



polish synchrotron  
radiation society



**SOLARIS**  
NATIONAL SYNCHROTRON  
RADIATION CENTRE

## SYNCHROTRON RADIATION IN NATURAL SCIENCE



### JOINT MEETING OF POLISH SYNCHROTRON RADIATION SOCIETY AND SOLARIS CENTRE USERS

11 – 13 September 2024



**Vol. 24, September 2024**

**Bulletin of Polish Synchrotron Radiation Society**

ISSN 1644-7190

# SYNCHROTRON RADIATION IN NATURAL SCIENCE

## Editor-In-Chief

### Edyta Piskorska-Hommel

Institute of Low  
Temperature  
and Structure Research  
Polish Academy of  
Sciences  
Wrocław, Poland



## Guest Editor

### Marcin Sikora

SOLARIS National  
Synchrotron Radiation  
Centre  
Jagiellonian University  
Kraków, Poland

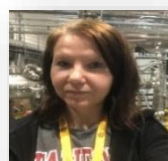


## Editorial board

### Co-Editor

#### Anna Bajorek

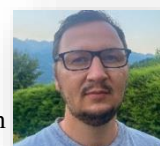
A. Chełkowski Institute  
of Physics University  
of Silesia in Katowice,  
Katowice, Poland



### Co-Editor

#### Maciej Jankowski

European Synchrotron Radiation  
Facility (ESRF)  
Experimental Division Algorithm  
and Data Analysis Group  
Grenoble, France



### Co-Editor

#### Agnieszka Cudek

SOLARIS National  
Synchrotron  
Radiation Centre,  
Kraków, Poland



### Co-Editor

#### Dagmara Chylewska- Olech

SOLARIS National  
Synchrotron  
Radiation Centre,  
Kraków, Poland



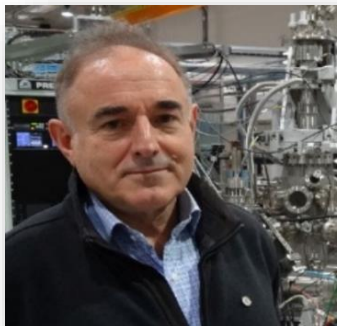
POLYX news – Paweł Korecki, SOLARIS  
CIRI news – Tomasz Wróbel, SOLARIS

**Cover image:** X-ray tomography of a crane fly (Diptera, Limoniidae: genus *Trichoneura*) - POLYX beamline. The tomogram was measured by POLYX beamline scientists during the realization of the Dr. Katarzyna Kopeć project from the Institute of Systematics and Evolution of Animals, Polish Academy of Sciences.



Ministry of Science and Higher Education  
Republic of Poland

The conference co-financed by the Ministry of Science and Higher Education Republic of Poland under the Programme Doskonała Nauka II.



Dear Readers,

It is our great pleasure to present to you this special edition of the Polish Synchrotron Radiation Society bulletin. It is exclusively devoted to the 3<sup>rd</sup> Joint Meeting of the Polish Synchrotron Radiation Society and the National Synchrotron Radiation Centre SOLARIS Users, held in Kraków from September 11 to 13, 2024.

Polish Synchrotron Radiation Society (PSRS) was launched in 1991 as the result of the initiative of the Polish group of researchers, who had already discovered the unique multidisciplinary research options created by the advent of synchrotron radiation (SR) facilities emerging in the 80s all over the world

and who identified, the benefits of promoting these exceptional opportunities amongst the Polish scientific community. Unavoidably, the dream of constructing an SR source in Poland emerged amongst the PSRS members at a certain stage. Due to their persisting efforts, supported by many individuals and research groups, the dream materialized in 2010 when the Ministry of Science and Higher Education allocated the relevant funds. In 2015, the National Synchrotron Radiation Centre SOLARIS was born, and in 2018, its infrastructure was opened for researchers. Since then, SOLARIS has been constantly developing its infrastructures, broadening its services in many research areas. Today, we offer 10 research infrastructures, including two cryo-EM microscopes, 5 times more than in 2018. We are keeping pace, and the construction of another 4 is in progress. Since the opening, more than 1000 Polish and foreign researchers have visited SOLARIS to carry out their measurements, many of them recurrently. Up to now, 316 SOLARIS-related research papers have been published as the result of their research. Together with 16 other European synchrotron and free electron laser facilities, we form the League of European Accelerator-based Photon Sources (LEAPS), whose primary goal is to ensure and promote the quality and impact of fundamental, applied and industrial research carried out at each facility to the greater benefit of European science and society which is also the mission of PSRS.

In 2020, following the practice of most of the SR sources, SOLARIS has decided to organize its Users' Meetings. However, taking into account the PSRS tradition of organizing since 1991 the National Symposium of Synchrotron Radiation Users (KSUPS), a foreseeable and valuable idea developed to merge those two meetings. Today, integrating the SR community in Poland and abroad, we are organizing a Joint Meeting of the Polish Synchrotron Radiation Society and the National Synchrotron Radiation Centre SOLARIS Users for the second time. Its purpose is to share and exchange research ideas, learn the progress in SR-based research, and report individual achievements. They will be presented during the meeting, and you will find the abstracts of the presentations, lectures, and posters in this bulletin. Hope you will find them interesting and inspiring.

Wishing you a very enjoyable and productive meeting,

On behalf of the Organizers,

Marek Stankiewicz

The Chairmen

## CONTENTS

□ Committees	p. 3
□ Invited speakers list	p. 4
□ Program of the Joint Meeting of PSRS Members and SOLARIS Centre Users	p. 5
□ Abstracts	p. 9
□ News	p. 97

## **Chairman**

Marek Stankiewicz

*SOLARIS National Synchrotron Radiation Centre, Jagiellonian University, PSRS*

## **Program Committee**

Marcin Sikora, *AGH University of Krakow, PSRS - Committee Chairman*

Edyta Piskorska-Hommel, *Institute of Low Temperature and Structure Research Polish Academy of Sciences, PSRS - Committee Secretary*

Anna Bajorek, *University of Silesia in Katowice, PSRS*

Paweł Korecki, *SOLARIS National Synchrotron Radiation Centre, Jagiellonian University, PSRS*

Maciej Kozak, *Adam Mickiewicz University, SOLARIS National Synchrotron Radiation Centre, Jagiellonian University, PSRS*

Ewa Partyka-Jankowska, *SOLARIS National Synchrotron Radiation Centre, Jagiellonian University*

Ryszard Sobierajski, *Institute of Physics Polish Academy of Sciences, PSRS*

Tomasz Wróbel, *SOLARIS National Synchrotron Radiation Centre, Jagiellonian University*

Marcin Zając, *SOLARIS National Synchrotron Radiation Centre, Jagiellonian University*

## **Organizing Committee**

Dagmara Chylewska-Olech, *SOLARIS National Synchrotron Radiation Centre*

Agnieszka Cudek, *SOLARIS National Synchrotron Radiation Centre*

Joanna Czapla-Masztafiak, *Institute of Nuclear Physics Polish Academy of Sciences, PSRS*

Marcin Klepka, *Institute of Physics Polish Academy of Sciences, PSRS*

Wiktor Kotlarz, *SOLARIS National Synchrotron Radiation Centre*

Joanna Kowalik, *SOLARIS National Synchrotron Radiation Centre*

Patrycja Pakońska, *SOLARIS National Synchrotron Radiation Centre*

Katarzyna Tokarz, *SOLARIS National Synchrotron Radiation Centre*

Agnieszka Witkowska, *Gdańsk University of Technology, PSRS*

Natalia Zapart, *SOLARIS National Synchrotron Radiation Centre*

## Invited speakers



**Dr. Artur Biela**

SOLARIS National Synchrotron Radiation Centre, Jagiellonian University, Kraków, Poland

*CryoEM – A perfect tool for investigation of protein cages polymorphism.*



**Prof. Guillaume Brotons**

Université Le Mans, France

*In-situ and operando synchrotron small angle X-ray scattering (SAXS) experiments, designed to understand nanoparticles assemblies in complex bio-environments.*



**Dr. Tim Butcher**

Paul Scherrer Institute (PSI), Villigen, Switzerland

*Development of Ptychographic Imaging with Soft X-Rays.*



**Prof. Mirosław Gilski**

Adam Mickiewicz University, Poznań, Poland

*Challenges of X-ray crystallography: Unusual molecular arrangements.*



**Prof. Nils Huse**

University of Hamburg, Germany

*Investigating the electronic structure of molecules in solution with X-ray spectroscopy.*



**Giuseppe Mercurio**

European XFEL, Hamburg, Germany

*Time-resolved RIXS and SAXS at the SCS instrument of European XFEL.*



**Prof. Aleksandra Mielewczyk-Gryń**

Gdańsk University of Technology, Gdańsk, Poland

*The importance of synchrotron studies in view of the development of hydrogen industry.*



**Dr. Martin Schnell**

CIC nanoGUNE, Spain

*Nano-FTIR spectroscopy of single cell sections.*

## Program of the Joint Meeting of PSRS Members and SOLARIS Centre Users

**Wednesday 11/09/2024**

**10:30 - 11:00 Registration and welcome coffee**

**11:00 - 11:50 Welcome session: Introduction to SOLARIS and PSRS**

Marek Stankiewicz, Jakub Szlachetko: Opening

Agnieszka Witkowska: Past and present of PSRS & ESUO

Adrianna Wawrzyniak: SOLARIS – Machine status

Marcin Sikora: SOLARIS – Research facilities

**11:50 – 13:00 Session: X-ray scattering in soft matter** (*Chair Marek Stankiewicz*)

Mirosław Gilski: Challenges of X-ray crystallography: Unusual molecular arrangements **L1**

Maciej Jankowski: Advanced software tools and workflows for synchrotron X-ray scattering analysis at ESRF from a user's perspective **O1**

Karolina Jurkiewicz: Studies of the local structure of amorphous pharmaceuticals using X-ray scattering **O2**

**13:00 – 15:00 Lunch**

**15:00 - 17:00 Session: Spectroscopy with synchrotron light (I)**

(*Chair Agnieszka Witkowska*)

Aleksandra Mielewczyk-Gryń: The importance of synchrotron studies in view of the development of hydrogen industry **L2**

Taymaz Tabari: Unveiling the active sites in co-containing perovskite-based photo-rechargeable batteries **O3**

Paulina Gwóźdź: Diving deep into non-stoichiometric perovskites: unveiling Co/Fe doping effects **O4**

Josef Hormes: Synchrotron radiation based techniques for agricultural research **O5**

Dominik Czernia: Plasma-enhanced Physical Properties of Mn(II)-Nb(IV) Molecular Magnet Investigated with EXAFS **S1**

Mohammad Sadegh Shakeri: Time-dependent oxidation state change during pulsed laser irradiation of colloids; an experimental XAFS study confirmed by computational analysis **S2**

Adam Czempik: Changes in the electronic structure of NiFe<sub>2</sub>O<sub>4</sub>@SiO<sub>2</sub> nanocomposites by synthesis process and annealing **S3**

**17:00 – 17:30 Coffee break**

**17:30 - 19:00 Session: Research opportunities and support for synchrotron users**  
(Chair *Edyta Piskorska-Hommel*)

Jakub Szlachetko: LEAPS consortium

Anna Wolska: ESRF access project **R1**

Wiktor Kotlarz: SOLARIS User Office

Danylo Babich: Light 4 project **R2**

Mikołaj Gołuński: Beyond open call – forms of access to SOLARIS **R3**

Robert Nietubyć: PoLFEL project **R4**

**19:00 – Conference picture**

**19:10 - 21:00 Poster session**



## Thursday 12/09/2024

### 09:00 - 10:30 Session: Microspectroscopy and imaging (I) (Chair Anna Bajorek)

Guillaume Brotons: In-situ and operando synchrotron small angle X-ray scattering (SAXS) experiments, designed to understand nanoparticles assemblies in complex bio-environments **L3**

Przemyslaw Rzepka: Quantitative locating titanium in the framework of titanium silicalite-1 by exploiting anomalous X-ray powder diffraction **O6**

Taoufik Lamrani: Studies of molecular order in itraconazole by X-ray diffraction **S4**

Franciszek Sobczuk: Ill – posed problems with noisy data: from optics to X-ray scattering **O7**

### 10:30 – 11:00 Coffee break

### 11:00 - 13:00 Session: Ultrafast processes studied with X-ray FEL radiation (Chair Jerzy Antonowicz)

Giuseppe Mercurio: Time-resolved RIXS and SAXS at the SCS instrument of European XFEL **L4**

Nils Huse: Investigating the electronic structure of molecules in solution with X-ray spectroscopy **L5**

Ryszard Sobierajski: Scientific Opportunities at XFEL **O8**

Tomasz Kołodziej: Towards new time and frequency standards with <sup>45</sup>Sc and EUXFEL **O9**

Oleksii Liubchenko: Ultrafast structural transformations in Fe studied by time-resolved XRD

### 13:00 – 15:00 Lunch

### 15:00 - 16:30 Session: Microspectroscopy and imaging (II) (Chair Paweł Korecki)

Tim A. Butcher: Development of ptychographic imaging with soft X-rays **L6**

Ewa Madej: How PEEM helps in the study of antiferromagnets? **O10**

Ewa Młyńczak: Ultrathin Sn deposited on Pt(111): growth and electronic structure **O11**

Paweł Nita: Observing barium oxide on W(110) by low-energy, thermionic and photoemission electron microscopy **O12**

### 16:30 – 17:00 Coffee break

### 17:00 - 18:00 SOLARIS guided tour

### 19:00 Networking meeting - Vanilla Aparthotel

## Friday 13/09/2024

### 09:00 - 11:00 Session: Microspectroscopy and imaging (II) (Chair Maciej Kozak)

Martin Schnell: Nano-FTIR spectroscopy of single cell sections **L7**

Artur Biela: CryoEM – A perfect tool for investigation of protein cages polymorphism **L8**

Michał Gućwa: CheckmyMetal (cmm): validating metal-binding sites in X-ray and Cryo-EM data **O13**

Oskar Siemianowski: How do plants manage their microelements? Untangling the Zn transport mechanisms between lateral roots **O14**

Joanna Ortyl: New polymeric materials based on cationic photopolymerisation processes for 3D printing technology (3D-VAT) based on digital light processing **O15**

### 11:00 – 11:30 Coffee break

### 11:30 - 13:20 Session: Spectroscopy with synchrotron light (II) (Chair Anna Wolska)

Łukasz Pluciński: On the origin of circular dichroism in ARPES spectra from graphene, WSe<sub>2</sub>, and other quantum materials **O16**

Jacek Kołodziej: Band-bending, Band-tailing, 2D Electron Gas at Te doped InAs Surfaces **O17**

Ashutosh Wadge: Unveiling impervious band crossings in the bulk of topological nodal-line semimetal ZrAs<sub>2</sub> **O18**

Marcin Rosmus: Electronic Structures of Dirac Semimetals LaCuSb<sub>2</sub> and LaAgSb<sub>2</sub> **O19**

Aleksandra Figura-Jagoda: Understanding the mechanism of beam damage on copper thin films **S5**

Marek Stęślicki: Absolute calibration of the solar X-ray spectrometer BRAXIS for a NASA MidEx mission **O20**

### 13:20 - 13:30 Closing remarks



The *Ultrafast processes studied with X-ray FEL radiation* session was co-organized by the Institute of Physics of the Polish Academy of Sciences and is supported by the Ministry of Science and Higher Education within a grant no. 2022/WK/13 which provides Polish scientists with access to the European XFEL.

## POSTERS

Poster N°	Presenting author	Abstract title
P1	Ryszard Sobierajski	<i>STRUCTURAL PATHWAYS FOR ULTRAFAST MELTING OF OPTICALLY EXCITED THIN POLYCRYSTALLINE PALLADIUM FILMS</i>
P2	Katarzyna Sowa	<i>Establishing detection limits for heavy elements in pigments based on 3d-metals with the use of synchrotron-based X-ray fluorescence spectroscopy</i>
P3	Patryk Grzywa	<i>What we breath in Krakow, Poland: winter and summer air in the prism of XAFS</i>
P4	Romisaa Abdelrahman	<i>The art ceramics from the Museum of Royal Wawel Castle's analyzed by X-Ray fluorescence technique</i>
P5	Dawid Surmik	<i>RESEARCH POTENTIAL OF THE POLISH SYNCHROTRON IN EXAMINING THE REMAINS OF ORGANIC MATTER IN FOSSILIZED BONES</i>
P6	Krzysztof Matlak	<i>NEW SCANNING TRANSMISSION X-RAY MICROSCOPE AT SOLARIS OPTIMIZED FOR FAST SCANNING AND ENVIRONMENTAL EXPERIMENTS</i>
P7	Danylo Babich	<i>X-ray Spectroscopy and Scattering with 20~fms Time Resolution at SwissFEL Bernina Endstation: Probing Ultrafast Dynamics of <math>[Fe(terpy)_2]^{2+}</math></i>
P8	Maciej Roman	<i>IR NANOSPECTROSCOPY AT THE CIRI BEAMLINE AT THE SOLARIS SYNCHROTRON</i>
P9	Joanna Depciuch	<i>Synthesis and dissolution of <math>Ce_xO_y</math> nanoparticles for catalytic application by in-situ liquid cell TEM</i>
P10	Joanna Sławek	<i>ARYA – new beamline for macromolecular x-ray crystallography at SOLARIS</i>
P11	Maciej Kozak	<i>SAXS/WAXS END STATION FOR SMAUG BEAMLINE</i>
P12	Grzegorz Ważny	<i>OPTIMIZATION OF MACROMOLECULE IMAGING IN CRYO-EM METHOD</i>

<b>Poster N°</b>	<b>Presenting author</b>	<b>Abstract title</b>
P13	Aleksandra Drzewiecka-Antonik	<i>STRUCTURAL STUDIES OF PLATINIUM COMPLEXES WITH THIOUREAS</i>
P14	Tetiana Zakusylo	<i>Observation of Rashba type spin splitting in Ge-doped PbSe ferroelectric semiconductor</i>
P15	Joanna Stępień	<i>EFFECTS OF NI/CO DOPING ON STRUCTURAL AND ELECTRONIC PROPERTIES OF 122 AND 112 FAMILIES OF EU BASED IRON PNICTIDES</i>
P17	Maciej Nowagiel	<i>Investigation of Local Order in Bi2O3-Al2O3-SiO2 Glasses and Nanomaterials Using ASTRA Beamline</i>
P18	Ryszard Stekla	<i>Sulfur K-edge XANES spectra of methyl and phenyl compounds: breaking new ground in organic compound research at the ASTRA beamline</i>
P19	Gabriela Imbir	<i>Evolution of the electronic structure of Cu nanoparticles at different oxidizing conditions</i>
P20	Paweł Winiarski	<i>Molecular insights of the oxidation process of iron oxide and cobalt ferrites nanoparticles incorporated in alginate fibers</i>
P21	Krzysztof Pitala	<i>Research at PIRX beamline</i>
P22	Lulu Alluhaibi	<i>Spectroscopic Synergy at the ASTRA Beamline: Combining X-ray Absorption and Raman Spectroscopy for Advanced Analysis of Complex Materials</i>
P23	Agnieszka Gładysz-Płaska	<i>THE USE OF SYNCHROTRON RADIATION IN THE STUDY OF THORIUM COMPLEXES WITH P-DONOR LIGANDS</i>
P24	Grzegorz Gazdowicz	<i>CAPABILITIES OF THE ASTRA BEAMLINE FOR X-RAY ABSORPTION SPECTROSCOPY IN LIFE SCIENCES AND AGRICULTURE: HIGHLIGHTS AND FUTURE PLANS</i>
P25	Agata Sabik	<i>Electronic structure of ZnIn<sub>2</sub>S<sub>4</sub> revealed by photoemission investigations</i>
P26	Jerzy Antonowicz	<i>Hydrostatic compression effects on metallic glasses - a combined XAFS and simulation study</i>
P27	Edyta Beyer	<i>PHYLIX - An advanced tool for complementary photoemission experiments</i>

