_O1 - PHELIX - a new tool for spectroscopic measurements - M. Szczepanik - SOLARIS National Synchrotron Radiation Centre		
		14:20	W2_O2 - Chemical Infrared Imaging - capabilities at the nanoscale - M. Roman - SOLARIS National Synchrotron Radiation Centre	12:40	T5_O2 - DEMETER - Dual Electron Microscopy and Spectroscopy Beamline - A. Mandzlik - SOLARIS National Synchrotron Radiation Centre		
		14:40	Coffee break	13:00	Lunch break		
		15:00	W3_IS1 - Applications of a high repetition rate XFEL in diffraction and scattering: Exploring more than three dimensions at the SPB/SFX Instrument of the European XFEL - J. Bielecki - European XFEL	14:30	T6_O1 - National Cryo-EM Centre at SOLARIS - M. Rawski - SOLARIS National Synchrotron Radiation Centre		
		16:30	W3_IS2 - Soft X-ray femtosecond time-resolved photoelectron spectroscopy opportunities at the European XFEL - M. Izquierdo - European XFEL	14:50	T6_O2 - ASTRA beamline: 'work horse' for absorption spectroscopy at tender and higher X-ray energies - A. Maximenko - SOLARIS National Synchrotron Radiation Centre		
		16:00	W3_IS3 - Time-resolved X-ray crystallography on membrane proteins: watching ions moving in time and space - P. Nogly - ETH Zurich	15:10	T6_O3 - PolyX beamline for microimaging and microspectroscopy at SOLARIS - K. Sowa - SOLARIS National Synchrotron Radiation Centre		
		16:30	W3_O1 - Correlation study of two timing tools at SwissFEL - W. Blochucki - Institute of Nuclear Physics, Polish Academy of Sciences	15:30	T6_O4 - Current status of Chemical Infrared Imaging CIRI (SOLAIR) beamline in Solaris - T. Wróbel - SOLARIS National Synchrotron Radiation Centre		
		16:50	Sponsor's speech - COMEF Sp. z o.o. sp.k. - nearSCOPE for nanoscale optical analysis - technology and applications - Dr. Suman Paul - Sales Application Engineer attocube systems AG	15:50	T6_O5 - SOLCRYS project - MX and SAXS beamline, updated status - M. Kozak - SOLARIS National Synchrotron Radiation Centre		
		17:05	Poster session	16:10	The NAA Laboratory - M. Silarski - Jagiellonian University		
				16:20	Conference Photo		
				16:30	Networking Meeting		

Next conference, **TECHNART 2023**, was organised in Lisbon from May 7-12, 2023.

During the conference, prof. Josef Hormes had the opportunity to present results demonstrating the applicability of the SOLARIS XAS-beamline in two poster sessions according to the Scientific programme: https://technart2023.com/wp-content/uploads/2023/05/programme_-_technart23.pdf

TIMETABLE

	07 May	08 May	09 May	10 May	11 May	12 May
08h30		Registration				
09h00		Opening session	Invited speaker	Invited speaker	Invited speaker	
09h20		Invited speaker				
10h00		OP	OP	OP	OP	
10h30						Visit to MNAZ
11h00		Coffee break	Coffee break	Coffee break	Coffee break	
11h30		OP	OP	OP	OP	
12h30						
13h00		Lunch break	Lunch break	Lunch break	Lunch break	
13h30						
14h00						
14h30		Invited speaker	Invited speaker	Invited speaker	Invited speaker	
15h00	Registration					
16h00		OP	OP & CS	OP	OP	
16h30		Coffee break	Coffee break	Coffee break	Coffee break	
17h00	Welcome reception	Poster Session 1	Poster Session 2	Poster Session 3	Poster Session 4	
18h00					Closing session	
18h30						
20h00				Conference dinner		

OP Oral Presentations
CS Commercial session

The topics and abstracts of both posters presented by prof. Josef Hormes are available in the Abstract Book <https://technart2023.com/wp-content/uploads/2023/05/Book-of-abstracts-technart23.pdf> (page 155 and 205)

Ancient glass samples from the Cathedral in Paderborn: an investigation using synchrotron radiation based techniques

Goals of this study:

- Determining the elemental composition of the samples: base material and additives
- Determining – if possible – the origin of the base material used for the fabrication of the samples (one of the glassworks?)
- Providing information about fabrication techniques by determining the chemical oxidation states of major elements.