<b>Poster N°</b>	<b>Presenting author</b>	<b>Abstract title</b>
P28	Yashasvi Mehra	<i>On-site Coulomb energy in TMDC compounds by resonant Photoemission</i>
P29	Sophia Kaleta	<i>Correlative Fluorescence and Soft X-Ray Microscopy in the Water Window Region in an Integrated Lab-based Setup</i>
P30	Anna Bajorek	<i>EXPLORING THE INFLUENCE OF VARIOUS NZFO CONTENT ON THE ELECTRONIC STRUCTURE IN NZFO/F-MWCNTS NANOCOMPOSITES FABRICATED VIA EX-SITU SYNTHESIS</i>
P31	Anna Janowska	<i>Molecular Dynamics Simulations of the Structure of Probucol Pharmaceutical in the Vitrified and Pressure-Densified Phases</i>
P32	Krystian Sokołowski	<i>Achieving enhanced microwave shielding efficiency with absorption-dominant effect in electrospun carbon nanofibers by tailoring the addition of Co/Ni phase</i>
P33	Karolina Kosowska	<i>LINEARLY POLARIZED INFRARED MICROSCOPY METHODS IN POLYMER SCIENCE</i>
P34	Nicolo Allasia	<i>A Multitechnique Integrated Approach for Unveiling the Monoatomic Nature and Properties of Active Centers in Single-Atom Catalysts</i>
P35	Rafał Fanselow	<i>Examining the electronic structure of zinc selenide quantum dots for the development of novel hybrid plasmonic materials</i>
P36	Angelika Kmita	<i>X-ray absorption spectroscopy of advanced aerogel/liquid metal composites</i>
P37	Agnieszka Sysło	<i>MORPHOLOGICAL ANALYSIS OF 3D PRINTED CARBON DOT-BASED HYDROGELS USING SEM/AFM/NANO-FTIR/S-SNOM</i>
P38	Elżbieta Tądel	<i>NANOCOMPOSITE FILTERS BASED ON CARBON NANOFIBERS AND TiO<sub>2</sub> NANOPARTICLES FOR WATER PURIFICATION USING PHOTOCATALYTIC PROCESS AND SOLAR ENERGY</i>

<b>Poster N°</b>	<b>Presenting author</b>	<b>Abstract title</b>
P39	Dorota Lachowicz	<i>EVALUATION OF THE EFFECT OF POLYMER ON THE STRUCTURE AND STABILITY OF COPPER-ZINC FERRITE NANOPARTICLES</i>
P40	Bartłomiej Lemieszek	<i>Enhanced electrochemical performance of partially amorphous <math>La_{0.6}Sr_{0.4}CoO_{3-\delta}</math> oxygen electrode materials for low-temperature solid oxide cells operating at 400 °C</i>
P41	Katarzyna Ostrowska	<i>Operando Observation of Electrocatalyst Active Species during the Glucose Electrooxidation Reaction</i>
P42	Tomasz Kołodziej	<i>POLYX@SOLARIS: LAYOUT, SPECIFICATION &amp; FIRST RESULTS</i>
P43	Natalia Olszowska	<i>DEVELOPMENT OF URANOS BEAMLINE INFRASTRUCTURE</i>
P44	Tomasz Kołodziej	<i>Optical Design And Numerical Simulation Of The Upcoming Beamlines At SOLARIS Centre</i>
P45	Wojciech Błachucki	<i>High resolution X-ray emission spectroscopy at the PolyX beamline of SOLARIS</i>
P46	Anna Wach	<i>Development of in situ/operando spectroscopy at SOLARIS synchrotron: a powerful approach towards understanding catalysts and electrocatalysts</i>
P47	Liana Socaciu-Siebert	<i>NAP-XPS Instrumentation and Applications</i>

# L1

## CHALLENGES OF X-RAY CRYSTALLOGRAPHY: UNUSUAL MOLECULAR ARRANGEMENTS

Mirosław Gilski<sup>1,2</sup>

<sup>1</sup>*Faculty of Chemistry, Adam Mickiewicz University, Poznan, Poland*

<sup>2</sup>*Institute of Bioorganic Chemistry, Polish Academy of Sciences, Poznan, Poland*

\*E-mail: mirek@amu.edu.pl

X-ray macromolecular crystallography is a leading method for understanding the three-dimensional structure of proteins and nucleic acids. Despite the development of new research methods, such as Cryo-EM, crystallographic studies remain the most precise and reliable. However, some cases require unique procedures and deep structural analysis. These "difficult cases" are often abandoned after initial failures. However, studying such structures provides a unique opportunity to learn about nature's surprising abilities to create sophisticated molecular systems with various applications. The presented examples include the following crystal structures: (i) A supramolecular complex formed by encapsulating C60 fullerene in a molecular container built from two resorcin[4]arene rims zipped together by peptidic arms hydrogen bonded into a cylindrical  $\beta$ -sheet [1]. (ii) The crystal structure of a DNA-RNA chimeric duplex in complex with Ba<sup>2+</sup> ions, exhibiting complicated twinning (a combination of threefold and twofold rotation) and structural pseudosymmetry [2,3]. (iii) The modulated crystal structure of the ANS complex of Hyp-1 protein with 36 protein molecules and 156 ANS ligands (~ 50 000 non-H atoms) in the asymmetric unit of the supercell and commensurate ninefold modulation, manifested in the diffraction pattern by a wave of reflection-intensity modulation [4]. (iv) The potassium-independent L-asparaginase from *Phaseolus vulgaris*, comprised of eight ( $\alpha\beta$ )<sub>2</sub> dimers (~36 000 non-H atoms) with rare  $P_2$  symmetry and pseudosymmetric 4<sub>1</sub>-like helical packing, featuring a huge 18-stranded  $\beta$ -sheet of each dimer extended in both directions by similar  $\beta$ -sheets of its neighbors. An infinite helix running throughout the crystal forms a "protein double-helix".

- [1] Gilski, M., Drozdal, P., Kierzek, R. & Jaskolski, M. (2016). *Acta Cryst.* **D72**, 211–223.
- [2] Luo Z., Dauter Z. & Gilski M. (2017). *Acta Cryst.* **D73**, 940–951.
- [3] Gilski M. *et al.* (2020). *Acta Cryst.* **B76**, 815-824.
- [4] Smietanska, J. *et al.* (2020). *Acta Cryst.* **D76**, 653-667.

## L2

### THE IMPORTANCE OF SYNCHROTRON STUDIES IN VIEW OF THE DEVELOPMENT OF HYDROGEN INDUSTRY

Aleksandra Mielewczyk-Gryń<sup>1,\*</sup>, Iga Szpunar<sup>2</sup>, Joanna Pośpiech<sup>1</sup>, Jagoda Budnik<sup>1</sup>, Francis Oseko<sup>1</sup>, Sebastian Wachowski<sup>1</sup>, Agnieszka Witkowska<sup>1</sup>, Daniel Jaworski<sup>1</sup>, Arkadiusz Dawczak<sup>1</sup>, Tadeusz Miruszewski<sup>1</sup>, Maria Gazda<sup>1</sup>

<sup>1</sup>*Faculty of Applied Physics and Mathematics, Gdańsk University of Technology*

<sup>2</sup>*Faculty of Telecommunication, Electronics and Informatics, Gdańsk University of Technology*

\*e-mail: alegryn@pg.edu.pl

Materials engineering is crucial for the hydrogen industry as it enables the development of efficient and safe hydrogen storage systems, enhances fuel cell components, and supports the creation of robust infrastructure. Advanced materials are essential for storing hydrogen at high densities, improving fuel cell performance, and preventing issues like metal embrittlement in pipelines and tanks. Moreover, by advancing materials, the industry can significantly reduce costs and enhance the safety and efficiency of hydrogen production, storage, and transportation, thereby accelerating the transition to a sustainable hydrogen economy.

Over the last decade, more specific and sophisticated measuring methods have been used to determine the properties of materials for engineering solutions. Amongst them, synchrotron-related techniques are more and more often used to facilitate different studies.

In our case, since we study ceramic materials for protonic ceramic fuel cells, the most important data input that we can gain from synchrotron-based techniques is the one coming from both x-ray diffraction studies as well as from x-ray absorption spectroscopy (XAS). The choice of these techniques is related to the information about both crystalline and electronic structure that we can have a grasp on and at the same time to the capabilities of investigating bulk samples. The additional advantage of these techniques is the capability to measure samples in different conditions.

This talk will present how the XAS along with data from different techniques can help in understanding of properties of materials for the hydrogen industry and how these techniques can be useful not only for physicists but also for chemists and engineers.

#### **Acknowledgments**

The authors acknowledge the CERIC-ERIC Consortium for access to the Elettra Sinchrotrone Trieste and financial support under proposals 20177009 and 20187079. We also acknowledge SOLARIS Centre for the access to the PIRX o 181MS001, 191011, 201036, 231033, 231061, and ASTRA 221014, 231063, beamlines, where the measurements were performed.



## L3

### *IN-SITU AND OPERANDO SYNCHROTRON SMALL ANGLE X-RAY SCATTERING (SAXS) EXPERIMENTS, DESIGNED TO UNDERSTAND NANOPARTICLES ASSEMBLIES IN COMPLEX BIO-ENVIRONMENTS*

Prof. Dr. Guillaume BROTONS

*IMMM, Institut des Molécules et des Matériaux du Mans, Le Mans Université / CNRS-UMR  
6283, France*

\*e-mail: guillaume.brotons@univ-lemans.fr

Over the last decades, advances in synchrotron instrumentation resulted in new strategies to collect X-rays at very small scattering angles. This signal contains all the features of the mesoscopic structure and interactions of nanoparticles in solutions or materials (SAXS techniques, X-ray coherent imaging, ...).

Synchrotrons somehow opened the way to in-situ time resolved and operando X-ray scattering experiments, which are changing our understanding of nanoscience by revealing how colloidal and molecular interactions come into play at small scales and times in solution.

To illustrate such approaches and to identify fundamental questions that remain to be answered in soft matter and biophysics, selected synchrotron experiments will be discussed from the perspective of health and environmental societal challenges:

in the field of galenic and medicine, for Drug Delivery Systems formulation via microfluidics;

in the field of biomaterials for synthetic bone transplant scaffold growth from bioglass nanoparticle solutions;

and in the field of nanoparticles plastic pollutants, in order to understand their fate in the environment and, more particularly, in biotic and abiotic aqueous compartments.

# L4

## TIME-RESOLVED RIXS AND SAXS AT THE SCS INSTRUMENT OF EUROPEAN XFEL

Giuseppe Mercurio<sup>1,\*</sup>

<sup>1</sup>*European XFEL, 22869 Schenefeld, Germany*

\*e-mail: giuseppe.mercurio@xfel.eu

The Spectroscopy and Coherent Scattering (SCS) instrument of the European X-ray free-electron laser (EuXFEL) provides time-resolved tools to investigate electronic, spin and lattice structure of complex materials and reveal the material dynamics on the nanometer length scale and the femtosecond time scale using optical lasers as pump and soft X-rays as probe.

Femtosecond lasers are important tools to modify and control the properties of quantum materials on ultrashort time scales. Resonant inelastic X-ray scattering (RIXS) spectroscopy has emerged over the last decades as a powerful method to explore low-energy orbital, spin, lattice and charge excitations in quantum materials. The main limiting factor to attain RIXS at high energy- and time-resolution is the low repetition rate and photon flux of the first-generation XFEL. Taking advantage of the Megahertz repetition rate of the EuXFEL, the high-resolution spectrometer of the Heisenberg User consortium (hRIXS) enables users to perform RIXS spectroscopy of material dynamics in nonequilibrium with unprecedented time- and energy-resolution [1]. We report from the user-assisted commissioning program addressing charge transfer (CT) excitations in NiO transition metal oxide. The paradigmatic charge transfer insulator and antiferromagnet NiO were excited across the CT gap by a 50 fs laser pulse at 266 nm. We observe the initial creation of localized charge transfer excitons, and their subsequent decay with a time constant of about 2 ps into a metastable state that persists over several tens of ps. These first results demonstrate the potential of time-resolved RIXS at MHz-repetition rate XFELs to explore nonequilibrium dynamics of quantum materials.

Furthermore, in the context of topological states of matter, a key challenge is the fast creation of topological phases, which requires massive reorientation of charge or spin degrees of freedom. Here we report the picosecond emergence of an extended topological phase that comprises many magnetic skyrmions [2]. The nucleation of this phase, followed in real time via single-shot small angle X-ray scattering (SAXS) after infrared laser excitation, is mediated by a transient fluctuation state. This state is enabled by the presence of a time-reversal symmetry-breaking perpendicular magnetic field and exists for less than 300 ps. These observations provide fundamental insights into the nature of topological phase transitions, and together with atomistic spin dynamics simulations, lead to a detailed microscopic understanding of all-optical topological switching.

[1] Schlappa et al., arXiv:2403.08461v1

[2] Büttner et al., Nature Materials 20, 30 (2021)

# L5

## INVESTIGATING THE ELECTRONIC STRUCTURE OF MOLECULES IN SOLUTION WITH X-RAY SPECTROSCOPY

Nils Huse,<sup>1,\*</sup>

<sup>1</sup>*University of Hamburg, Department of Physics, 22761 Hamburg, Germany*

\*e-mail: nils.huse@uni-hamburg.de

This contribution will present applications of soft and tender X-ray absorption spectroscopy (XAS) and resonant inelastic X-ray scattering (RIXS) to small molecules in solution to probe their electronic charge density by and of quantum chemical modeling. This information allows to correlate charge density and molecular structure in order to understand their interplay and thereby inform on basic principles of chemical bonding as well as light induced reactions.

Heteroatoms in small organic molecules strongly influence function and chemical reactivity. Such atoms, thus, present good targets of element-specific probes such as X-ray absorption and emission spectroscopy. XAS is not only specific to a chemical element but also to its chemical environment, allowing to distinguish bond order and valence charge differences of atoms of a particular element. RIXS as a form of resonant Raman scattering can provide vibrational and valence excitation spectra from tens of meV to tens of eV. Applications of XAS and RIXS to core-level resonances of nitrogen and sulfur atoms in fully solvated organic molecules provide observables that can be compared to quantum chemical simulations. In combination with pulsed ultraviolet (UV) lasers, time-resolved spectroscopy enables spectral measurement of transient photoproducts to study photochemical reaction pathways with elemental specificity.

The molecules that were studied include formamides<sup>1</sup> (as important solvents and building blocks of peptides), diazines<sup>2,3,4,5</sup> (as building blocks of molecules important in biological contexts such as DNA) and disulfides<sup>6</sup> (containing a sulfur-sulfur bond which represents an important bond motif in proteins and materials).

---

<sup>1</sup> M. Ochmann, V. Vaz da Cruz, S. Eckert, N. Huse, A. Föhlisch, *Chem. Comm.* **58**, 8834-8837 (2022)

<sup>2</sup> S. Eckert, V. Vaz Da Cruz, M. Ochmann, I. Von Ahnen, A. Föhlisch and N. Huse, *J. Phys. Chem. Lett.* **35**, 3-8643 (2021)

<sup>4</sup> A. Freibert, D. Mendive-Tapia, N. Huse, O. Vendrell, *J. Chem. Theory Comput.* **20**, 2167-2180 (2024)

<sup>5</sup> A. Freibert, D. Mendive-Tapia, O. Vendrell, N. Huse, 'A fully dynamical description of time-resolved resonant inelastic X-ray scattering of pyrazine', *Phys. Chem. Chem. Phys.* **accepted** (2024)

# L6

## DEVELOPMENT OF PTYCHOGRAPHIC IMAGING WITH SOFT X-RAYS

Tim A. Butcher<sup>1,2\*</sup>

<sup>1</sup>*Paul Scherrer Institut, 5232 Villigen PSI, Switzerland*

<sup>2</sup>*Max Born Institute for Nonlinear Optics and Short Pulse Spectroscopy,  
12489 Berlin, Germany*

\*e-mail: tim.butcher@psi.ch

X-ray microscopy in the soft X-ray regime allows chemical and magnetic characterization of numerous technologically relevant materials. The visualization of magnetic or ferroelectric textures is enabled by dichroic contrasts with circularly or linearly polarized X-rays at the L-edges of 3d transition metals and M-edges of the rare earths. Scanning transmission X-ray microscopy (STXM) is well established at synchrotron light sources, but the coherent diffractive imaging method of ptychography is necessary to unlock spatial resolutions below 10 nm. This technique is well suited to study ferroic orders in nanoparticles or thin films of materials such as the room temperature multiferroic bismuth ferrite [1]. An overview of results obtained with the new SOPHIE endstation (Soft X-ray Ptychography Highly Integrated Endstation) of the Microspectroscopy group at the Swiss Light Source (Villigen, Switzerland) and currently at the SoftiMAX beamline at MAX IV (Lund, Sweden) will be given.

[1] T. A. Butcher et al. *Adv. Mater.* 36, 23 (2024); <https://doi.org/10.1002/adma.202311157>

# L7

## NANO-FTIR SPECTROSCOPY OF SINGLE CELL SECTIONS

Martin Schnell

*CIC nanoGUNE, Tolosa Hiribidea, 76, E-20018 Donostia / San Sebastian*

\*e-mail: mschnelloptics@gmail.com

We demonstrate high-sensitivity near-field infrared (IR) spectroscopy (nano-FTIR) for the label-free investigation of single cell cuts. We show that IR absorption of individual sub-cellular regions can be spectroscopically measured and small but consistent spectral differences can be resolved. This capability has the potential to pinpoint chemical changes at the cellular ultrastructural level when disease occurs. We will also discuss that nano-FTIR can be combined with synchrotron light sources for single-shot characterization of molecular vibrations but also phononic and plasmonic excitations in a large spectral range with nanoscale spatial resolution.

# L8

## CRYOEM – A PERFECT TOOL FOR INVESTIGATION OF PROTEIN CAGES POLYMORPHISM

Artur Biela<sup>1,\*</sup>

<sup>1</sup>National Synchrotron Radiation Center SOLARIS, 30-392 Kraków, Poland

\*E-mail: artur.biela@uj.edu.pl

Protein cages are complex, symmetrical, often spherical and hollow structures. They are of great interest to researchers because of their ability to act as protective containers for the delivery of medically useful substances to cells. The design and construction of artificial, fully synthetic protein cages is an approach by which it is possible to create cages with non-standard properties that do not occur naturally in nature. Determining the structures of artificial protein cages can confirm that they do (or do not) match the assumptions set out in the original design. Cryogenic electron microscopy (cryoEM) has proven to be an ideal method for this type of analysis.

This work will be a summary of what have been done in this field, especially with use of cryoEM as a tool for deciphering structural details of modified protein cages; both: natural (based on MS2 bacteriophage<sup>1</sup>) and artificial (based on trp-attenuation protein (TRAP)<sup>2-5</sup>). The polymorphism discussed here will be induced by an experimentator and his/her design. In both cases (MS2 and TRAP cages) the polymorphism has never been seen nor described before.

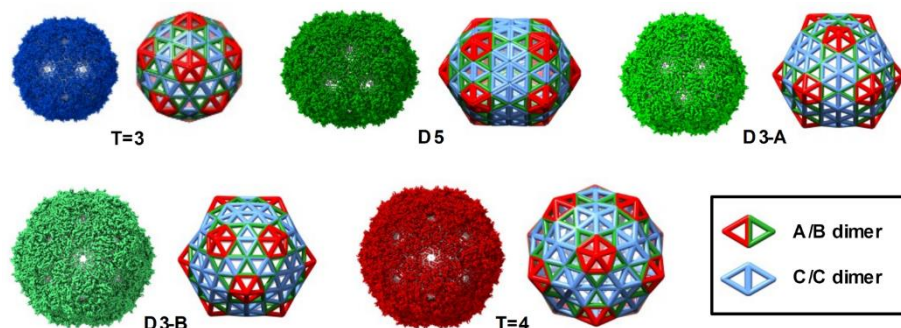


Figure 1. Polymorphic variants of MS2 VLPs with their respective wireframe models

1. Biela, A. *et al.* Programmable polymorphism of a virus-like particle. *Communications Materials* 3, 7 (2022)
2. Stupka, I. *et al.* Chemically induced protein cage assembly with programmable opening and cargo release. *Science Advances* 8, (2022)
3. Sharma, M. *et al.* Shape-Morphing of an Artificial Protein Cage with Unusual Geometry Induced by a Single Amino Acid Change. *ACS Nanoscience Au* 2, 5 (2022)
4. Majsterkiewicz, K. *et al.* Artificial protein cage with unusual geometry and regularly embedded gold nanoparticles. *Nano Letters*. 8 (2022)
5. Stupka, I. *et al.* An artificial protein cage made from a 12-membered ring. *Journal of Material Chemistry B*. (2023)

# O1

## ADVANCED SOFTWARE TOOLS AND WORKFLOWS FOR SYNCHROTRON X-RAY SCATTERING ANALYSIS AT ESRF FROM A USER'S PERSPECTIVE

Maciej Jankowski,<sup>1</sup>

<sup>1</sup> *The European Synchrotron Radiation Facility – ESRF, 71 Avenue des Martyrs, CS  
40220, Grenoble Cedex 9, 38043 France*

\*E-mail: [maciej.jankowski@esrf.fr](mailto:maciej.jankowski@esrf.fr)

In this presentation, we will take the scientific perspective of a researcher working at the synchrotron beamline and utilizing the available software tools. As a user coming to the synchrotron, it's essential to understand the software tools and workflows that are at your disposal and how they can facilitate efficient data analysis in synchrotron X-ray scattering techniques.

We will introduce the collaborative software tools and workflows utilized at the ESRF synchrotron for data analysis related to X-ray scattering techniques. Specifically, we'll present key software technologies such as EWOKS, integrated with BLISS software for beamline control, SILX, a Python package offering essential tools for data science and analysis, and tools dedicated to the reduction of X-ray diffraction data from 2D X-ray detectors.

Additionally, we will look at the digital ecosystem at ESRF, including the Linux cluster for data analysis, the Virtual Infrastructure for Scientific Analysis (VISA) platform, and the web-based environment for working with Jupyter notebooks. These platforms and tools are crucial in accelerating scientific discoveries and advancing synchrotron radiation research.

## STUDIES OF THE LOCAL STRUCTURE OF AMORPHOUS PHARMACEUTICALS USING X-RAY SCATTERING

Karolina Jurkiewicz,<sup>1,\*</sup> Taoufik Lamrani,<sup>1</sup> Joanna Grelska,<sup>1</sup> and Anna Janowska,<sup>1</sup>

<sup>1</sup>*Institute of Physics, University of Silesia in Katowice, 41-500 Chorzów, Poland*

\*E-mail: karolina.jurkiewicz@us.edu.pl

Low aqueous drug solubility in pharmaceuticals is a pervasive issue. It is estimated that around 70% of pipeline drugs in development today are poorly soluble molecules. Amorphization and formation of solid dispersions using crystalline structures of active pharmaceutical ingredients is one of the most effective methods to enhance their solubility and bioavailability as well as to reduce side effects. However, different methods of the production (vitrification, milling, compression, solvation) of amorphous-like drugs and applied conditions (temperature, pressure, frequency) may affect their atomic-scale structure and yield different properties such as physical stability and solubility. Therefore, the characterization of the correlations between the preparation method, structure and properties is a prerequisite to the wider commercialization of amorphous-like drugs.

In this contribution, we would like to present our recent studies of the atomic and supramolecular structure of amorphous-like pharmaceuticals (such as ritonavir, probucol, itraconazole) using laboratory and synchrotron X-ray scattering methods, including high-pressure in-situ X-ray diffraction and pair-distribution function. The analysis of very subtle differences in the amorphous-like structures is supported by molecular dynamics simulations and modeling, vibrational and dielectric spectroscopy, and other complementary techniques. We will demonstrate that the amorphous like-phases, which give very similar, on the first sight, diffraction patterns, may significantly differ in the intermolecular architecture, degree of the local order and the size of coherent domains, H-bonding pattern, and molecular conformations.

Authors acknowledge financial support from the National Science Centre (Poland), grant number: Opus 21 No. 2021/41/B/NZ7/01654, and the European Synchrotron Radiation Facility (ESRF), Grenoble, France, ID15B and ID22 beamlines (proposals: SC-5158, HC5404). The access to ESRF was financed by the Polish Ministry of Education and Science – decision number: 2021/WK/11.



## UNVEILING THE ACTIVE SITES IN CO-CONTAINING PEROVSKITE-BASED PHOTORECHARGEABLE BATTERIES

Taymaz Tabari,<sup>1,\*</sup> Przemysław Łabuz,<sup>1</sup> Alexey Makimenko,<sup>2</sup> Zbigniew Sojka,<sup>1</sup>  
and Wojciech Macyk<sup>1</sup>

<sup>1</sup>*Faculty of Chemistry, Jagiellonian University, 30-387, Kraków, Poland.*

<sup>2</sup>*SOLARIS National Synchrotron Radiation Centre, Jagiellonian University, 30-392, Kraków, Poland*

*\*E-mail: taymaz.tabari@uj.edu.pl*

The growing interest in flexible electronics and artificial intelligence has heightened the need for multifunctional power sources, drawing attention from scientific and technological sectors. Photo-rechargeable batteries are central to developing efficient self-powering devices, particularly lithium-ion batteries (LIBs), which are commercially successful with a theoretical energy density of 400 W h kg<sup>-1</sup>. However, lithium is limited, and its electrolytes are toxic and flammable. Alternatively, zinc-ion batteries (ZIBs), with safe aqueous electrolytes, abundant zinc, and effective oxygen evolution and reduction catalysts, offer a theoretical energy density of 1350 W h kg<sup>-1</sup>, making them a promising LIB replacement. ZIB performance relies on efficient oxygen evolution (OER) and reduction (ORR) reactions. IrO<sub>2</sub> and Pt are active OER and ORR electrocatalysts, which are rare and costly. The ABO<sub>3</sub> perovskites, with tunable structures, allow manipulation of A- and B-sites with different atoms. B-sites are crucial in reactions like OER and ORR, and changes in A- and B-site compositions affect their catalytic properties and electronic structure.<sup>1</sup> The electronic properties of electrocatalysts were analyzed using X-ray absorption and UV photoelectron spectroscopies. Controlling cobalt ion oxidation states enhances battery capacity and energy density, while ORR activity is influenced by oxygen vacancies related to the Co<sup>2+</sup>/Co<sup>3+</sup> ratio and the high spin d<sup>7</sup> electron configuration.<sup>2</sup>

### Acknowledgments

The work was financially supported by “Excellence Initiative — Research University” program at the Jagiellonian University in Kraków (U1U/W20/NO/17.05) and the National Science Centre, Poland (2022/45/B/ST5/04087). AM acknowledges the Polish Ministry for Higher Education for “Support for research and development with the use of research infrastructure of the National Synchrotron Radiation Centre SOLARIS” (1/SOL/2021/2) and EU Horizon2020 program (952148-Sylinda) for developing ASTRA beamline.

### References

- (1) Tabari, T.; Kobieliusz, M.; Duch, J.; Singh, D.; Kotarba, A.; Macyk, W. *Applied Catalysis B: Environmental* **2020**, 272, 118952.
- (2) Tabari, T.; Łabuz, P.; Singh, D.; Maximenko, A.; Gryboś, J.; Mathur, S.; Sojka, Z.; Macyk, W. *Applied Catalysis B: Environment and Energy* **2024**, 358, 124425.

## DIVING DEEP INTO NON-STOICHIOMETRIC PEROVSKITES: UNVEILING CO/FE DOPING EFFECTS

Paulina Gwóźdz, <sup>1,\*</sup> Alexey Maximenko<sup>2</sup>, Agnieszka Łącz<sup>1</sup>, Ewa Drożdż<sup>1</sup>

<sup>1</sup> AGH University of Krakow, Faculty of Materials Science and Ceramics  
al. A. Mickiewicza 30, 30-059 Krakow, Poland

<sup>2</sup> SOLARIS National Synchrotron Radiation Centre, Jagiellonian University,  
Krakow, 30-392, Poland

\*E-mail: gwozdz@agh.edu.pl

Perovskite materials with the general formula  $ABO_3$  have shown significant potential in applications for catalysis and in electrochemical devices. The functional properties of these materials can be controlled by doping with selected metals, primarily d-block elements. This doping process involves introducing atoms on aliovalent or/and isovalent oxidation states into the perovskite lattice, replacing host atoms, and thereby altering the crystal structure, electron band configuration, and defect chemistry. These changes can modify the material's functional properties.

Materials based on the binary system  $CaTiO_3$ - $SrTiO_3$  modified with cobalt (Co) or iron (Fe) were prepared using the modified citrate method. For each dopant (Co, Fe), two series of materials were obtained, differing in the presence of a 5% deficiency in the Ca/Sr sublattice and calcium content. All compositions were obtained in form of powders after calcination at  $900^\circ\text{C}$  and characterized in terms of their structure (XRD, XAS), microstructure (SEM), and reducibility in an  $H_2$ -containing atmosphere (TPR). The aim of this study was to investigate the incorporation of Co or Fe into the perovskite structure, the potential formation of oxides, and the effect of non-stoichiometry in the A sublattice (Sr/Ca) on the amount of dopant incorporated into the titanium sublattice.

The primary objective was to assess the impact of these modifications on the electronic and local structure of cobalt and iron dopants. Incorporating small amounts of a modifier into a perovskite structure presents unique analytical challenges, as traditional methods such as X-ray diffraction (XRD) often fail to detect these small quantities or identify amorphous phases within the material. To address these challenges, advanced techniques such as X-ray absorption spectroscopy (XAS) combined with temperature-programmed reduction (TPR), were employed. This approach provides a detailed understanding of the material's composition.

### Acknowledgments

Acknowledgments: Research project supported by the subsidy no. 16.16.160.557 of the Polish Ministry of Science and Education. Part of the experimental results were accomplished by using of ASTRA beamline at SOLARIS synchrotron which development was supported within the EU Horizon2020 program (952148-Sylinda).

SYNCHROTRON RADIATION BASED TECHNIQUES  
FOR AGRICULTURAL RESEARCH

Josef Hormes<sup>1,2\*</sup>, Lisa Langlois<sup>2</sup>, Alexey Maximenko<sup>3</sup>, Henning Lichtenberg<sup>4</sup>,  
Alexander Prange<sup>4</sup>

<sup>1</sup> Institute of Physics, Rheinische Friedrich-Wilhelms- University, Nussallee 12,  
D-53115 Bonn, (Germany)

<sup>2</sup> Center for Advanced Microstructures and Devices (CAMD), Louisiana State University,  
6980 Jefferson Hwy., Baton Rouge, LA 70806, (USA)

<sup>3</sup> SOLARIS, National Synchrotron Radiation Centre, Jagiellonian University,  
ul. Czerwone Maki 98, 30-392 Krakow (Poland)

<sup>4</sup> Hochschule Niederrhein, University of Applied Sciences, Reinarzstr. 49, D-47805 Krefeld  
(Germany)

\*Email: Hormes@physik.uni-bonn.de

Macrominerals (e.g. Ca, P, Na, S) and microminerals (e.g. Fe, Mn, Cu, Zn, Se) are of crucial importance for the wellbeing and a healthy development not just for humans but also for animals and plants. In most cases the origin of these nutrients are minerals in the soil (and in some cases also fertilizers) taken up by plants before going as food either directly or via animals into the human body. Today for humans also the uptake via food supplements is quite common. In many cases the biological/chemical reactions taking place during all these processes are not well understood and specifically for many elements the chemical form with the best bioavailability is not known!

Here synchrotron radiation (SR) based techniques are extremely useful for improving the understanding of these processes. SR based X-ray fluorescence, for example, gives quantitative information about the elemental composition of minerals in soil, plants, and food. However, more important is the information about the chemical state of a specific element and the changes of this state on its way into the human body! This information is provided element specific and without any wet-chemistry by X-ray absorption spectroscopy.

In this talk examples will be presented for the analysis of minerals in plants, food, and food supplements. “Quasi in-situ measurements” will be discussed as a demonstration of the capability of SR techniques for the investigation of the processes taking place at the uptake of minerals by plants, animals and humans.

QUANTITATIVE LOCATING TITANIUM IN THE FRAMEWORK OF  
TITANIUM SILICALITE-1 BY EXPLOITING ANOMALOUS X-RAY  
POWDER DIFFRACTION

Przemyslaw Rzepka,<sup>1,2,3\*</sup> Matteo Signorile,<sup>4</sup> Thomas Huthwelker,<sup>5</sup> Stefano Checchia,<sup>6</sup>  
Francesca Rosso,<sup>4</sup> Silvia Bordiga,<sup>4</sup> Jeroen A. van Bokhoven<sup>2,3</sup>

<sup>1</sup> *J. Heyrovsky Institute of Physical Chemistry Dolejškova 2155/3, 182 23 Prague 8,  
Czech Republic*

<sup>2</sup> *Institute for Chemical and Bioengineering, ETH Zurich; 8093 Zurich, Switzerland* <sup>3</sup>  
*Paul Scherrer Institute, Center for Energy and Environmental Sciences, PSI; 5232  
Villigen, Switzerland*

<sup>4</sup> *Department of Chemistry, NIS and INSTM Reference Centre, Università di Torino,  
Via G. Quarello 15, I-10135 and Via P. Giuria 7, I-10125, Torino, Italy*

<sup>5</sup> *Swiss Light Source, PSI; 5232 Villigen, Switzerland*

<sup>6</sup> *ID 15A, European Synchrotron Radiation Facility 71 Avenue des Martyrs, 38000  
Grenoble, France*

\*E-mail: [przemyslaw.rzepka@jh-inst.cas.cz](mailto:przemyslaw.rzepka@jh-inst.cas.cz)

One of the major challenges in developing improved zeolite-based catalysts is the lack of methods for accurately locating light heteroatoms on the T-sites within zeolite frameworks. Titanium silicalite-1 (TS-1), a Ti-containing zeolite-type catalyst, is commonly employed in partial oxidation reactions using H<sub>2</sub>O<sub>2</sub>, such as aromatic hydroxylation and olefin epoxidation. The configuration of titanium sites, which replace silicon in the zeolite framework, plays a crucial role in controlling the reaction mechanism. However, these sites remain unidentified, hindering a fundamental understanding of the catalytic processes involved.

This study aims to quantitatively determine the distribution of heteroatoms within the zeolite-type framework using anomalous X-ray powder diffraction (AXRD) and by examining changes in the titanium X-ray scattering factor near the Ti K-edge (4.96 keV). Two TS-1 samples, each containing approximately 2 Ti atoms per orthorhombic unit cell with 12 T-sites, were analyzed. The results revealed that about half of the titanium atoms were predominantly located at sites T3 and T9, with the remaining titanium dispersed among various T-sites within both frameworks. One of the structures exhibited significant non-framework titanium within the micropores of a more distorted lattice. In both samples, isolated titanium atoms were more prevalent than dinuclear species, which could only potentially emerge at site T9 with a substantial energy penalty and were not detected.

Franciszek Sobczuk<sup>1\*</sup><sup>1</sup>*Solaris National Synchrotron Radiation Centre, Jagiellonian University,**Czerwone Maki 98, 30-392 Kraków, Poland*\*E-mail: [franciszek.sobczuk@uj.edu.pl](mailto:franciszek.sobczuk@uj.edu.pl)

Solving of **inverse problems** is a crucial challenge in many fields of experimental physics. For example, in high resolution optical spectroscopy, deconvolution of the light spectrum from interferograms is frequently needed. From mathematical point of view it could be treated as a solution of the Friedholm equation of the first kind

$$g(x) = \int_a^b k(x, s)u(s)ds \quad (1)$$

with respect to the function  $u(s)$ , where  $k(x, s)$  is an apparatus function of the used interferometer [1]. From the other side, the same mathematical problem emerges in the processing of data originating from X-ray synchrotron radiation scattering experiments, for example SAXS (*small angle X-ray scattering*) technique [2]. In this case, inverse Fourier transform of square of the auto-correlation function  $\rho^2(r)$

$$I(q) = 4\pi \int_0^\infty r^2 \rho^2(r) \frac{\sin qr}{qr} dr \quad (2)$$

is measured with respect to the momentum transfer variable  $q$ . In order to process the data one have to deconvolve the function  $\rho^2$ .

In the most general way this kind of problem could be described using operator equation

$$Ks = u,$$

where  $K$  is some known operator which describes operation of the experimental setup, vector  $u$  represents the data and  $s$  is the searched observable. Unfortunately, almost all inverse problems emerging from experimental data are so called **ill – posed problems with noisy data**. It means, that it is impossible to solve it by simple inversion of the operator  $K$  and some regularization method is required.

During my presentation I will show how the Tikhonov regularization method [3] could be applied for the optical problem (1). I will also present some suggestions how this solution could be re-implemented for the SAXS problem (2).

- [1] B. Heeg, J.B. Abbiss, *Piezospectroscopic imaging with a tunable Fabry–Perot filter and Tikhonov reconstruction*, Optics Letters **32**, 7, 859-861 (2007).
- [2] S.P. Meisburger, D. Xu, N. Ando, *REGALS: a general method to deconvolve X-ray scattering data from evolving mixtures*, IUCrJ **8**, 2, 225-237 (2021).
- [3] J. Honerkamp, J. Weese, *Tikhonovs regularization method for ill-posed problems*. Continuum Mech. Thermodyn **2**, 17–30 (1990).

## SCIENTIFIC OPPORTUNITIES AT XFEL

Ryszard Sobierajski<sup>1,\*</sup>, Wojciech Gawęda<sup>2</sup>, Adam Glinka<sup>2</sup>, Katarzyna Jarzemska<sup>3</sup>,  
Radosław Kamiński<sup>3</sup>, Maciej Kozak<sup>2</sup>, Jacek Kubicki<sup>2</sup>, Dagmara Milewska<sup>4</sup>

<sup>1</sup> *Instytut Fizyki PAN, al. Lotników 32/46, 02-668 Warszawa*

<sup>2</sup> *Wydział Fizyki, Uniwersytet im. Adama Mickiewicza w Poznaniu, ul. Uniwersytetu  
Poznańskiego 2, 61-614 Poznań*

<sup>3</sup> *Wydział Chemii, Uniwersytet Warszawski, Żwirki i Wigury 101, 02-089, Warszawa*

<sup>4</sup> *Narodowe Centrum Badań Jądrowych, ul. Andrzeja Soltana 7, 05-400 Otwock-Świerk*

\*E-mail: [ryszard.sobierajski@ifpan.edu.pl](mailto:ryszard.sobierajski@ifpan.edu.pl)

The European X-ray Free Electron Laser (EuXFEL) is an international laboratory where intense ultrashort pulses X-rays are generated and applied in scientific research. It contributes to the significant expansion of our knowledge in many scientific disciplines (m.in. medicine, pharmacology, chemistry, materials science, nanotechnology, energy and electronics) and the emergence of new technologies affecting our daily lives [1]. During the presentation, a Project financed by the Ministry of Science and Higher Education to support the Polish scientific community in the use of new research opportunities offered by EuXFEL will be presented [2]. The project includes the following activities:

1. training in basic knowledge of XFEL applications and research techniques used, including several months of internships for young researchers at institutions participating in XFEL research and a lecture on XFEL for undergraduate and doctoral students;
2. funding the participation of Polish scientists in conferences and workshops on XFEL research;
3. assistance in establishing or expanding scientific contacts with EuXFEL employees and/or research groups carrying out similar research in Poland and abroad;
4. assistance in the preparation of research projects in competitions for measurement time on XFEL sources, also by performing pilot and complementary studies.

The lecture will end with a presentation by the Network of Centres of Excellence in the field of research using XFEL (CD XFEL), in which the above program is implemented.

[1] [https://biuletyn.synchrotron.org.pl/wp-content/uploads/2023/12/Biuletyn\\_all\\_12\\_2023.pdf](https://biuletyn.synchrotron.org.pl/wp-content/uploads/2023/12/Biuletyn_all_12_2023.pdf)

[2] [www.ifpan.edu.pl/cd-xfel](http://www.ifpan.edu.pl/cd-xfel)

Co-financed by the Ministry of Science and Higher Education program "Support for the participation of Polish research teams in international research infrastructure projects", based on contract No. 2022/WK/13.

TOWARDS NEW TIME AND FREQUENCY STANDARDS WITH  $^{45}\text{Sc}$  AND  
EuXFELTomasz Kołodziej<sup>1\*</sup><sup>1</sup>*SOLARIS National Synchrotron Radiation Centre, Jagiellonian University, Kraków,  
Poland*

\*E-mail: t.kolodziej@uj.edu.pl

Nowadays, the most precise clocks are atomic clocks. These devices use the transition of cesium ( $^{133}\text{Cs}$ ) atoms between two electronic states to control the frequency and they can measure time with an accuracy of 1 second within 300 million years. To improve this precision, scientists want to use the resonant transition between the ground and excited levels of the nuclei of long-lived isomers.

An international team of scientists from the United States and Europe led by Yuri Shvyd'ko of Argonne National Laboratory (USA), with the participation of Tomasz Kołodziej of SOLARIS, excited successfully for the first time with x-rays an isomeric state in Scandium-45 – the sharpest quantum transition in hard x-ray regime.

European XFEL in the so-called self-seeding mode provided an X-ray beam with an appropriate spectral density to excite the desired resonance. At the MID beamline, 25-micrometer thick scandium foils were irradiated with an X-ray laser beam, and resonance was observed by the time-delayed emission of the characteristic  $K_{\alpha}$  and  $K_{\beta}$  radiation by scandium atoms. Using sophisticated noise reduction techniques and high-resolution X-ray optics, the resonant transition energy was determined with an unprecedented accuracy to 5 decimal places, (12.38959 keV). The width of the resonance is about a million times smaller than in the Mössbauer isotope of iron  $^{57}\text{Fe}$  (it still remains to be measured precisely in the further steps), which in turn gives a time measurement accuracy on the order of 1 s per 300 billion years, i.e. 1,000 times better than previously achieved in atomic clocks.