14 glass samples from the Cathedral of Paderborn and several samples from two glassworks operated in the 12th century near Paderborn were included in the study. Age of samples from 777 and 1000 to Romantic time

EXPERIMENTAL TECHNIQUES

- X-ray fluorescence spectroscopy and X-ray absorption spectroscopy (XANES) measurements at various beamlines and synchrotrons (CAMD, SOLARIS, SLIRI): excitation energy for XRF at all beamlines 10 keV, 5 keV, and 3 keV; double crystal monochromators with Si(111) or Si(422) crystals according to the required energy range.

RESULTS and DISCUSSION

Fig. 1a and 1b shows six "typical examples" the fluorescence spectra of 3 glasses in the high energy range between 6.0 and 15 keV (1a) and in the low energy range (1b) between 2 and 7 keV. Spectra are normalized to the Compton peak.

Fig. 1a XRF spectra 200-2000 eV range
Fig. 1b XRF spectra 200-2000 eV range
Fig. 1c XRF spectra DOM and glasswork samples

Major XRF Observations

- 3 different groups of samples: DOM 1, 2 and 3 in Fig. 1a and Fig. 1b are representatives of these groups:
- High concentration of Pb in group 1 and 2 – for groups 1 and 2 lead was used for reducing the melting temperature!
- High Ca/K ratio for group 3 (DOM 3) – Group 3: ashes from branches and trunks used for reducing melting temperature
- Concentrations of trace elements (K, Ti, V, and Cr) in group 3 (DOM 3) is different from group 1 (DOM 1) and 2 (group 2) – group 3 samples fabricated at a different glasswork than group 1 and group 2
- Very similar element distribution for group 1 and Glasswork Föllenberg (Fig. 1 c) – group 1 was fabricated at this glasswork

Fig. 2: Ca-K-XANES spectra

- DOM 1 (group 1) and DOM 2 (Group 2) very similar spectra – similar fabrication process
- Spectra from same group (DOM 5 and 7) have same spectra
- "Stronger" pre-edge line for group 1 and 2 – higher melting temperature than group 3

Fig. 3: Cu-K-XANES spectra

- Different spectra for samples from the same Group (DOM 3, DOM 5), same glasswork
- Difference can also be seen optically:
 - Full 20: light green transparent
 - DOM 5: dark green opaque
 - Full 3 and DOM 3: in between

Acknowledgement:
Part of this work was supported by the European Union's Horizon 2020 Research and Innovation Program under grant agreement No. 952148 (SYLINDA-Project)

X-ray absorption near edge structure (XANES) spectra: A thermometer for the firing temperature of ceramics?

Problem: Determining from X-ray absorption spectra (XANES) quantitatively the "highest" temperature at which a ceramic artefact has been used/fired?

Investigated samples: Poverty Point Objects (PPOs) – 3000 years old ceramic objects and "PPOs" items made from "original clay" heated to different temperatures (up to ~800°C in oxidizing or reducing atmosphere)

Experimental Techniques: X-ray absorption spectroscopy (XANES) at various synchrotrons (SOLARIS, CAMD, SLIRI) using double crystal monochromators

RESULTS and DISCUSSION

Fig. 2a Ca-K-XANES spectra of four forms made PPOs
Fig. 2b: Pre-edge region of the Ca-K-XANES spectra
Fig. 2c: Calibration curves obtained by the analysis of the pre-edge peaks and white line area under shoulder

Major observations Ca-K-edge

- Ca-K-XANES spectra show temperature dependent differences A–D (Fig. 2a); changes don't depend on atmosphere!
- The quantitative evaluation of feature A and B provides the two "calibration curves" of Fig. 2c
- Using calibration curves a firing temperature of ~500 ± 50 °C was determined for several PPOs – reasonable for a wood fire!