The resonant excitation of the scandium-45 isomer together with precise determination of the resonance energy (previously known only with an accuracy of  $\pm 50$  eV) opens up completely new possibilities for the construction of ultra-precise clocks (the so-called atomic nuclear clock), in spectroscopy and metrology with previously unattainable resolutions, and new measurements of basic physical quantities.

**Reference:**

Shvyd'ko, Y., Röhlberger, R., Kocharovskaya, O., (...) & Kołodziej, T. “Resonant X-ray excitation of the nuclear clock isomer  $^{45}\text{Sc}$ ”, *Nature* **622**, 471–475 (2023)

## HOW PEEM HELPS IN THE STUDY OF ANTIFERROMAGNETS?

E. Madej<sup>1,\*</sup>, K. Freindl<sup>1</sup>, J. Korecki<sup>1</sup>, N. Kwiatek<sup>1,2</sup>, E. Młyńczak<sup>1</sup>,D. Wilgocka-Ślęzak<sup>1</sup>, M. Zając<sup>2</sup>, N. Spiridis<sup>1</sup><sup>1</sup>*Jerzy Haber Institute Of Catalysis And Surface Chemistry Polish Academy Of Sciences,  
Krakow, Poland*<sup>2</sup>*Solaris National Synchrotron Radiation Centre, Jagiellonian University, Krakow, Poland*

\*e-mail: ewa.madej@ikifp.edu.pl

Antiferromagnetic (AFM) films are components of spintronic devices due to robustness against magnetic field perturbations, fast spin dynamics, and lack of stray fields. Here, we use an ultrathin ferromagnetic (FM) epitaxial Co layer to control the antiferromagnetic state of a hematite film on Pt(111), similarly as previously presented for the CoO/Fe system [1].

The XMCD-PEEM (Co edge) and XMLD-PEEM (Fe edge) measurements were performed at the SOLARIS synchrotron [2]. PEEM images of FM Co domains in 1 nm Co/ $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> and AFM domains in 10 nm  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> in the as-grown sample are shown in the left column in Fig. 1. By using permanent magnets (140 mT), we were able to remagnetize the sample in the PEEM microscope. Noteworthy, while the bare hematite film resisted the magnetic field, the AFM  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> domains beneath the Co layer followed the remagnetization process of the cobalt film, as shown in the middle and right columns, for the magnetic field perpendicular and parallel to the direction of the X-ray beam, respectively. This observation confirms the expectation that the Pt/hematite/FM system is very promising from the perspective of spintronic applications [3].

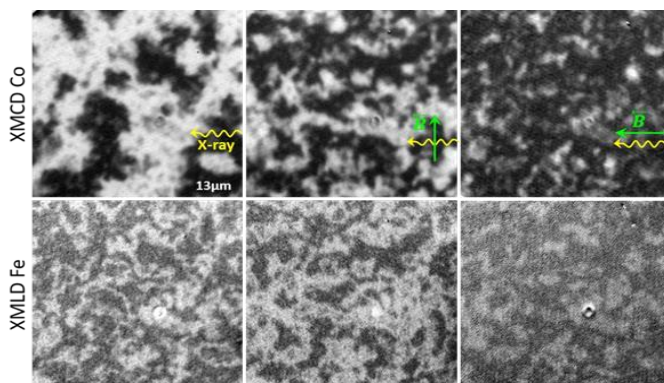


Fig 1. PEEM images of FM Co domains (top) and AFM  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> domains (bottom row) in Co/ $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> system. Arrows show orientations of the X-ray beam and external magnetic field.

Research funded by National Science Centre, Poland, grant number 2020/39/B/ST5/01838.

[1] M. Ślęzak et al., Sci. Rep. Vol 9, 2019, 8188-8193

[2] J. Szlachetko et al., Poland, Eur. Phys. J. Plus. Vol 138, 2023, 1-10

[3] A. Kozioł-Rachwał et al., Phys. Rev B. Vol 106, 2022, 104419



## Ultrathin Sn deposited on Pt(111): growth and electronic structure

E. Młyńczak<sup>1</sup>, D. Wilgocka-Ślęzak<sup>1</sup>, E. Madej<sup>1</sup>, A. Surendran<sup>1</sup>, S. Shaju<sup>1</sup>, G. Bihlmayer<sup>2</sup>  
and N. Spiridis<sup>1</sup>

<sup>1</sup>*Jerzy Haber Institute of Catalysis and Surface Chemistry, Polish Academy of Sciences,  
Poland*

<sup>2</sup>*Peter Grünberg Institute, Forschungszentrum Jülich, Germany*

Email: ewa.mlynczak@ikifp.edu.pl

Sn films grown on Pt(111) have been the subject of considerable scientific interest thanks to their interesting catalytical properties. It is known that adding Sn to Pt results e.g. in improved stability, much higher selectivity for isomerization and aromatization in hydrocarbon conversion reactions as well as improved performance in the CO oxidation [1]. However, the mechanism responsible for such beneficial effects is not clear yet, with the effects of strain and modification of the electronic structure suggested to play a role [2].

We have studied the Sn growth on Pt(111) at room temperature using low energy electron microscopy (LEEM) tracking changes in the sample structure with the amount of deposited material. Among others, we have identified the  $\sqrt{3} \times \sqrt{3}$  (R 30°) room temperature (RT) phase, present for approximately 0.3 ML coverage, which we have further investigated using photoemission electron microscopy (PEEM) at the DEMETER beamline in Solaris synchrotron in Krakow. When slightly larger amount of Sn grown on Pt(111) is annealed to 200°C, a high temperature (HT) phase is formed, showing LEED with the same  $\sqrt{3} \times \sqrt{3}$  (R 30°) pattern. We have studied the electronic structure of both RT and HT phases using angle-resolved photoelectron spectroscopy at the Phelix beamline in Solaris. We will discuss the experimental electronic band structures in comparison to the theoretical results as given by the *ab initio* slab calculations performed within the generalized gradient approximation (GGA). The electronic structure of the RT phase compares well to the theoretically expected for the Sn atoms adsorbed in the hollow sites of the Pt(111) surface, while the electronic bands of the experimental HT phase correspond to the Pt<sub>2</sub>Sn surface alloy.

[1] H. J. Wallander et al. J. Phys. Chem. C 126, 6258 (2002)

[2] J. R. Kitchin et al. Phys. Rev. Lett. 93, 156801 (2004)

This research was funded by National Science Centre, Poland (NCN), grant number 2022/46/E/ST3/00184.

OBSERVING BARIUM OXIDE ON W(110) BY LOW-ENERGY,  
THERMIONIC AND PHOTOEMISSION ELECTRON MICROSCOPY

Clara Gutierrez-Cuesta<sup>1</sup>, Pawel Nita<sup>2, 3\*</sup>, Natalia Kwiatek<sup>3, 4</sup>, José Emilio Prieto<sup>1</sup>  
and Juan de la Figuera<sup>1</sup>

<sup>1</sup>*Instituto de Química Física Blas Cabrera (IQF), CSIC, 28006 Madrid SPAIN*

<sup>2</sup>*Faculty of Physics, Astronomy and Applied Computer Science, Jagiellonian University,  
30-348 Kraków, Poland,*

<sup>3</sup>*SOLARIS NSRC, 30-392 Kraków, Poland*

<sup>4</sup>*ICSC PAS, 30-239 Kraków, Poland*

\*E-mail: pawel.nita@uj.edu.pl

The deposition of alkali earth metals on transition metals is one of the classical problems in surface science, initiated by the discovery of the increased thermal emission of such cathodes [1]. Here we grow barium oxides by high temperature oxygen-assisted molecular beam epitaxy (HOMBE) on the W(110) surface, observing the growth front in real time and real space in low-energy electron microscopy, obtaining tens of micrometer wide islands. They are characterized by selected area x-ray absorption and photoemission spectroscopy by means of the photoemission microscope at the DEMETER beamline in the Solaris synchrotron, determining that the islands are of subnanometric height barium peroxide. When the sample is heated above 600°C, strong electron emission is observed, allowing for the observation of the islands in ThEEM (Thermionic Electron Emission Microscopy). Following Sheikh et al [2] we measure the thermionic emission spectra and the photoemission spectra obtained with a Hg lamp to determine the work function of the islands. In the future, we plan to tune the growth, potentially allowing for “design cathodes” where the thermionic emission takes place from well-defined distribution of objects.

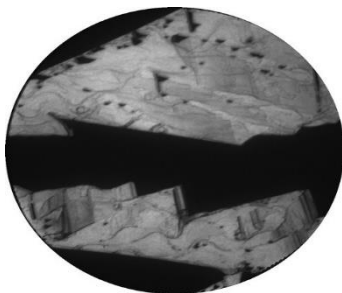


Figure 1. Thermionic Electron Microscopy image of barium oxide islands. The field of view is 50  $\mu\text{m}$ .

**Acknowledgment:** This research was funded by Grant TED2021-130957B-C54 funded by MCIN/AEI/10.13039/501100011033, and by the "European Union NextGenerationEU/PRTR" and the SciMat Priority Research Area budget under the program Excellence Initiative - Research University at the Jagiellonian University in Kraków - Grant No. 75.1920.2021

### References

- [1] L.R. Koller, The physics of electron tubes, MacGrawHill, New York (1937).  
[2] M. Sheikh et al., APL Materials **12**, (2024) 061105.

## CHECKMYMETAL (CMM): VALIDATING METAL-BINDING SITES IN X-RAY AND CRYO-EM DATA

Michal Gucwa<sup>1,2,3</sup>, Vanessa Bijak<sup>1</sup>, Krzysztof Murzyn<sup>2\*</sup>, Wladek Minor<sup>1\*</sup>

<sup>1</sup>*Department of Molecular Physiology and Biological Physics, University of Virginia, Charlottesville 22908, USA*

<sup>2</sup>*Department of Computational Biophysics and Bioinformatics, Jagiellonian University, Krakow, Poland*

<sup>3</sup>*Doctoral School of Exact and Natural Sciences, Jagiellonian University, Krakow, Poland*

\*E-mail: Wladek Minor [wladek@minorlab.org](mailto:wladek@minorlab.org) and Krzysztof Murzyn [krzysztof.murzyn@uj.edu.pl](mailto:krzysztof.murzyn@uj.edu.pl)

Identifying and characterizing metal-binding sites (MBS) within macromolecular structures is imperative for elucidating their biological functions. CheckMyMetal (CMM) is a web-based tool that facilitates the interactive validation of MBS in structures determined through X-ray crystallography (XRC) and cryo-electron microscopy (cryo-EM). Recent updates to CMM have significantly enhanced its capability to efficiently handle large datasets generated from cryo-EM structural analyses. In this study, we address various challenges inherent in validating MBS within both X-ray and cryo-EM structures. Specifically, we examine the difficulties associated with accurately identifying metals and modeling their coordination environments, considering the ongoing reproducibility challenges in structural biology and the critical importance of wellannotated, high-quality experimental data. CMM employs a sophisticated framework of rules rooted in the valence bond theory for MBS validation. We explore how CMM's validation parameters correlate with the resolution of experimentally derived structures of macromolecules and their complexes. Additionally, we showcase CMM's practical utility by analyzing a representative cryo-EM structure. Through a comprehensive examination of experimental data, we demonstrate CMM's capability to advance MBS characterization and identify potential instances of metal misassignment.

CheckMyMetal is available at: <https://cmm.minorlab.org/>

## HOW DO PLANTS MANAGE THEIR MICROELEMENTS? UNTANGLING THE ZN TRANSPORT MECHANISMS BETWEEN LATERAL ROOTS

Oskar Siemianowski\*, and Magdalena Pypka,

*Department of Plant Metal Homeostasis, Faculty of Biology, University of Warsaw,  
Miecznikowa 1 st., 02-096 Warsaw, Poland*

\*E-mail: o.siemianowski@uw.edu.pl/presenting author

Plants provide nearly all the calories and micronutrients required for the human diet. Plant productivity and nutritional value are influenced by the uptake and distribution of microelements, such as zinc, which is essential for plant development. Zn is absorbed by plant roots from the soil and transported to the shoots, yet the mechanisms governing Zn distribution within and between plant organs are not well understood. This study investigates these mechanisms, particularly under conditions of partial zinc deficiency.

The objective was to determine the mechanisms of Zn distribution between lateral roots by analyzing Zn distribution and speciation in plants grown in both Zn-heterogeneous (parts of the root system in Zn-sufficient and other parts in Zn-deficient conditions) and Zn-homogeneous media (either Zn-sufficient or Zn-deficient). Achieving high sensitivity and minimal sample preparation was crucial for preserving Zn distribution and its chemical forms, which was accomplished using the POLYX ( $\mu$ XRF) setup.

Roots were mounted between 3,6 $\mu$ m foil sandwich, allowing for fresh sample analysis. We were able to achieve spot resolution up to 5  $\mu$ m but most efficient (time/results) were  $\mu$ XRF maps were acquired with 100  $\mu$ m resolution. The results (Fig 1) demonstrated a strong Zn signal within whole root system, that is in parts that were grown in Zn deficient and Zn sufficient medium. Those results indicate Zn transport from Zn-sufficient to Zn-deficient roots. Zn was also not uniformly distributed, suggesting the presence of storage sites within the root system. Higher Zn levels in upper roots suggested that younger roots have a greater capacity for Zn uptake.

This study successfully utilized the POLYX beamline to analyze Zn distribution in plant root systems, revealing significant insights into Zn transport mechanisms. Our findings highlight the dynamic nature of Zn redistribution in plants, especially under nutrient deficiency, and provide a basis for further studies on nutrient transporters responsible for Zn distribution within plants.

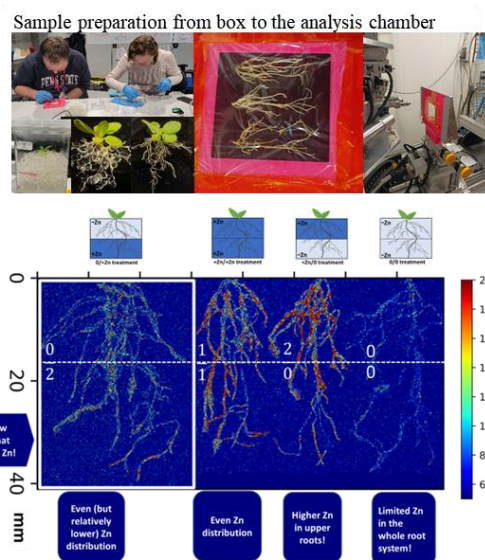


Fig 1 Zn elemental maps shows that Zn is distributed between lateral roots within the root system. Representative roots grown in homogenous (0/0 and 1/1  $\mu$ M Zn) and heterogeneous (2/0 and 0/2  $\mu$ M Zn) medium. Spot size is 100  $\mu$ m the background intensity was cut off (scale started at certain indicated count) and images in white rectangle were measured not simultaneously with 3 other roots systems.

NEW POLYMERIC MATERIALS BASED ON CATIONIC  
PHOTOPOLYMERISATION PROCESSES FOR 3D PRINTING  
TECHNOLOGY (3D-VAT) BASED ON DIGITAL LIGHT PROCESSING

Joanna Ortyl<sup>\*1,2,3</sup>, Filip Petko<sup>1,2</sup>, Andrzej Swięży<sup>1,2</sup>, Patrycja Środa<sup>1,2</sup>, Paweł Niezgoda<sup>1,3</sup>,  
Patryk Szymaszek<sup>1</sup>, Magdalena Jankowska<sup>1</sup>, Jakub Pietraszewski<sup>1</sup>, Kamil Pulit<sup>1</sup>

<sup>1</sup>*Wydział Inżynierii i Technologii Chemicznej, Politechnika Krakowska, Warszawska 24,  
31-155 Kraków*, <sup>2</sup>*Photo HiTech Ltd., Bobrzyńskiego 14, 30–348 Kraków*, <sup>3</sup>*Photo4Chem Ltd.,  
Lea 114, 31-133 Kraków*

\*E-mail: jortyl@chemia.pk.edu.pl

3D-VAT printing is an excellent alternative to the traditional preparation of 3D objects from polymeric materials, reducing costs and increasing the resolution of objects. The use of cationic 3D-VAT printing unfortunately hits a number of limitations. One of these is the lack of suitable photoinitiators that absorb in the emission range of the light sources used in printers (around 405 nm).[1] Most of the commonly used iodonium salts are diaryl derivatives proposed by Crivello in the 1970s. They show only residual light absorption above 300 nm and require photosensitizers or special light sources to efficiently initiate polymerization.[2] It is therefore essential to develop advanced iodonium salts that absorb longer wavelength light and efficiently generate superacid (which is the actual initiator of cationic polymerization).

The new innovative design of chromophores makes it possible to obtain iodonium salts in a selective manner, which was previously impossible with more refined chromophores.[3,4] Furthermore, the design used has made it possible to obtain the first symmetric iodonium salts equipped with an extended chromophore with a double bond.[5] Such advances in the structure of iodonium salts have made it possible to obtain compounds with excellent absorption properties extending into the visible range. The new iodonium salts are able to efficiently photolyze the cationic polymerization under 365 nm and 405 nm LED irradiation and can photoinitiate the cationic polymerization of monomers such as epoxides and vinyl ethers.

This design leads to a significant improvement in photoinitiating properties, allowing the developed salts to be used in such advanced applications as cationic 3D-VAT printing allowing prints with a resolution superior to those obtained with commercial photoinitiating systems.

The present work was funded by the OPUS project LAP - NCN contract number 2020/39/I/ST5/03556.

#### References

- [1] S.C. Ligon, R. Liska, J. Stampfl, M. Gurr, R. Mülhaupt, *Chem Rev* 2017;117:10212–90.
- [2] J. V. Crivello, J. H. W. Lam, *Macromolecules* 1977;10:1307–15.
- [3] F Petko, M. Galek, E. Hola, R. Popielarz, J. Ortyl, *Macromolecules* 2021;54:7070–87.
- [4] F. Petko, A. Świeży, M. Jankowska, P. Stalmacha, J. Ortyl, *Polym. Chem.*, 2023,14, 3018-3034
- [5] F Petko, M. Galek, E. Hola, M. Topa-Skwarczyńska, et al., *Chem Mater* 2022;2022:10077–92.

On the origin of circular dichroism in ARPES spectra from graphene,  $WSe_2$ ,  
and other quantum materials

H. Boban<sup>1</sup>, M. Qahosh<sup>1</sup>, X. Hou<sup>2</sup>, T. Sobol<sup>2</sup>, E. Beyer<sup>2</sup>, M. Szczepanik<sup>2</sup>, Simone Mearini<sup>1</sup>,  
V. Feyer<sup>1</sup>, F. Lüpke<sup>3</sup>, C. M. Schneider<sup>1</sup>, J. Henk<sup>4</sup>, and L. Plucinski<sup>1,5</sup>

<sup>1</sup>Peter Grünberg Institute PGI-6, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

<sup>2</sup>Solaris National Synchrotron Radiation Centre, Jagiellonian University, Czerwone  
Maki 98, 30-392 Kraków, Poland

<sup>3</sup>Peter Grünberg Institute PGI-3, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

<sup>4</sup>Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle (Saale),  
Germany

<sup>5</sup>II. Institute of Physics, RWTH Aachen University, 52074 Aachen, Germany

Email: l.plucinski@fz-juelich.de

On the example of graphene, we will discuss various contributions to circular dichroism in angle-resolved photoemission (CD-ARPES) [1,2] which include phase shifts of the participating partial waves [3], the interatomic phase shifts [4], and the CD due to elastic scattering of an excited electron [5]. Multiple scattering calculations are performed using the EDAC cluster code [6]. Subsequently, we perform similar analysis for  $WSe_2$ , a material where orbital characters are relatively well-defined.

Finally, a simple interatomic interference model that qualitatively explains asymmetric spin-polarized ARPES (spin-ARPES) spin texture from  $WTe_2$  single crystal surface [4] is presented.

This study aims to investigate how CD-ARPES and spin-ARPES techniques can contribute to a better understanding of topological materials.