Major observations Fe-K-edge

- Also Fe-K-XANES spectra show temperature dependent differences: A–C in Fig. 3a
- Spectral changes depend on the atmosphere!
- Increase of pre-edge peak as f₀ of temperature = less centrosymmetric site (Fig. 3b)
- Fe-K-XANES can be used for a quantitative determination of firing temperature

Conclusion

Temperature dependent changes in the Ca-K and Fe-K spectra of ceramic can be used for the quantitative determination of firing temperature.

Major observation at Si-K-edge:

- No significant changes in the Si-K-XANES spectra up to 800°C
- No significant modifications in the chemical environment of Si
- Si XANES not suitable for determination of firing temperature

Acknowledgement:
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Next conference, the **Molecules & Light, V Autumn Meeting of the Polish Photochemistry Group**, was mainly dedicated to young scientists. This meeting took place in Krakow on September 24-27, 2023 (<https://ml2023.org/>). During the poster session young researchers from SOLARIS (Lulu Alluhaibi, PhD and Grzegorz Gazdowicz) presented results of their experiments conducted on the SOLARIS XAS-beamline.

ASTRA BEAMLINE AT SOLARIS: XAS IN THE TENDER AND HARD X-RAY RANGE

G.Gazdowicz¹, A. Maximenko¹, H. Lichtenberg², M.Piszak¹, A. Prange³ and J. Hormes³

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² Hochschule Niederrhein University of Applied Sciences, Krefeld, Germany
³ Institute of Physics, Rheinische Friedrich-Wilhelm-University Bonn, Germany

BEAMLINE LAYOUT

- Bending magnet beamline dedicated for XAS - X-ray Absorption Spectroscopy.
- Energy range: 1-15 keV, Flux: 10¹⁹ photons per second
- Measurements in low vacuum or ambient pressure - only one Kapton window along the beam path.
- Safe and handy operation - no radiation hutch.

END STATION

- Transmission and Fluorescence measurement modes
- Simultaneous reference measurement for precise calibration control
- Absorber concentration from 100% to 10ppm
- Possibility of collecting XRF spectra

CAPABILITIES

It is possible to elucidate absorption fine structure of elements:

- from Sodium to Bromine - K-edge
- from Krypton to Bismuth - L-edge
- from Polonium to Uranium - N-edge

Available L_{2,3} absorption edges

Element	L ₂ Edge (eV)	L ₃ Edge (eV)
Na	1046.7	1070.8
Mg	1486.4	1500.0
Al	1911.7	1998.7
Si	2344.8	2484.5
P	2774.1	2957.0
S	3206.9	3548.3
Cl	3696.4	4048.8
Ar	4182.1	4548.5
K	4641.3	5047.0
Ca	5091.3	5544.0
Sc	5541.3	6040.0
Ti	5991.3	6536.0
V	6441.3	7032.0
Cr	6891.3	7528.0
Mn	7341.3	8024.0
Fe	7791.3	8520.0
Co	8241.3	9016.0
Ni	8691.3	9512.0
Cu	9141.3	10008.0
Zn	9591.3	10504.0
Ga	10041.3	11000.0
Ge	10491.3	11496.0
As	10941.3	11992.0
Se	11391.3	12488.0
Br	11841.3	12984.0
Kr	12291.3	13480.0
Rb	12741.3	13976.0
Sr	13191.3	14472.0
Zr	13641.3	14968.0
Nb	14091.3	15464.0
Mo	14541.3	15960.0
Tc	14991.3	16456.0
Ru	15441.3	16952.0
Rh	15891.3	17448.0
Pd	16341.3	17944.0
Ag	16791.3	18440.0
Cd	17241.3	18936.0
In	17691.3	19432.0
Sn	18141.3	19928.0
Sb	18591.3	20424.0
Te	19041.3	20920.0
I	19491.3	21416.0
Xe	19941.3	21912.0
Ba	20391.3	22408.0
Hf	20841.3	22904.0
Ta	21291.3	23400.0
W	21741.3	23896.0
Re	22191.3	24392.0
Os	22641.3	24888.0
Ir	23091.3	25384.0
Pt	23541.3	25880.0
Au	23991.3	26376.0
Hg	24441.3	26872.0
Tl	24891.3	27368.0
Pb	25341.3	27864.0
Bi	25791.3	28360.0
Po	26241.3	28856.0
At	26691.3	29352.0
Rn	27141.3	29848.0
Ac	27591.3	30344.0
Th	28041.3	30840.0
Pa	28491.3	31336.0
U	28941.3	31832.0
Np	29391.3	32328.0
Pu	29841.3	32824.0
Am	30291.3	33320.0
Cm	30741.3	33816.0
Bk	31191.3	34312.0
Cf	31641.3	34808.0
Es	32091.3	35304.0
Fm	32541.3	35800.0
Mendelevium	32991.3	36296.0
Nobelium	33441.3	36792.0
Lanthanum	33891.3	37288.0
Cerium	34341.3	37784.0
Praseodymium	34791.3	38280.0
Neodymium	35241.3	38776.0
Europium	35691.3	39272.0
Gadolinium	36141.3	39768.0
Terbium	36591.3	40264.0
Dysprosium	37041.3	40760.0
Ytterbium	37491.3	41256.0
Lutetium	37941.3	41752.0