[1] arXiv:2309.02187 (2023)

[2] JESRP 258, 147219 (2022)

[3] JESRP 214, 29 (2017)

[4] PRL 130, 146401 (2023)

[5] JJAP 32, L1480 (1993)

[6] PRB 63, 75404 (2001)

## BAND-BENDING, BAND-TAILING, 2D ELECTRON GAS AT TE DOPED INAS SURFACES

Jacek Kołodziej<sup>1\*</sup>, Mariusz Garb<sup>1</sup>, Natalia Olszowska<sup>2</sup>, Marcin Rosmus<sup>2</sup>, Dawid Wutke<sup>1</sup>

<sup>1</sup>*Marian Smoluchowski Institute of Physics, Jagiellonian University, Prof. S. Łojasiewicza 11, PL-30348 Kraków, Poland*

<sup>2</sup>*Solaris National Synchrotron Radiation Centre, Jagiellonian University, Czerwone Maki 98, 30-392 Kraków, Poland*

\*e-mail: [jj.kolodziej@uj.edu.pl](mailto:jj.kolodziej@uj.edu.pl)

Using photoelectron spectroscopy (PES), we study InAs(001) and InAs(110) surfaces, doped with Te atoms to induce strong band-bending phenomena and a formation of two-dimensional electron gases (2DEGs). The band structure of the 2DEGs as well as the coexisting 3D bulk electronic structure are investigated. We discuss several details of the investigated surface electronic structures, including the band tailing, the nonlocality, the many-body effects.

UNVEILING IMPERVIOUS BAND CROSSINGS IN THE BULK OF TOPOLOGICAL  
NODAL-LINE SEMIMETAL  $\text{ZrAs}_2$

A. S. Wadge,<sup>1\*</sup> K. Zberecki,<sup>2</sup> B. J. Kowalski,<sup>3</sup> D. Jastrzebski,<sup>1,3</sup> P. K. Tanwar,<sup>1</sup>  
P. Iwanowski,<sup>3</sup> R. Diduszko,<sup>3</sup> A. Moosarikandy,<sup>1</sup> M. Rosmus,<sup>4</sup> N. Olszowska,<sup>4</sup>  
and A. Wisniewski<sup>1,3</sup>

<sup>1</sup>International Research Centre MagTop, Institute of Physics, Polish Academy of  
Sciences, Aleja Lotnikow 32/46, PL-02668 Warsaw, Poland

<sup>2</sup>Faculty of Physics, Warsaw University of Technology, Koszykowa 75, PL-00662,  
Warsaw, Poland

<sup>3</sup>Institute of Physics, Polish Academy of Sciences, Aleja Lotnikow 32/46, PL-02668  
Warsaw, Poland

<sup>4</sup>National Synchrotron Radiation Centre SOLARIS, Jagiellonian University, Czerwone  
Maki 98, PL-30392 Cracow, Poland

\*e-mail: [wadge@magtop.ifpan.edu.pl](mailto:wadge@magtop.ifpan.edu.pl)

Topological nodal line semimetals (TSMs) are a fascinating class of materials, distinguished by their unique electronic structures and symmetry-driven properties.  $\text{ZrAs}_2$  is a notable example, featuring nodal lines in momentum space dictated by non-symmorphic symmetries. In this work, we combine angle-resolved photoemission spectroscopy (ARPES) and density functional theory (DFT) calculations to investigate the electronic characteristics of  $\text{ZrAs}_2$ .

Using ARPES, we have mapped the Fermi surface and observed impervious band crossings resistant to gap opening, providing experimental validation of non-symmorphic symmetry-protected nodal lines in  $\text{ZrAs}_2$ . The ARPES measurements reveal distinctive surface and bulk states at varying photon energies, linked to these nodal lines. Supported by DFT calculations, we uncover robust band crossings at specific points within the Brillouin zone, particularly around the S point (see Figure 1). Detailed slab calculations further illuminate the surface bands and bulk states near these crossings, reinforcing our experimental observations. These findings significantly advance our comprehension of  $\text{ZrAs}_2$ 's electronic structure and contribute to the broader understanding of TSMs. ([A. Wadge et al. Phys. Rev. B 110, 035142 \(2024\)](#))

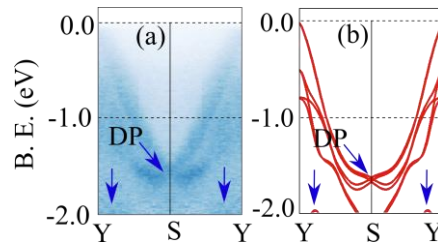


Figure 1 (a) ARPES result showing symmetry protected band crossing in support with (b) DFT calculations



Electronic Structures of Dirac Semimetals LaCuSb<sub>2</sub> and LaAgSb<sub>2</sub>

Marcin Rosmus<sup>1,\*</sup>, Natalia Olszowska<sup>1</sup>, Zbigniew Bukowski<sup>2</sup>, Przemysław Piekarczyk<sup>3</sup>,  
Andrzej Ptok<sup>3</sup> and Paweł Starowicz<sup>4</sup>

<sup>1</sup>*Solaris National Synchrotron Radiation Centre, Jagiellonian University, Czerwone Maki 98,  
30-392 Kraków, Poland*

<sup>2</sup>*Institute of Low Temperature and Structure Research, Polish Academy of Sciences, P.O. Box  
1410, 50-950 Wrocław, Poland*

<sup>3</sup>*Institute of Nuclear Physics, Polish Academy of Sciences, W. E. Radzikowskiego 152, PL-  
31342 Kraków, Poland* <sup>4</sup>*Marian Smoluchowski Institute of Physics, Jagiellonian University,  
Prof. S. Łojasiewicza 11, PL-30348 Kraków, Poland*

\*Email: marcin.rosmus@uj.edu.pl

Dirac semimetals LaCuSb<sub>2</sub> and LaAgSb<sub>2</sub> have garnered significant research interest due to their unique electronic properties, characterized by Dirac-like linear band dispersions and the existence of Dirac fermions [1]. Electronic structure of both materials is investigated using Angle-Resolved Photoemission Spectroscopy (ARPES) and Density Functional Theory (DFT) calculations. LaCuSb<sub>2</sub> is a superconductor exhibiting nodal lines and linear bands indicative of Dirac fermions, which contribute to its complex electronic structure [2]. In contrast, LaAgSb<sub>2</sub> displays charge density wave (CDW) order with two distinct transition temperatures and linear magnetoresistance. Despite the shared Dirac-like characteristics, the two compounds exhibit distinct electronic structures and different physical properties [3]. LaAgSb<sub>2</sub> manifests pronounced CDW phases, while LaCuSb<sub>2</sub> lacks CDW formation despite stronger Fermi surface nesting, underscoring fundamental differences in their electronic behaviors. This comparative analysis provides insights into the differences between these two semimetals, contributing to our understanding of the complex interactions governing their electronic properties and the topological phenomena in Dirac semimetals.

[1] P. Ruszała, et al, Computational Materials Scienc, **154**, 106-110 (2018)

[2] M. Rosmus, et al, Materials, **15**, 7168 (2022)

[3] M. Rosmus, et al, Journal of Alloys and Compounds, 1002, 175298 (2024)

## Absolute calibration of the solar X-ray spectrometer BRAXIS for a NASA MidEx mission

Marek Stęślicki,<sup>1,\*</sup> Żaneta Szaforz<sup>1</sup>, Janusz Sylwester<sup>1</sup>, Mirosław Kowaliński<sup>1</sup>, Jarosław Bąkała<sup>1</sup>, Daniel Ścisłowski<sup>1</sup>, Piotr Podgórski<sup>1</sup>, Tomasz Mrozek<sup>1</sup>

<sup>1</sup> *Centrum Badań Kosmicznych PAN Zakład Fizyki Słońca, Kopernika 11, 51-622*

*Wrocław, Poland*

Email:: sm@cbk.pan.wroc.pl

Solar flares are the most energetic events in the Solar System and a major driver of space weather. Developed spectrometer BRAXIS aims to observe selected lines of highly ionized elements from a wide range of soft X-ray radiation (1.8-22.4 Å). Such observations will enable the determination of physical parameters prevailing in the hot plasma of the solar corona, as well as its chemical composition. Such data seem necessary to understand the processes occurring during solar flares. We will present the approach to the absolute calibration of a very precise X-ray spectrometer developed for the DAISI mission using Astra line in the SOLARIS synchrotron.

# R1

## POLISH PARTICIPATION IN THE ESRF - A GRANT OF THE MINISTRY OF SCIENCE AND HIGHER EDUCATION

Anna Wolska,<sup>1,\*</sup> Anna Reszka,<sup>1</sup> Joanna Libera<sup>1</sup>

<sup>1</sup> *Institute of Physics Polish Academy of Sciences, Al. Lotników 32/46 PL-02668 Warsaw, Poland*

\*E-mail: wolska@ifpan.edu.pl

The European Synchrotron Radiation Facility (ESRF) is an international research infrastructure located in Grenoble (France) financed by the contributions paid by the Member Countries (contribution above 4 %) and Scientific Associated Members (below 4 %). Poland is one of the others with a contribution of 1% of the infrastructure budget. Polish contribution to the ESRF is possible thanks to the grant from the **Ministry of Science and Higher Education**. The grant is led by the *National Consortium of Scientific Institutions Interested in the Use of the European Synchrotron Radiation Source in Grenoble* and coordinated by Institute of Physics, Polish Academy of Sciences. It officially started in April 2021 and will end in March 2026.

In the current Ministry grant, not only a 1% contribution to the ESRF is included, but also a co-financing of participation in conferences for scientists with Polish affiliation presenting the results of research conducted at the ESRF. The funding regulations are available on the project website: <https://esrf.ifpan.edu.pl/> together with many other information concerning the National Consortium implementing the grant, news, reports, statistics, proposals submission deadlines, interesting publications and webinars.

Research results presented at conferences or published in scientific journals must include acknowledgments to the grant financing Poland's access to the ESRF: *The access to the ESRF was financed by the Polish Ministry of Science and Higher Education, dec. no. 2021/WK/11*. These are measurable project results which influence whether the Ministry will continue financial support, and therefore whether Polish scientists will continue to have access to the ESRF.

## R2

### ADVANCING UKRAINIAN SCIENCE: THE MICRO/NANO BEAMLINE AT SOLARIS UNDER THE 'LIGHT FOR UKRAINE' INITIATIVE

Danyo Babich,<sup>1,\*</sup> Anna Wach,<sup>2</sup> Jakub Szlachetko<sup>2</sup>, Alexander Kordyuk<sup>3</sup>, Leonid Rivkin<sup>1</sup>,  
Luc Patthey<sup>1</sup>

<sup>1</sup> *Paul Scherrer Institut, Villigen, Switzerland*

<sup>2</sup> *SOLARIS National Synchrotron Radiation Centre, Jagiellonian University, Kraków,  
Poland*

<sup>3</sup> *G.V.Kurdyumov Institute for Metal Physics, Kiev 03142, Ukraine*

\*E-mail: danylo.babich@psi.ch

The "Light for Ukraine" project represents a significant initiative aimed at revitalizing the Ukrainian scientific community by constructing a dedicated Ukrainian beamline at the SOLARIS synchrotron in Krakow, Poland. Initiated by the League of European Accelerator-based Photon Sources (LEAPS), this project is strongly supported by SOLARIS and PSI. The project will see the refurbishment and transfer of equipment as for example the U19 undulator from the Swiss Light Source (SLS) to SOLARIS. The U19 undulator will enable a broad spectrum of scientific investigations, producing high-brightness X-rays in the tender to hard X-ray range.

This presentation will provide an overview of the "Light for Ukraine" beamline project, highlighting recent scientific findings from the micro-XAS beamline at SLS and X-ray spectroscopy research at the Swiss Free Electron Laser (SwissFEL). These examples will showcase the advanced research capabilities that will be accessible to Ukrainian scientists through this new facility.

The new micro/nano beamline will not only create unprecedented research capabilities but also catalyze the Ukrainian scientific community's shift towards utilizing large-scale synchrotron radiation facilities. It will serve as a vital tool for Ukrainian research groups, enabling them to enhance their studies and forge connections with other leading facilities worldwide, such as free electron lasers and synchrotrons.

Additionally, the presentation will outline potential research findings of Ukrainian scientists, emphasizing the importance of international collaborations and support in rebuilding the Ukrainian scientific landscape. The "Light for Ukraine" beamline at SOLARIS is set to illuminate the path for cutting-edge research and innovation in Ukraine, fostering a new era of scientific advancement.

## R3

### BEYOND OPEN CALL – FORMS OF ACCESS TO SOLARIS

Mikolaj Golunski,<sup>1,\*</sup>

<sup>1</sup>*SOLARIS National Synchrotron Radiation Centre, 30-392 Krakow, Poland*

\*E-mail: mikolaj.golunski@uj.edu.pl

Scientists interested in conducting research using synchrotron radiation can access the SOLARIS infrastructure for free through regular scientific access. Based on biannual open calls for proposals, this system ensures fairness and equality. The main scoring factor is scientific merit, which guarantees that everyone, regardless of their background or affiliation, has an equal chance to conduct their research with synchrotron radiation.

It comes with a cost, though—the research should be published. We understand that for many private entities, this cost is too much; they need their research to be confidential. As SOLARIS aims to help foster progress in a broad spectrum of fields, we cannot turn our backs on the private sector. That is why we have industrial-type access to our infrastructure. In the talk, I will present how such access works.

There are still some situations when even regular researchers must pay for the measurements, including in-house ones from other Jagiellonian University departments. As it might seem strange to some, the reason why such a situation might happen will be explained using a Glacios CryoEM as an example.

Lastly, I will touch on the exciting potential that comes with our participation in international programmes and consortia such as NEPHEWS or ERIC. These collaborations can help scientists gain a broader perspective on their research, allowing them to conduct measurements not only at SOLARIS but also at many other facilities across Europe and the world.

# R4

## The project of PolFEL laboratory

Robert Nietubyc

*National Centre for Nuclear Research, Świerk, Sołtana 7, 05-400 Otwock, Poland*

\*E-mail:robert.nietubyc@ncbj.gov.pl

Polfel will be a combined facility providing electromagnetic radiation in the range from THz to EUV and 9 MeV electron beam for ultra-fast electron diffraction (UED). THz radiation and electron beams will be generated with two separate superconducting, cw operating linacs, while electromagnetic radiation in other ranges will be sourced from solid state lasers and from plasma jet, as harmonic radiation induced with those lasers. Experimental setups available at the facility launch will be fitted for THz transmission and reflection measurements in temperature range down to 5 K, for time- and angle-resolved photoemission, and for femtoseconds resolved electron diffraction on solid and gaseous samples. Beam dynamical simulations and mechanical design of accelerators have been concluded allowing for procurement and civil engineering works to proceed. The installation will begin at NCBJ in the half of 2025 aiming at the commissioning and first light in 2026.

# S1

## PLASMA-ENHANCED PHYSICAL PROPERTIES OF Mn(II)-Nb(IV) MOLECULAR MAGNET INVESTIGATED WITH EXAFS

Dominik Czernia,<sup>1,\*</sup> Piotr Konieczny,<sup>1</sup> and Alexey Maximenko<sup>2</sup>

<sup>1</sup>*Institute of Nuclear Physics PAN, ul. Radzikowskiego 152, 31-342 Kraków, Poland*

<sup>2</sup>*National Synchrotron Radiation Centre SOLARIS, Jagiellonian University, ul.*

*Czerwone Maki 98, 30-392 Kraków, Poland*

\*E-mail: dominik.czernia@ifj.edu.pl

Molecular magnets are promising materials for applications in modern technologies such as spintronics, quantum computing, magnetic refrigeration, bistable switches, and active sensors. A key challenge in this class of materials is obtaining systems with high enough Curie temperature  $T_C$  to effectively utilize their properties at a reasonable temperature range, at least at a liquid nitrogen boiling point of 77 K. The primary approach of the molecular magnetism community is to engineer materials at the molecular level by selecting appropriate synthetic building blocks and procedures. Another method is the plasma treatment of the materials. This is a cost-effective and fast technique successfully used to alter the net magnetic moment, magnetic hysteresis loop, and  $T_C$  in ceramics, thin films, and nanoparticles. Despite promising prospects, plasma irradiation was never used in molecular magnets.

To address this research gap, we studied how plasma irradiation affects the magnetic properties of  $\{[\text{Mn}^{\text{II}}(\text{H}_2\text{O})_2]_2[\text{Nb}^{\text{IV}}(\text{CN})_8] \cdot 4\text{H}_2\text{O}\}_n$  molecular magnet, which is known for its magnetocaloric effect and magnetic sponge behavior. Using plasma treatment,  $T_C$  raised by 20% from 49 K to 72 K. X-ray powder diffraction (XRD) confirmed the crystallographic structure remains unchanged, with a slight contraction of the unit cell that increased the superexchange coupling constants by 20%, as determined by the mean-field approximation model.

The X-ray absorption near edge structure (XANES) for Nb  $L_2$ - and  $L_3$ -edges and extended X-ray absorption fine structure (EXAFS) for the Mn K-edge were analyzed to investigate how the local structures of the magnetic metal centers are affected by plasma irradiation. The results point to the shortening of the interatomic distances after plasma irradiation by 1-2%. Consequently, the first coordination shell is closer to Mn by approximately 0.02 Å, which confirms the qualitative conclusions drawn from the XRD measurement. This leads to the modification of superexchange coupling constants that are sensitive to interatomic distances, as determined by the Bethe-Slater curve. The increase in  $T_C$  was probably an effect of the desorption of four or fewer molecules of water of crystallization, while all four coordinated water molecules were maintained.

Our findings demonstrate that plasma-induced modifications in molecular systems are a quick, reliable, and effective way to obtain unique magnetic phases that would otherwise be unattainable. Such changes can then be investigated in detail using synchrotron methods, generating fresh perspectives on achieving high- $T_C$  systems for technological purposes.

## Time-dependent oxidation state change during pulsed laser irradiation of colloids; an experimental XAFS study confirmed by computational analysis

Mohammad Sadegh Shakeri, Zaneta Swiatkowska-Warkocka  
 Institute of Nuclear Physics Polish Academy of Sciences, 31342 Krakow,  
 Poland  
 ms.shakeri@ifj.edu.pl

When a suspension is irradiated with a laser pulse, the electromagnetic wave is locally absorbed by the suspended agglomerates, resulting in a temperature rise. Depending on their temperature, possible phase formations/transitions take place in a short time of the pulse duration. Immediately, the particles are cooled to ambient temperature by thermal equilibrium with the solvent molecules, which are transparent to the laser beam. This process is alternatively repeated during pulsed laser irradiation of suspensions (PLIS), initially known as pulsed laser melting in liquid (PLML). In 2007, scientists reported for the first time that unlike the laser ablation process used to produce smaller nanoparticles, PLML uses lower laser fluences and forms larger particles than the original constituents by melting. In our latest publications [M.S.Shakeri, et al. *Adv. Funct. Mater.* 2023, 33, 2304359], we proposed that during melting of nanoparticles physical phase transitions and chemical oxidation/reduction processes will occur. We used linear combination fitting of Extended X-ray Absorption Fine Structure (EXAFS) spectra (Figure 1) not only to determine the chemical composition of samples, but also to recognize which one of physical/chemical transitions control the formation of various phases. EXAFS spectra were used to interpret both the mechanism and exact composition of samples.

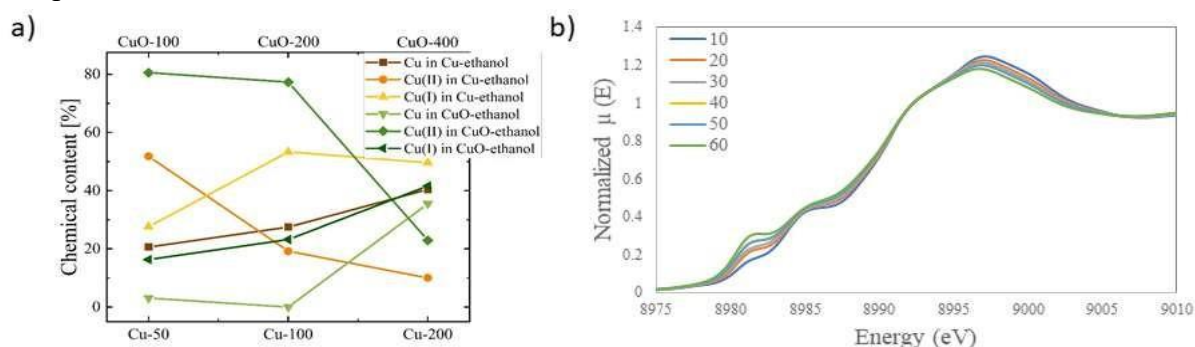


Fig. 1. The exponential/logarithmic changes of chemical composition derived from LCF of EXAFS spectra

Hopefully, our investigation led to proposing a scientifically acceptable mechanism for particle formation and as a next logical step we tried to dig more into the analyzing the oxidation states by altering the synthesizing parameters using X-ray absorption spectroscopy (XAS) method. We successfully conducted XAS spectra for powders resulted from pulsed laser irradiation of CuO/Fe<sub>3</sub>O<sub>4</sub>/organic solvent colloids. X-ray Absorption Near Edge Spectra (XANES) showed the meaningful change in oxidation state of both copper and iron K-edges. We also tried to use Feff code in order to analyze how the structural changes interpret the observed variations in XANES spectra.