XANES

XANES - X-ray Absorption Near Edge Structure contains information about:

- Oxidation state of elements (shift of absorption edge)
- Chemical environment around absorber
- type of ligands; coordination number;
- degree of symmetry (spectral fingerprint, prepeaks, white line intensity)

EXAFS

EXAFS - Extended X-ray Absorption Fine Structure contains information about:

- Distances between absorber and surrounding atoms
- Number and type of atoms in each coordination shell
- Level of structural disorder

DEVELOPMENT

Raman spectroscopy:

- Two wavelength laser excitation system
- Raman spectrometer and microscope (simultaneous and independent operation)

In situ measurements:

- Temperature cell
- Electrochemical cell
- Flow cell
- In situ cell - controlled atmosphere for catalytic reactions

Photoluminescence of Thiazolothiazoles and Their Metal Complexes

INTRODUCTION: Thiazolothiazoles are bicyclic aromatic compounds with four heteroatoms. Despite high stability, relatively simple synthesis and interesting photophysical and electrochemical properties, they have not attracted much attention. Due to planarity of the central ring system, they undergo efficient stacking in the solid state, which may lead, after appropriate doping, to high conductivity of these materials. Along with possible diversity of substitutions, thiazolothiazoles are an ideal playground for photophysical and molecular electronics.

SYNTHESIS ROUTE:

RESULTS & DISCUSSION:

X-ray absorption fine structure spectroscopy (XAFS) at sulfur K-edge indicates the effects of electron-withdrawing group (b12) and Electron Donating Groups (b3 & b8) on electronic structure of the bicyclic thiazolothiazole moiety

CONCLUSIONS: Thiazolothiazoles show remarkable EXAFS and XANES spectra features: the aromatic core is very stable and does not undergo any significant changes in the presence of either electron donating and electron withdrawing groups. EXAFS indicates the importance of long-range interactions at solid state, which is also reflected in the solid state luminescence spectra.

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3. Summary

Participation in prestigious conferences with a wide audience provided an opportunity to enhance the visualization of the Sylinda project and demonstrate the capabilities of SOLARIS. In addition, participation in the conferences through the Sylinda project has significantly contributed to strengthening the position of the SOLARIS infrastructure in the world-wide large-scale Research Infrastructure community. Moreover, the widely promoted use of the SOLARIS XAS-beamline has increased the number of academic and industrial users interested in using it for their experiments.

Demonstration of SOLARIS XAS-beamline capabilities at international conferences will be consistently performed, to establish SOLARIS position in the research environment.



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