This work is mostly supported by the Polish National Science Centre Program No. 2018/31/B/ST8/03043. It is also supported partially by the Polish National Science Centre Program No. 2022/06/X/ST3/01743. The computational works were done in cooperation with Prometheus Cluster, Cyfronet, AGH University of Science and Technology, Krakow using Grant No. PLG/2022/015573. The X-ray absorption spectroscopy measurements were performed at the SOLARIS synchrotron center in Krakow, Poland, under experiment number 221926 and Elettra synchrotron facility, under the proposal number 20232086.



CHANGES IN THE ELECTRONIC STRUCTURE OF  $\text{NiFe}_2\text{O}_4@\text{SiO}_2$  NANOCOMPOSITES  
BY SYNTHESIS PROCESS AND ANNEALING

Adam Czempik,<sup>1,\*</sup> Anna Bajorek,<sup>1</sup> Ewa Partyka-Jankowska,<sup>2</sup> Tomasz Sobol,<sup>2</sup>  
Magdalena Szczepanik,<sup>2</sup> Jerzy Kubacki,<sup>1</sup> Barbara Liszka,<sup>1</sup> Fabien Grasset,<sup>4,5</sup> Krystian Prusik,<sup>1</sup>  
Joanna Klimontko,<sup>1</sup> Sandy Auguste,<sup>3</sup> Anthony Rousseau,<sup>3</sup> and Nirina Randrianantoandro<sup>3</sup>

<sup>1</sup> *University of Silesia in Katowice, 40-007 Katowice, Poland*

<sup>2</sup> *SOLARIS National Synchrotron Radiation Centre, 30-392 Krakow, Poland*

<sup>3</sup> *Le Mans Université, 72085 Le Mans, France*

<sup>4</sup> *Université de Rennes, 35000 Rennes, France*

<sup>5</sup> *National Institute for Materials Science, Tsukuba, 305-0044, Japan*

\*E-mail: adam.czempik@us.edu.pl

Nickel ferrite  $\text{NiFe}_2\text{O}_4$  (NFO) magnetic nanoparticles are promising materials for magnetic hyperthermia in cancer treatment [1]. To enhance biocompatibility and chemical stability, the nanoparticles can be embedded in silica, forming  $\text{NFO}@\text{SiO}_2$  nanocompounds.

For our research,  $\text{NFO}@\text{SiO}_2$  was obtained using two methods: co-precipitation followed by microemulsion [1] and the wet-chemical method (WCM) [2]. Annealing at various temperatures was performed to enhance the stability of NFO and improve the properties of the nanocompounds. The structural, electronic and magnetic properties were tested, among others, using X-ray absorption spectroscopy at SOLARIS at PHELIX and PIRX beamlines.

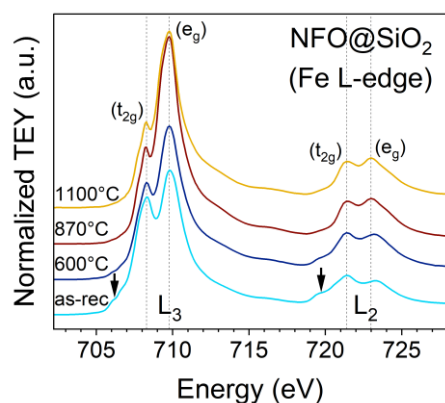


Figure 1 – X-ray absorption spectrum of  $\text{NFO}@\text{SiO}_2$ , obtained by WCM, reveals the influence of annealing temperature on the electronic structure of iron, including the presence of  $\text{Fe}^{3+}$  and some traces of  $\text{Fe}^{2+}$  (marked by arrows).

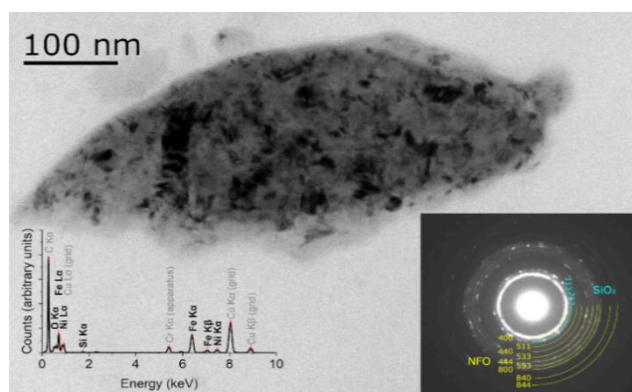


Figure 2 - Transmission electron microscopy image of  $\text{NFO}@\text{SiO}_2$  obtained by WCM and annealed at  $1100^\circ\text{C}$ .

The results of energy dispersive spectroscopy (bottom left) and selective area electron diffraction (bottom right) confirm the presence of expected elements and phases: nickel ferrite (NFO, ref. 01-090-8282) and cristobalite  $\alpha$  ( $\text{SiO}_2$  ref. 00-039-1425).

[1] A. Czempik et al., *Ceramics International* 50 (2024) 20473- 20494

[2] Y Ichiyanagi et al., *phys. stat. sol. (c)* 1, No. 12, 3485–3488 (2004)

STUDIES OF MOLECULAR ORDER IN ITRACONAZOLE BY X-RAY  
DIFFRACTION

Taoufik Lamrani,<sup>1,\*</sup> Paulina Jesionek,<sup>2,3</sup> Magdalena Tarnacka,<sup>1</sup> Barbara Hachuła,<sup>2</sup>  
Daniel Zakowiecki<sup>4</sup>, Ewa Ozimina-Kamińska<sup>3</sup>, Kamil Kamiński<sup>1</sup>, Karolina Jurkiewicz<sup>1</sup>

<sup>1</sup>*Institute of Physics, University of Silesia in Katowice, 75 Pułku Piechoty 1, 41-506  
Chorzów, Poland, taoufik.lamrani@us.edu.pl.*

<sup>2</sup>*Institute of Chemistry, University of Silesia in Katowice, ul. Szkolna 9, 40-007 Katowice,  
Poland.*

<sup>3</sup>*Department of Pharmacognosy and Phytochemistry, Medical University of Silesia in  
Katowice, ul. Jagiellońska 4, 41-200 Sosnowiec, Poland.*

\*E-mail: taoufik.lamrani@us.edu.pl

Liquid crystals (LCs) with a molecular organization between crystalline and amorphous states have gained significant attention in pharmaceutical research due to their unique properties. These systems can form diverse mesophases with orientational order (e.g., nematic and smectic) through thermotropic or lyotropic transitions. The ability to modulate and control these transitions is crucial, as they significantly impact liquid crystalline compounds' physicochemical characteristics and performance in drug delivery applications.

This study investigates the structural properties of solid-state phases of itraconazole (model thermotropic LC) with different degrees of molecular order produced by vitrification and cryo-milling. While standard vitrification of itraconazole isotropic liquid down to room temperature results in the formation of glass with some degree of smectic order, cryo-milling easily destroys not only crystalline order but also smectic organization of molecules into layers, omitting the melting. The structural properties of such prepared non-crystalline, glassy phases of itraconazole were studied using X-ray diffraction and completed by calorimetry, dielectric spectroscopy, and solubility studies. Although extending the milling time does not destroy the *N* alignment of molecules, it does frustrate their nearest-neighbor organization. The higher degree of the intermolecular disorder translates into faster dynamics of cryo-milled species, which never matches that observed for the vitrified phase. Moreover, structures of itraconazole obtained by cryo-milling are much more physically stable and soluble.

The obtained results can guide the formulation of ultrastable LC pharmaceuticals with tunable molecular order and solubility.

Authors acknowledge financial support from the National Science Centre (Poland), grant number: Opus 21 No. 2021/41/B/NZ7/01654, and the European Synchrotron Radiation Facility (ESRF), Grenoble, France, ID22 beamline (proposal HC5404). The access to ESRF was financed by the Polish Ministry of Education and Science – decision number: 2021/WK/11.

## Understanding the mechanism of beam damage on copper thin films

Aleksandra Figura-Jagoda,<sup>1,\*</sup> Caroline Hain<sup>2</sup>, Michał Hubczak<sup>3</sup>, Sylwia Klejna<sup>1</sup>,  
Artur Kwiatkowski<sup>3</sup>, Krzysztof Maćkosz<sup>2</sup>, Camilla Minzoni<sup>2</sup>, Joanna Stępień<sup>1,4</sup>,  
Aleksandra Szkudlarek<sup>1</sup>, Ivo Utke<sup>2</sup>, Marcin Zając<sup>4</sup> and Marcin Sikora<sup>1,4</sup>

<sup>1</sup>*Academic Centre for Materials and Nanotechnology AGH, 30-055 Kraków, Poland*

<sup>2</sup>*Empa - Swiss Federal Laboratories for Materials Science and Technology, 3603 Thun,  
Switzerland*

<sup>3</sup>*Faculty of Physics and Applied Computer Science AGH, 30-055 Kraków, Poland*

<sup>4</sup>*SOLARIS National Synchrotron Radiation Centre, 30-392 Kraków, Poland*

\*E-mail: afigura@agh.edu.pl

Thin films are important element of modern science and technology. They find wide range of applications in technology, from catalytic conversion of water to hydrogen and oxygen to electronic modules such as processors and random-access memories. To obtain best quality thin films, surface sensitive analysis is crucial – not only with respect to roughness or chemical composition but also the bonds and local atomic environment. The latter two are probed with the use of synchrotron methods, such as X-ray absorption spectroscopy (XAS) or X-ray photoelectron spectroscopy (XPS). Nowadays synchrotron methods are getting more advanced and open to different ideas and measurement techniques.

Surface sensitive spectroscopies, such as X-ray absorption spectroscopy (XAS) and X-ray photoelectron spectroscopy (XPS) provide key information for understanding chemistry of a deposition process of thin films, but only if researchers are aware of unwanted effects that affects spectral shape, such as damage/evaporation of film due to heating the sample by strong X-ray beam [1] or reducing effective charge of some elements [2, 3]. These effects are well known in XPS, while changes in XAS have been barely studied.

In XAS study we have observed that L edge of copper in thin films exposed to focused synchrotron beam show a strong reduction in the intensity of Cu-II feature and increase in the intensity of spectral features corresponding to Cu-I and metallic copper. Preliminary measurements showed that this effect is strongly associated with the intensity and energy of photon beam, but can also depend on the thickness of the film, substrate, and deposition method. One of the hypotheses of the origin of the strong radiation damage of copper is that the native oxide layer caused by film exposure to air reacts with hydro carbide contamination deposited by X-ray beam. Understanding the mechanisms of copper reduction can also provide ideas for how to prevent this effect without damaging the sample.

[1] E.L. Bright, et al., *J. Synchrotron Rad.* (2021), 28, 1377–1385

[2] L. Monico, et al., *Anal. Chem.* (2020), 92, 14164–14173

[3] F. Stellato, et al., *Metallomics*, (2019), 11, 1401

# P1

## STRUCTURAL PATHWAYS FOR ULTRAFAST MELTING OF OPTICALLY EXCITED THIN POLYCRYSTALLINE PALLADIUM FILMS

J. Antonowicz<sup>1</sup>, A. Olczak<sup>1</sup>, K. Sokolowski-Tinten<sup>2</sup>, P. Zalden<sup>3</sup>, I. Milov<sup>4</sup>,  
P. Dzięgielewski<sup>1</sup> and R. Sobierajski<sup>5,\*</sup>

<sup>1</sup>*Faculty of Physics, Warsaw University of Technology, Koszykowa 75, 00-662 Warsaw,  
Poland,*

<sup>2</sup>*Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of  
Duisburg-Essen, Lotharstrasse 1, 47048 Duisburg, Germany,*

<sup>3</sup>*European XFEL, Holzkoppel 4, 22869 Schenefeld, Germany,*

<sup>4</sup>*Industrial Focus Group XUV Optics, MESA+ Institute for Nanotechnology, University  
of Twente, Drienerlolaan 5, 7522 NB Enschede, Netherlands,*

<sup>5</sup>*Institute of Physics Polish Academy of Sciences, al. Lotników 32/46, 02-668 Warsaw,  
Poland.*

\*E-mail: ryszard.sobierajski@ifpan.edu.pl

Due to its extremely short timescale, the non-equilibrium melting of metals is exceptionally difficult to probe experimentally. The knowledge of melting mechanisms is thus, to a large extent, based on the results of theoretical predictions and computer modeling. This work reports on the ultrafast melting of thin polycrystalline Pd films studied by an optical laser pump – X-ray free-electron laser probe technique and two-temperature model molecular dynamics simulations [1]. By acquiring the X-ray diffraction snapshots with a picosecond resolution, we capture the sample's atomic structure during its transition from the crystalline to the liquid state. Bridging the timescales of the experiment and the simulation allows us to formulate a comprehensive microscopic picture of the melting transition. We demonstrate that the melting process gradually accelerates with the increasing density of the absorbed energy. The molecular dynamics simulations reveal that the transition mechanism progressively varies from heterogeneous, initiated inside structurally disordered grain boundaries, to homogenous, proceeding catastrophically in the crystal volume on a picosecond timescale.

[1] J. Antonowicz et al., *Acta Materialia* 276 (2024) 120043

## P2

### ESTABLISHING DETECTION LIMITS FOR HEAVY ELEMENTS IN PIGMENTS BASED ON 3D-METALS WITH THE USE OF SYNCHROTRON-BASED X-RAY FLUORESCENCE SPECTROSCOPY

Paweł Wróbel,<sup>1,2</sup> Anna Osojca,<sup>3</sup> Katarzyna Piekło,<sup>3</sup> Katarzyna M. Sowa,<sup>1,\*</sup>

Tomasz Kołodziej,<sup>1</sup> Paweł Korecki,<sup>1,4</sup> Zbigniew Ingłot,<sup>3</sup>

Magdalena Kluz-Pękalska,<sup>3</sup> and Jakub Szlachetko,<sup>1</sup>

<sup>1</sup>*SOLARIS National Synchrotron Radiation Centre, Jagiellonian University,  
30-392 Krakow, Poland*

<sup>2</sup>*Faculty of Physics and Applied Computer Science, AGH University of Krakow,  
30-059 Krakow, Poland*

<sup>3</sup>*Ingłot Sp. Z O. O., 37-700 Przemyśl, Poland*

<sup>4</sup>*Institute of Physics, Jagiellonian University, 30-348 Krakow, Poland*

*\*E-mail: k.sowa@uj.edu.pl*

Pigments based on 3d transition metals are widely used in cosmetic industry, thus detection of contamination with heavy elements is of highest importance. Many methods are used to determine the concentration of elements with a variety of detection limits and often specific requirements for material preparation. Among these methods, energy dispersive X-ray fluorescence spectroscopy (EDXRF) is an attractive tool as it provides very low detection limits (as low as sub ppm levels) without any sample preparation. On the other hand detection of trace amounts of heavy elements in pigments is very challenging due to the elemental complexity and strong spectral interferences.

The goal of this research was to check feasibility of assessment of the concentration and detection limits of lead in three eyeshadows coloured with the 3d metals such as Cr, Fe, Ti, Zn prepared in a form of pellets at PolyX beamline [1] at SOLARIS NSRC [2]. The results of the quantification will be confronted with the results gathered with ICP-OES spectrometer after acid digestion. The challenges and limitations will be discussed as well.

[1] K.M. Sowa et. al. Nuclear Instruments and Methods in Physics Research B 538 (2023) 131–137

[2] J. Szlachetko et al. The European Physical Journal Plus (2023) 138:10

The work is supported under the Polish Ministry and Higher Education project: “Support for research and development with the use of research infrastructure of the National Synchrotron Radiation Centre SOLARIS” under contract nr 1/SOL/2021/2

## P3

### What we breath in Krakow, Poland: winter and summer air in the prism of XAFS

Patryk Grzywa<sup>1</sup>, Alexey Maximenko<sup>2</sup>, Romisaa Gamal Mahmoud Abdelarhman<sup>1</sup>,  
Paweł Wróbel<sup>1,2</sup>, Filip Baran<sup>1</sup>, Lucyna Samek<sup>1\*</sup>

<sup>1</sup>*AGH University of Krakow, Faculty of Physics and Applied Computer Science  
30-059 Krakow, Poland*

<sup>2</sup>*SOLARIS National Synchrotron Radiation Centre Jagiellonian University,  
30-392 Kraków, Poland*

\*E-mail: [Lucyna.Samek@fis.agh.edu.pl](mailto:Lucyna.Samek@fis.agh.edu.pl) corresponding

During our beamtime on 25-26 March 2024 and 10 May 2024 the XANES technique (SOLARIS ASTRA beamline) has been used to study absorption K-edges of sulphur, chlorine, potassium, iron and zinc of 8 aerosols samples (PM<sub>2.5</sub>) collected in Krakow during summer and winter 2018/2019 and 2020/2021. A set of 17 reference samples (sulfides, sulphates and bisulphates of NH<sub>4</sub>, K, Na, Ca, Zn, Fe and Cu, potassium chloride, potassium carbonate and bicarbonate, potassium nitride) was studied as well. The results show that PM<sub>2.5</sub> XANES spectra at S absorption K-edge have different characteristics in summer and winter. Samples of PM<sub>2.5</sub> collected in summer contain mostly sulfates. On the other hand, spectra from samples collected in winter additionally contain peaks of KHSO<sub>4</sub>, NaHSO<sub>4</sub>, NH<sub>4</sub>HSO<sub>4</sub>, ZnS and sulphur in organic compounds. The Table 1 below shows our XANES results at the K-edge of potassium with the contribution of each compound to potassium in PM<sub>2.5</sub> samples collected in winter. The highest contribution to potassium has KHSO<sub>4</sub>. The contribution is in the range 31-46%. The lower contribution to potassium is observed for KHCO<sub>3</sub> and K<sub>2</sub>SO<sub>4</sub>. The obtained results for potassium K-edge confirm the results from sulphur K-edge, that during winter bisulphates are present in particulate matter.

**Acknowledgements:** This study was supported by SOLARIS project no 232073 and the Ministry of Science and Higher Education, grant number 16.16.220.842. Thank you Grzegorz Gazdowicz and Lulu Alluhaibi for the support during the measurements.

Table 1. The determined contribution of chemical compounds to PM<sub>2.5</sub> at the K-edge of potassium.

Compound	09/01/2019	15/01/2019	11/01/2021	17/01/2021
K <sub>2</sub> HPO <sub>4</sub>	3%	3%	11%	6%
K <sub>2</sub> SO <sub>4</sub>	21%	31%	23%	39%
KHCO <sub>3</sub>	19%	22%	20%	19%
KHSO <sub>4</sub>	45%	31%	46%	38%
KNO <sub>3</sub>	13%	-----	-----	-----

### The art ceramics from the Museum of Royal Wawel Castle's analyzed by X-Ray fluorescence technique

Romisaa Gamal Mahmoud Abdelrahman<sup>1,3</sup>, Bartłomiej Makowiecki<sup>2</sup>, Lucyna Samek<sup>1\*</sup>

<sup>1</sup>*AGH University of Krakow, Faculty of Physics and Applied Computer Science, 30-059 Krakow, Poland*

<sup>2</sup>*Royal Wawel Castle's, Ceramic and Glass Department, Wawel 5 PL 31-001 Kraków, Poland*

<sup>3</sup>*Future University in Egypt (FUE), Faculty of Engineering and Technology, Egypt*

\*E-mail: Lucyna.Samek@fis.agh.edu.pl corresponding author

This research aims to develop a methodology for determining the origin and historical context of ceramic art objects from the Museum of Royal Wawel Castle's collection. The doctoral dissertation focuses on using X-ray fluorescence (XRF) spectroscopy to analyze the elemental composition of these ceramics. By examining the elemental data, the research seeks to uncover the provenance and production techniques of the artifacts. Five ceramic samples from Wawel Castle were analyzed using X-ray fluorescence (XRF), revealing detailed information about the concentration of various elements and compounds. The measurements were performed on M4 TORNADO Plus, BRUKER spectrometer. The concentrations of the following elements: Na, Mg, Al, Si, P, S, K, Ca, Ti, V, Cr, Mn, Fe, Ni, Cu, Zn, Ga, Ge, As, Br, Rb, Sr, Y, Zr, Ba and Pb were determined. The correlations between concentrations were calculated. Graphical Plot between  $K_2O/SiO_2$  versus  $Al_2O_3/SiO_2$  and ternary plots for  $(Na_2O+Al_2O_3)$ ,  $SiO_2$ ,  $Al_2O_3$  and  $CaO$ ,  $SiO_2$ ,  $Al_2O_3$  were performed, respectively. These findings provide insights into the materials' origins and manufacturing processes. Conducted in collaboration with the Wawel Royal Castle Museum, this study combines art history, archaeology, and materials science to enhance our understanding of the ceramics' historical and cultural significance. Plans include applying for a research grant to expand this study and develop a standardized methodology for future research. This project aims to deepen scientific knowledge of ceramic artifacts and inform curatorial and conservation practices.

**Acknowledgements:** *This study was supported by the program “Excellence initiative—research university” for the University of Krakow together with the subsidy of the Ministry of Science and Higher Education, grant number 16.16.220.842.*

## RESEARCH POTENTIAL OF THE POLISH SYNCHROTRON IN EXAMINING THE REMAINS OF ORGANIC MATTER IN FOSSILIZED BONES

Dawid Surmik,<sup>1,\*</sup>

*<sup>1</sup>Paleoecology and Taphonomy Research Group, Institute of Earth Sciences, Faculty of Natural Sciences, University of Silesia in Katowice, Ul. Będzinska 60, 41-200 Sosnowiec, Poland*

\*E-mail: dawid.surmik@us.edu.pl

Molecular paleontology is the study of organic matter remnants in the fossilized bones of extinct animals. The development of new sensitive research techniques based on synchrotron radiation allows the identification of remains of organic matter (e.g. proteins) in paleontological material. Research conducted at the SOLARIS National Synchrotron Radiation Centre is carried out on two research lines: PolyX and CIRI. In the first one, X-ray absorption spectroscopy is applied to examine iron oxide-mineralized, biological microstructures reminiscent of fossilized red blood cells, which were obtained from the Cretaceous (about 80 million years old) carnivorous dinosaur bone samples. Here, an attempt to evaluate the properties of iron was made, to determine its origin from the genuine iron-containing hemoproteins from dinosaur blood.

In another project, using the CIRI beamline research infrastructure, the "soft tissue" samples extracted from the bones of Triassic dinosaurs (about 80 million years old) were examined. The morphological features of these soft structures suggest that they are perfectly preserved, still flexible fragments of original blood vessels and extracellular matrix. The research hypothesis tested in this study is that genuine bone proteins (especially collagen) will be characterized by specific bio-signatures and fingerprint signals (e.g., amide bands), so it can confirm the proteinaceous origin of the examined soft structures and even provide clues to their endogenous source.

Although the collected data are of excellent quality, their clear interpretation is still problematic, so further studies on larger numbers of samples are advisable. The samples examined so far, are very valuable for an author as well as for the National Synchrotron Radiation Centre scientists, from a methodological point of view, and will be used to check and improve beamlines performance.



NEW SCANNING TRANSMISSION X-RAY MICROSCOPE AT SOLARIS  
OPTIMIZED FOR FAST SCANNING AND ENVIRONMENTAL EXPERIMENTS

K. Matlak,<sup>1,\*</sup> B. Wolanin,<sup>1</sup> M. Brzyski<sup>1</sup>, P. Nowak<sup>1</sup>, A. Mandziak<sup>1</sup>,  
P. Nita<sup>1,2</sup>, M. Zając<sup>1</sup> and Tolek Tyliszczak<sup>1,3</sup>

<sup>1</sup>*SOLARIS National Synchrotron Radiation Centre, Jagiellonian University, Kraków, PL*

<sup>2</sup>*Faculty of Physics Astronomy and Applied Computer Science, Jagiellonian University,  
Kraków, PL*

<sup>3</sup>*Lawrence Berkeley National Laboratory, 1 Cyclotron Rd., Berkeley CA94720, USA*

\*E-mail: krzysztof.matlak@uj.edu.pl

The SOLARIS National Synchrotron Radiation Centre is a 1.5 GeV 3rd generation synchrotron located in Krakow, Poland. As a low energy storage ring, this facility is going to specialize in building its beamlines mostly in the soft X-ray region. One of them is the DEMETER beamline, on which the Scanning Transmission X-ray Microscopy (STXM) is located. The beamline is a classic Plane Grating Monochromator (PGM) design with an Elliptically Polarizing Undulator (EPU) as a source and works in 100-2000 eV photon energy range. The STXM microscope has been designed and built in-house. The main goal of the design is to provide a universal microscope that can be easily reconfigured to a specific experiment. Microscope's relatively compact chamber enables faster sample load/unload and more economical purging with pure He, when a sample cannot be subjected to vacuum.

Our STXM design is based on the Advanced Light Source (ALS) beamline 5.3.2 STXM [1] but there is a significant difference. The microscope does not have sample stages in the direction of the X-ray beam. It has the Order Sorting Aperture (OSA) motion in this direction, instead. This modification reduces sample vibration and helps in the focusing procedure. Additionally, a custom Field-Programmable Gate Array (FPGA) is used there for timing, acquisition and fast shutter control.

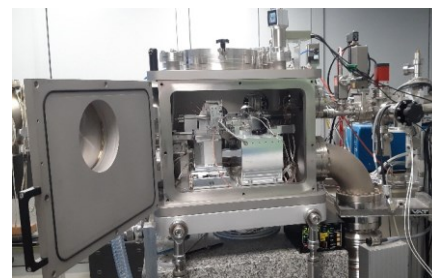


Figure 1: The STXM at SOLARIS

This STXM is operating on a modern undulator beamline, therefore acquisition time of a single-pixel can be less than 1ms, enabling fast scanning. To maintain the sample position with changing X-ray energy, we use a laser interferometer in a closed loop feedback. This STXM design is suitable for commercial electrochemical cell made by Hummingbird Scientific and also good for using a big matrix detectors for operating in ptychography mode in the future. Thanks to the use of an undulator with variable polarization, it is possible to perform measurements using the XMCD or XMLD effect for magnetic samples.

Apart of our STXM design and capability details, some example results of recent experiments will be presented.

References: [1] A. L. D. Kilcoyne, et al. (2003), *J. Synchrotron Rad.* 10, (125–136).

X-RAY SPECTROSCOPY AND SCATTERING WITH 20~FMS TIME RESOLUTION AT SWISSFEL BERNINA ENDSTATION: PROBING ULTRAFAST DYNAMICS OF  $[\text{Fe}(\text{TERPY})_2]^{2+}$

Danyo Babich<sup>1\*</sup>, Marius Hervé<sup>2</sup>, Serhane Zerdane<sup>1</sup>, Xin Liu<sup>1</sup>, Roman Mankowsky<sup>1</sup>, Mathias Sander<sup>1</sup>, Shih-Wen Huang<sup>1</sup>, Marc Alias-Rodríguez<sup>3</sup>, Claudio Cirelli<sup>1</sup>, Grigory Smolentsev<sup>1</sup>, Miquel Huix-Rotllant<sup>3</sup>, Eric Colet<sup>2</sup>, Marco Cammarata<sup>2</sup>, Henrik Till Lemke<sup>1</sup>

<sup>1</sup>Paul Scherrer Institut, Villigen, Switzerland

<sup>2</sup>Univ Rennes, CNRS, IPR - UMR 6251, F-35000 Rennes, France

<sup>3</sup>Aix-Marseille Univ, CNRS, ICR, 13013 Marseille, France

\*E-mail:danylo.babich@psi.ch

Time-resolved X-ray spectroscopy and scattering techniques at X-ray free electron lasers (XFELs) are powerful tools for studying chemical dynamics on ultrafast timescales. Comprehensive insights of even disordered molecules in solution can be gained for the electronic state, local structure, and solvation structure using X-ray emission spectroscopy (XES), X-ray absorption spectroscopy (XAS), and X-ray solution scattering (XSS), respectively [Zhang et al. 2014].

Detailed views into ultrafast electronic dynamics, however, may be obscured through a limitation in temporal resolution. As shown in Transition metal compounds showing charge transfer as well as spin transitions upon optical excitation, valuable insights about their mechanism can be gained by especially studying the initial cascade of electronic state transitions [Lemke et al. 2017].

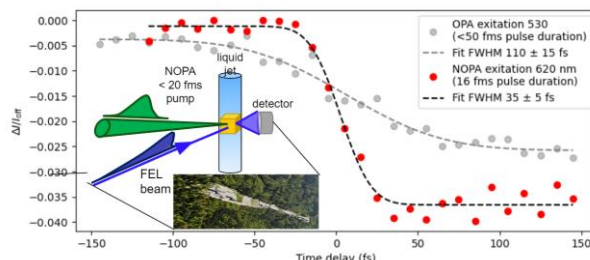


Fig. 1 Time resolved XANES measuring dynamics of the charge transfer state. at pre-edge region (7,113.5 eV) with and without ultrashort NOPA excitation performed at SwisFEL Bernina endstation

We show FEL-based results of different X-ray techniques using a newly developed NOPA laser system providing tunable pulses that allow better control of the ultrafast excitation at a timescale of the order of initial transition rates. The study has been performed on  $[\text{Fe}(\text{terpy})_2]^{2+}$ , an example of molecular Iron model complexes showing ultrafast charge transfer decaying into a cascade of spin transitions. The initial subpicosecond dynamics may depend on optical excitation parameters, such as wavelength, bandwidth, and time duration. Fig. 1 shows a significant improvement in the time of transient XANES changes measured at the pre-edge region (7,113.5eV) with a tunable ultrashort NOPA.

IR NANOSPECTROSCOPY AT THE CIRI BEAMLINE AT THE SOLARIS  
SYNCHROTRONMaciej Roman,<sup>1,\*</sup> Tetiana Stepanenko,<sup>2,1,3</sup> and Tomasz P. Wrobel<sup>1</sup><sup>1</sup>*SOLARIS National Synchrotron Radiation Centre, Jagiellonian University, Czerwone  
Maki 98, 30-392 Krakow, Poland*<sup>2</sup>*Doctoral School of Exact and Natural Sciences, Jagiellonian University, Lojasiewicza  
11, 30-348 Krakow, Poland*<sup>3</sup>*AGH University of Krakow, Mickiewicza 30, 30-059 Krakow, Poland*

\*E-mail: maciej.roman@uj.edu.pl

Infrared (IR) microspectroscopy is a microscale, label-free, nondestructive, and information-rich technique successfully applied for years in biological and material science. However, due to the diffraction limit, the lateral resolution of IR measurements can achieve approx. 3–10  $\mu\text{m}$  (wavelength dependent). On the other hand, the rapid development of nanotechnology has created a need for extensive research at the nanoscale. Several new IR techniques have been proposed, including Atomic Force Microscopy – IR (AFM-IR), and scattering-type Scanning Near-field Optical Microscopy (s-SNOM), to overcome the diffraction limit of IR light. The CIRI beamline provides access to a neaSCOPE microscope (attocube systems AG, Germany) that applies AFM-IR and s-SNOM techniques for nanoscale IR imaging and spectroscopy. It is possible through a combination of IR spectroscopy with AFM providing the chemical composition of the sample with a spatial resolution of less than 20 nm. In our studies, IR nanospectroscopy techniques are applied to investigate selected biological samples such as erythrocytes, cell membranes, and lipid bilayers. Since erythrocytes show a unique biconcave structure and pivotal role in oxygen transport, nanoscale investigation of their membranes is of great interest. However, due to the shape and size of cells, they remain difficult to image giving strong artifacts in s-SNOM images. On the other hand, erythrocyte “ghosts”, which after collapsing become more flat and easier to measure, can be easily analyzed for the chemical composition of the cell membrane with a nanoscale spatial distribution. Lipid bilayers are other examples of bionanomaterials that can be successfully studied using IR nanospectroscopy. s-SNOM images and AFM-IR spectra were measured to investigate the heterogeneity of DPPC:DOPC:POPC and DOPC:SM:CHL systems. IR nanospectroscopy techniques allow the identification of sample areas with different chemical compositions.

## Acknowledgments

This project is executed under the provision of the Polish Ministry of Science and Higher Education project “Support for research and development with the use of research infrastructure of the National Synchrotron Radiation Centre SOLARIS” under contract nr 1/SOL/2021/2. This work was supported by the National Science Centre, Poland (Grant No. 2023/49/N/ST4/04046).

Synthesis and dissolution of  $Ce_xO_y$  nanoparticles for catalytic application by  
in-situ liquid cell TEM

J. Depciuch<sup>1,\*</sup>, T. Tarnawski<sup>1</sup>, A. Maximenko<sup>2</sup>, Krzysztof Matlak<sup>2</sup>, M. Pawlyta<sup>3</sup>,  
M. ParlinskaWojtan<sup>1</sup>

<sup>1</sup> *Institute of Nuclear Physics Polish Academy of Sciences, PL-31-342 Krakow, Poland*

<sup>2</sup> *SOLARIS National Synchrotron Radiation Centre, Czerwone Maki 98, 30-392 Krakow,  
Poland*

<sup>3</sup> *Department of Engineering Materials and Biomaterials, Silesian University of Technology,  
Gliwice, 44-100, Poland*

\*e-mail: joanna.depciuch@ifj.edu.pl

Liquid cell TEM (LC-TEM) allows to observe *in situ* dynamic processes occurring during reactions in liquid inside the TEM. Using LC-TEM technique, most important stages of growth dynamics dependence on the ion concentration, the initialization of growth sites or particle synthesis in liquid can be investigated. Synthesis and dissolving of  $Ce_2O$  NPs and electrochemical properties of this binary catalyst ( $Ce_2O@Pd$  NPs/C) were studied.

Dynamic processes were observed in real-time using LC-TEM. The electrochemical activity of the  $Ce_2O@Pd$  NPs/C catalyst towards ethanol oxidation reaction (EOR) was evaluated. In-situ FTIR measurements were used to establish the catalytic activity and stability of  $Ce_2O@Pd$  NPs. X-ray absorption near edge structure (XANES) and X-ray diffraction (XRD) were used to determine the oxidation state of  $Ce_2O$  before and after ethanol oxidation reaction.

The LC-TEM experiment showed, that depending on the beam energy, the  $Ce_2O$  NPs were synthesized or dissolved. The electrochemical results showed, that the presence of  $Ce_2O$  NPs as a substrate for Pd NPs enhances the EOR. XANES and XRD measurements proved, that the synthesized  $Ce_2O$  NPs were stable even after EOR and it was composed of two phases.

Using LC-TEM, synthesis, dissolution and decoration of  $Ce_2O$  by Pd NPs was observed. The combination of XANES and XRD measurements gave detailed information about the structure of  $Ce_2O$  NPs and changes of this structure caused by EOR reaction. Finally, the presence of Pd NPs on the  $Ce_2O/C$  catalyst leads enhancement of the EOR.

**Funding:** This research was founded by the grant from the National Science Foundation 2019/35/B/ST5/04140.

## ARYA – NEW BEAMLINER FOR MACROMOLECULAR X-RAY CRYSTALLOGRAPHY AT SOLARIS

J. Sławek<sup>1\*</sup>, T. Kołodziej<sup>1</sup>, P. Grudnik<sup>2</sup>, M. Kozak<sup>1</sup>

<sup>1</sup>*SOLARIS National Synchrotron Radiation Centre, Jagiellonian University, Kraków,  
Poland*

<sup>2</sup>*Malopolska Centre of Biotechnology, Jagiellonian University, Kraków, Poland*

\*E-mail: joanna.slawek@uj.edu.pl

Macromolecular crystallography is a powerful technique used to determine the three-dimensional structures of biological macromolecules, such as proteins, nucleic acids, and large complexes, at atomic resolution. By analyzing X-ray diffraction patterns, researchers can reveal precise molecular architecture, which is crucial for understanding the function, mechanisms, and interactions of the investigated macromolecules. Synchrotron radiation plays a key role in advancing structural biology by providing intense, highly collimated X-ray beams with tunable wavelengths. This allows for collecting high-quality diffraction data from even the smallest or poorly ordered crystals, facilitating the determination of structures that are challenging or impossible to solve using conventional X-ray sources. The enhanced brightness and flexibility of synchrotron light have led to significant breakthroughs in drug design, enzyme mechanisms, and the exploration of complex biological systems.

The ARYA beamline, formerly known as the SOLCRYS beamline, will be a fully tunable and highly automated system operating at an energy range of 5-16 keV. Crystals will be mounted on a goniostat and rotated in the X-ray beam with high speed and precision. The reflections scattered on the crystal will be recorded by a high-resolution detector. The entire measurement process will be fully automated, allowing the testing of several dozen crystals per day. Data collected will be processed using various software packages, automatically solving the structures of the examined objects. In addition to routine crystallographic experiments for macromolecules, ARYA will offer additional measurement capabilities such as high-pressure measurements in DACs, temperature control from room temperature to 100K, and crystallographic fragment screening. The beamline will also be equipped with a fluorescence detector crucial for measuring samples containing metals. Currently, the beamline is under construction. The first planned user experiments are scheduled for 2027.

## SAXS/WAXS END STATION FOR SMAUG BEAMLIN

Maciej Kozak<sup>1,2</sup>, Joanna Sławek<sup>1</sup>, Tomasz Kołodziej<sup>1</sup>, Agnieszka Klonecka<sup>1</sup>, Franciszek Sobczuk<sup>1</sup>, Marcin Brzyski<sup>1</sup>, Michał Taube<sup>2</sup>, Daria Wojciechowska<sup>2</sup>, Ewa Banachowicz<sup>2</sup>

<sup>1</sup>*Solaris National Synchrotron Radiation Centre, Jagiellonian University, Czerwone Maki 98, 30-392 Cracow, Poland*

<sup>2</sup>*Department of Biomedical Physics, Adam Mickiewicz University, ul. Uniwersytetu Poznańskiego 2, 61-614 Poznań, Poland*

*\*e-mail: ma.kozak@uj.edu.pl*

The SMAUG experimental beamline, dedicated to X-ray scattering studies using synchrotron radiation, is a joint initiative of Adam Mickiewicz University in Poznań (AMU) and Jagiellonian University. It is financed by a project from the Ministry of Science and Higher Education (Poland) that was granted to AMU. The research at SMAUG will be conducted using synchrotron radiation obtained from the BM02 bending magnet. The energy range of synchrotron radiation from 6 to 15 keV with an intensity of up to 1012 photons/second will be available for experiments on liquid and solid samples.

The end station of the SMAUG beamline will be based on the SAXS/WAXS XEUSS 3.0 UHR system (XENOCSS, Grenoble, France). This equipment will be modified in a way that allows for direct connection to the optical section of the SMAUG beamline. Moreover, two laboratory high flux X-ray microsources (Cu Ka and Mo Ka) will be installed, which will be used in interrupted periods in standard synchrotron operation, allowing for the operation continuity of the SMAUG beamline. The available energy range of synchrotron radiation allows for high-pressure SAXS studies, therefore the end station is equipped with a dedicated chamber for high pressure studies in a solution up to 600 MPa. This setup will allow for monitoring conformational changes in biomacromolecules (proteins, nucleic acids) or pressure-induced phase transitions in polymers, liquid crystals, or lipids. Moreover, at the end station will be possible to conduct SAXS/WAXS studies in a wide temperature range, SEC-SAXS, rheo-SAXS and DSC-SAXS measurements. The end station is expected to be installed in the new experimental hall of the SOLARIS synchrotron in December 2024.

## OPTIMIZATION OF MACROMOLECULE IMAGING IN CRYO-EM METHOD

Grzegorz Ważny<sup>1,2,\*</sup>, Michał Rawski<sup>1</sup> and Sebastian Glatt<sup>3</sup>

<sup>1</sup>*SOLARIS National Synchrotron Radiation Centre, Jagiellonian University, Krakow, Poland*

<sup>2</sup>*Doctoral School of Exact and Natural Sciences, Jagiellonian University, Krakow, Poland*

<sup>3</sup>*Malopolska Center of Biotechnology, Jagiellonian University, Krakow, Poland*

\*E-mail: grzegorz.wazny@uj.edu.pl

The total electron dose ( $e^-/A^2$ ) is a critical parameter in a single particle cryo-EM method. A higher dose allows to achieve a higher signal to noise ratio, which should give a better quality of final macromolecule reconstruction, but also causes a bigger beam-induced motion. Too high dose can destroy the most sensitive parts of observed particles. In general, it is known how to determine the optimal dose for proteins and DNAs for obtaining a high resolution of reconstruction. Unfortunately, for RNA radiation damage problem is not clearly understood. In my PhD research, I will try to find answers to a few essential questions about the resistance of nucleotides to beam radiation:

1. Which nucleotide is the most sensitive to beam radiation and which one is most resistant?
2. Do RNA nucleotide/base pairs react differently to radiation damage than unpaired RNA nucleotides?
3. Which pair of RNA nucleotides is the most sensitive/resistant to radiation damage?
4. Are non-canonical pairs more resistant to radiation than canonical ones?
5. Do bound protein partners influence the beam affected nucleotide pairs?

To reach these aims, I've collected a dataset on the transmission electron microscope (TFS Krios G3i) for human type Ribosome and *E.coli* Ribosome with dose  $160 e^-/A^2$  (160 frames) and  $80 e^-/A^2$  (80 frames) accordingly. Next, I sliced each movie for a sequence of frames. This procedure should deliver information on the impact of dose on the degree of particle destruction and how beam-induced motion changes the final reconstruction resolution.

## STRUCTURAL STUDIES OF PLATINIUM COMPLEXES WITH THIOUREAS

Aleksandra Drzewiecka-Antonik,<sup>1,\*</sup> Anna Wolska,<sup>1</sup> Paweł Rejmak,<sup>1</sup> Daniel Szulczyk,<sup>2</sup>  
Alexey Maximenko,<sup>3</sup> and Marcin T. Klepka<sup>1</sup>

<sup>1</sup>*Institute of Physics Polish Academy of Sciences, 02-668 Warsaw, Poland*

<sup>2</sup>*Medical University of Warsaw, 02-097 Warsaw, Poland*

<sup>3</sup>*SOLARIS National Synchrotron Radiation Centre, 30-392 Krakow, Poland*

\*E-mail: adrzew@ifpan.edu.pl

Most approved therapeutics are organic compounds, however, metal complexes have the potential to offer more diverse properties that can be tuned in order to achieve specific functions [1]. Over the last three decades, there has been increasing interest in platinum complexes with *N,S*-donor ligands as thiourea derivatives. Such complexes may exhibit either higher anticancer activity or reduced toxicity compared to known metal containing drugs, such as *cisplatin* or *carboplatin*.

Platinum complexes with compounds containing three thiourea moieties in their structure (Fig. 1) were synthesized in order to compare their cytotoxic activities with those of initial ligands and reference drugs. The synthesized compounds have been structurally characterized by elemental analysis, ATR-IR, UV-Vis and X-ray photoelectron spectroscopies. More detailed information about the metal-thiourea ligand interaction has been obtained by applying the X-ray absorption spectroscopy (the ASTRA beamline). Density functional theory has been applied to determine the molecular structure of platinum complexes.

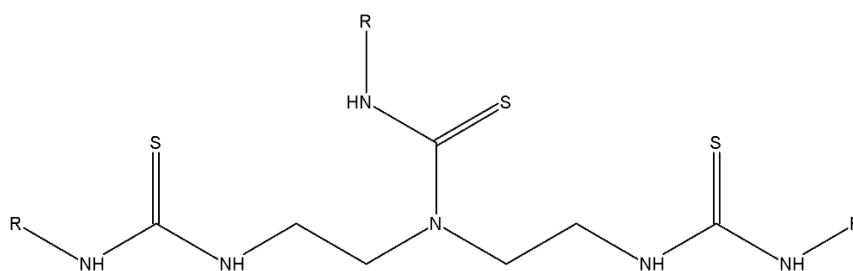


Figure 1. The molecular structure of initial thiourea ligands; R: phenyl or cyclohexyl.

The authors acknowledge SOLARIS Centre for the access to the ASTRA beamline, under the provision of the Polish Ministry of Science and Higher Education project "Support for research and development with the use of research infra-structure of the National Synchrotron Radiation Centre SOLARIS" under contract no. 1/SOL/2021/2. We gratefully acknowledge Poland's high-performance Infrastructure PLGrid (ACK Cyfronet) for providing computer facilities and support within computational grant no. PLG/2022/015746.

## Reference

[1] *Chem. Soc. Rev.*, 2022, **51**, 2544-2582.



OBSERVATION OF RASHBA TYPE SPIN SPLITTING IN GE-DOPED PbSe  
FERROELECTRIC SEMICONDUCTOR

T. Zakusylo,<sup>1,\*</sup> G. Krizman,<sup>1</sup> M. Hajlaoui,<sup>1</sup> T. Takashiro,<sup>1</sup> L. Sajeev,<sup>2</sup> M. Rosmus,<sup>3</sup>  
N. Olszowska,<sup>3</sup> O. Caha,<sup>2</sup> and G. Springholz<sup>1</sup>

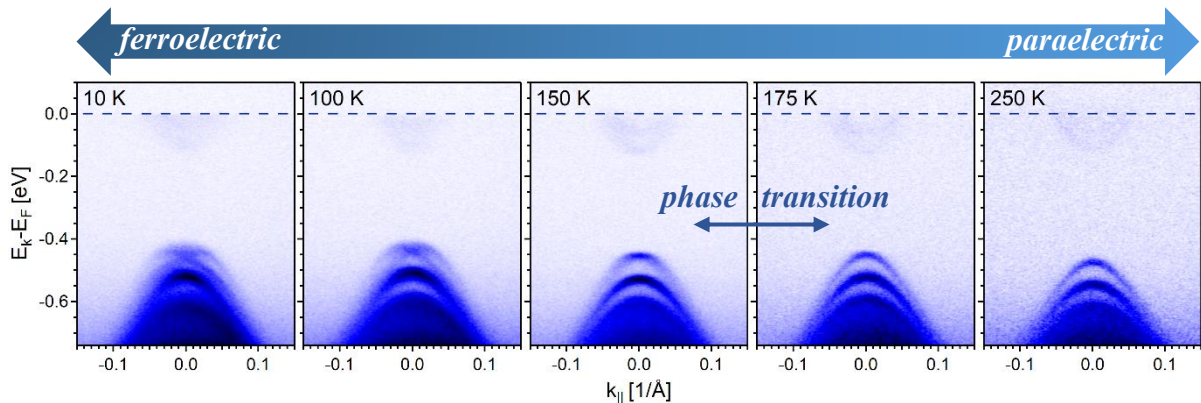
<sup>1</sup>*Institute of Semiconductor and Solid State Physics, Johannes Kepler University, 4040,  
Linz, Austria*

<sup>2</sup>*Department of Condensed Matter Physics, Masaryk University, 602 00, Brno, Czech  
Republic*

<sup>3</sup>*National Synchrotron Radiation Centre SOLARIS, Jagiellonian University, 30-349  
Krakow, Poland*

\*E-mail: tetiana.zakusylo@jku.at

Ferroelectric Rashba semiconductors exhibiting a giant Rashba type spin splitting of ferroelectric origin are a new class of multifunctional materials promising for spintronics yet still lacking experimental realization. In the present work, the ferroelectric Rashba effect is demonstrated for the first time in Germanium-doped PbSe quantum wells by means of temperature-dependent angle resolved photoemission spectroscopy (ARPES) spanning over the whole temperature range of the ferroelectric phase transition from room temperature down to 10 K, with particular attention to the Rashba splitting at the band edges at the high symmetry  $\Gamma$  and M points. The results (Fig.1) unveil a temperature-dependent Rashba type spin splitting that diminishes gradually as the system undergoes a phase transition from ferroelectric to paraelectric phase. Above the ferroelectric transition temperature  $T_C$ , sharp nondegenerate bands are observed, which indicates the absence of any surface-induced Rashba effect. Thus, the temperature-dependent lifting of the Kramer's spin degeneracy below the  $T_C$  is clearly of the ferroelectric origin. This demonstrates Ge-doped PbSe as a promising new compound for ferroelectric Rashba semiconductor applications.



**Figure 1.** Temperature-dependent Rashba type spin splitting in  $\text{Pb}_{1-x}\text{Ge}_x\text{Se}$  quantum wells caused by the ferroelectric phase transition occurring at a critical  $T_C \sim 170$  K for  $x_{\text{Ge}} = 8\%$  in this case. ARPES maps were recorded along the M–K direction from 10 K to 250 K at a photon energy  $h\nu = 18$  eV at the URANOS beamline of SOLARIS.

EFFECTS OF NI/CO DOPING ON STRUCTURAL AND ELECTRONIC  
 PROPERTIES OF 122 AND 112 FAMILIES OF EU BASED IRON PNICTIDES

Joanna Stępień<sup>1,\*</sup>, Damian Rybicki<sup>2</sup>, Marcin Sikora<sup>1,3</sup>, Zbigniew Bukowski<sup>4</sup>, Michał Babij<sup>4</sup>, Łukasz Gondek<sup>2</sup>, Czesław Kapusta<sup>2</sup>, Tomasz Strączek<sup>3</sup>, Kamil Goc<sup>2</sup>, and Danilo Oliveira De Souza<sup>5</sup>

<sup>1</sup>*AGH University of Science and Technology, Academic Centre for Materials and Nanotechnology, al. A. Mickiewicza 30, 30-059 Krakow, Poland*

<sup>2</sup>*AGH University of Science and Technology, Faculty of Physics and Applied Computer Science, al. A. Mickiewicza 30, 30-059 Krakow, Poland*

<sup>3</sup>*National Synchrotron Radiation Centre SOLARIS, Jagiellonian University, Czerwone Maki 98, 30-392 Krakow, Poland*

<sup>4</sup>*Institute of Low Temperature and Structure Research, Polish Academy of Sciences, ul. Okólna 2, 50-422 Wrocław, Poland*

<sup>5</sup>*ELETTRA Sincrotrone Trieste S.C.p.A., S.S. 14 Km 163.5, 34149 Trieste, Italy*

\*E-mail: [jstepien@agh.edu.pl](mailto:jstepien@agh.edu.pl)

Superconductivity in high-temperature superconductors such as cuprates or iron pnictides is typically achieved by hole or electron doping. It is of great interest to understand how doping affects their structural and electronic properties leading to superconductivity.

Iron pnictides are a family with the second highest  $T_c$  values after the cuprates and there are already many families of iron pnictides known. One of the most intensively studied is the 122 family ( $AFe_2As_2$ , where  $A = Ca, Sr, Ba, Eu$ , etc.) In this family superconductivity can be induced by mechanical pressure, by isovalent substitution and by electron or hole doping on Fe or As sites. Another family, which has not received as much scientific attention so far, is the 112 family ( $AFeAs_2$ , where  $A = Ca, Sr, Ba, Eu$ , etc.). The most noticeable difference between 122 and 112 families is the crystal structure: in 122 families there are two alternating layers of A and Fe-As while in the 112 family every second Fe-As layer is replaced by As in zig-zag chains.

We conducted Fe and As K edge x-ray absorption spectroscopy measurements on several electron doped compounds from the 112 and 122 family of Eu-based iron pnictides. XANES and EXAFS confirm that Co and Ni dopants are located at Fe sites. For both families we found an electronic charge redistribution between As and Fe occurring with doping. The changes in charge distribution are stronger in the 112 family and more affect As than Fe site, which indicates that additional charges are predominantly localized on the dopant site<sup>1</sup>.

<sup>1</sup>Stępień, J., Rybicki, D., Sikora, M. *et al. Sci Rep* **13**, 13123 (2023). <https://doi.org/10.1038/s41598-023-40419-8>

#### Acknowledgements

We acknowledge financial support by National Science Centre, Poland (Grant No. 2018/30/E/ ST3/00377).

## XAFS STUDY ON THE $\text{Ca}_{10}\text{Ni}_{0.5}(\text{VO}_4)_7$ CALCIUM ORTHOVANADATE

Anna Wolska<sup>1,\*</sup>, Houri S. Rahimi Mosafer<sup>1</sup>, Christine Martin<sup>2</sup>, Wojciech Paszkowicz<sup>1</sup>,  
Alexey Maximenko<sup>3</sup> and Marcin Klepka<sup>1</sup>

<sup>1</sup>*Institute of Physics Polish Academy of Sciences, Al. Lotników 32/46 PL-02668 Warsaw, Poland*

<sup>2</sup>*Laboratoire CRISMAT, Normandie Université, ENSICAEN, UNICAEN, CNRS, 14050 Caen,  
France*

<sup>3</sup>*SOLARIS National Synchrotron Radiation Centre, ul. Czerwone Maki 98, PL-30392 Krakow,  
Poland*

\*E-mail: wolska@ifpan.edu.pl

Calcium orthovanadate  $\text{Ca}_3(\text{VO}_4)_2$  belongs to a large family of whitlockite-structure orthovanadates. They crystallize in the  $R3c$  space group where the Ca atoms are located in five inequivalent sites. In the unsubstituted crystals a small fraction (typically up to ~10%) of Ca atoms can be replaced by others, of valences from +1 to +4, without a change of structure. In such cases, the corresponding structural modification consists of a partial or full replacement of Ca atoms at one (substitutionally ordered compound) or more of Ca sites (disordered compound) by the substituting atom. The whitlockite-type orthophosphates and orthovanadates jointly substituted with one divalent and one trivalent metal are of interest since they are considered for applications in optoelectronics, being potentially useful for white light generation.

In this work we have focused on the calcium orthovanadate doped with Ni atoms, namely the  $\text{Ca}_{10}\text{Ni}_{0.5}(\text{VO}_4)_7$  crystal. Our aim was to determine the host site for Ni ions. The perfect technique for such a case is the X-ray absorption fine structure spectroscopy (XAFS) which probes the local neighborhood around specific element. The XAFS measurements were performed at the ASTRA beamline at the SOLARIS synchrotron (Kraków, Poland). The Ni K-edge had been measured in the fluorescence mode at room temperature.

The analysis revealed that the Ni atoms mainly locate at M5 site, the only regular octahedral site for Ca, with six oxygen atoms in the nearest neighborhood.

The authors acknowledge SOLARIS Centre for the access to the ASTRA beamline, under the provision of the Polish Ministry of Science and Higher Education project "Support for research and development with the use of research infra-structure of the National Synchrotron Radiation Centre SOLARIS" under contract no. 1/SOL/2021/2.

Investigation of Local Order in Bi<sub>2</sub>O<sub>3</sub>-Al<sub>2</sub>O<sub>3</sub>-SiO<sub>2</sub> Glasses  
and Nanomaterials Using ASTRA Beamline

Maciej Nowagiel<sup>1,\*</sup>, Alexey Maximenko<sup>2</sup>, Marek Wasiucionek<sup>1</sup>,  
and Tomasz K. Pietrzak<sup>1</sup>

<sup>1</sup>*Faculty of Physics, Warsaw University of Technology, 00-662 Warszawa, Poland*

<sup>2</sup>*Solaris National Synchrotron Radiation Centre, Jagiellonian University, 30-392  
Kraków, Poland*

\*E-mail: maciej.nowagiel.dokt@pw.edu.pl

Bi<sub>2</sub>O<sub>3</sub>-Al<sub>2</sub>O<sub>3</sub>-SiO<sub>2</sub> bismuth oxide glasses have been observed as an interesting starting system for the stabilization of several crystal structures of Bi<sub>2</sub>O<sub>3</sub> [1]. In particular,  $\delta$ -Bi<sub>2</sub>O<sub>3</sub> is a candidate material for oxide ion conducting membranes in intermediate-temperature fuel cells. This phase is, however, stable only in the high-temperature range (>730°C). We observed the confinement of  $\delta$ -like nanograins in an amorphous matrix down to room temperature. The physical explanation of this phenomenon is not clear yet. There are a few working hypotheses:

1. stabilization due to the nanometric size of grains and the influence of the glassy matrix,
2. incorporation of glass-forming dopants into the crystal structure,
3. formation of non-stoichiometric Bi<sub>2</sub>O<sub>4-x</sub> due to the presence of Bi<sup>5+</sup> ions.

Local arrangement around Si, and Al atoms has already been investigated by MAS NMR. However, it was impossible to collect similar data for Bi atoms because of their exceptionally broad NMR spectrum. In this case of X-ray absorption spectroscopy measurements at ASTRA beamline could give a solution.

A unique property of the ASTRA beamline is its wide range of energy which covers all the required energies for elements present in bismuth-alumino-silicate glasses and nanomaterials. Namely, the Bi L<sub>3</sub>-absorption bismuth edge (13.4 keV) and Al, Si K-absorption edges (1.56 keV and 1.84 keV, respectively).

In this work, we study the stabilization mechanism down to room temperature of a  $\delta$ -like bismuth oxide phase confined in a glassy matrix. We want to determine the local environment of Bi and check whether Bi<sup>5+</sup> ions are present in the structure of studied materials. Investigation of the L<sub>3</sub>-absorption edge of Bi may be helpful to exclude the third of the working hypotheses if no presence of Bi<sup>5+</sup> is detected. Studies on the local environment of Bi and Si by XANES/EXAFS and Al by XANES would also support the other two hypotheses by revealing the local environment of these atoms and can be compared with the previous MAS-NMR investigation. During the presentation, the project overview through the prism of XAS measurements will be presented.

References:

[1] T.K. Pietrzak *et al.* Sci. Rep. 11 (2021) 1–12.

## Sulfur K-edge XANES spectra of methyl and phenyl compounds: breaking new ground in organic compound research at the ASTRA beamline

Ryszard Stekla<sup>\*1,2</sup>, Alexander Prange<sup>3</sup>, Josef Hormes<sup>4</sup>, Henning Lichtenberg<sup>3</sup>, Alexey Maximenko<sup>1</sup>

<sup>1</sup> NSRC SOLARIS 30-392 Krakow, Poland,

<sup>2</sup> AGH University of Krakow, 30-059 Krakow, Poland,

<sup>3</sup> Niederrhein University of Applied Sciences, 47805 Krefeld, Germany,

<sup>4</sup> University of Bonn, 53113 Bonn, Germany

\*correspondence E-mail:stekla@student.agh.edu.pl

ASTRA is an X-ray absorption spectroscopy beamline specially constructed for measurements in the tender energy range of X-rays. One major field of activity is XANES and EXAFS spectroscopy at the sulfur K-absorption edge. Investigating the atomic environment of sulfur atoms in different materials, especially the local bond structure, plays an important role in petrochemistry and polymer science. Sulfur can form up to six bonds by donating, and up to two bonds by accepting electrons due to vacant **3p** orbitals. The strength of these chemical bonds is influenced not only by its electronegativity difference but also by surrounding ligands<sup>i</sup>. The complexity of sulfur bonds is associated with shifts in energy levels caused by orbital hybridization. Hybridization modifies the electronic structure of a molecule, impacting the lowest unoccupied molecular orbital (LUMO), and consequently, the molecule's chemical behavior<sup>ii</sup>. A bond's impact on orbital occupation depends on its ionic character — the more ionic the bond towards the target atom, lower the energy required to transfer the electron. The more occupied the orbitals, lower the photon energy required to temporarily transfer electrons from the **1s** orbital to the Rydberg states. Therefore, the local bond structure of sulfur in different organic compounds can be easily investigated using X-ray absorption fine structure (XAFS) spectroscopy.

Several years ago, researchers from the University of Bonn measured a comprehensive set of XANES spectra at the S K-edge of rare organic sulfur compounds with methyl and phenyl groups, sometimes bonded with extra oxygen bonds, at different synchrotrons (in Germany and the USA) before ASTRA was built. Unfortunately these spectra were no longer available as data files, but only printed on paper. Scientists at ASTRA are now digitizing the data and adding it to ASTRA's XAS spectra library. Moreover, they performed an analysis of the spectra combined with the FEFF simulations. During the presentation, the main features of the spectra will be related to sulfur bonds with carbon, oxygen and other sulfur atoms and further discussed.

This work is a stepping stone for ASTRA's beamline users conducting similar studies about organic compounds, providing the beamline with a XANES library of unique sulfur-containing compounds.

**Acknowledgements:** The further development of the ASTRA beamline for measuring at low photon energies was supported within the EU Horizon2020 programme (952148-Sylinda).

<sup>i</sup> Sulfur X-ray Absorption and Vibrational Spectroscopic Study of Sulfur Dioxide, Sulfite, and Sulfonate Solutions and of the Substituted Sulfonate Ions X<sub>3</sub>CSO<sub>3</sub> - (X) H, Cl, F) E. D. Risberg, L. Eriksson, J. Mink, L. G. M. Pettersson, M. Y. Skripkin, M Sandstrom

<sup>ii</sup> Functional Groups and Sulfur K-Edge XANES Spectra: Divalent Sulfur and Disulfides A. Mijovilovich, L. G. M. Pettersson, F. M. F. de Groot, B. M. Weckhuysen

EVOLUTION OF THE ELECTRONIC STRUCTURE OF CU  
NANOPARTICLES AT DIFFERENT OXIDIZING CONDITIONS

Gabriela Imbir<sup>1,\*</sup>, Anna Wach<sup>2</sup>, Joanna Czapla-Masztafiak<sup>1</sup>, Wojciech Błachucki<sup>1</sup>,  
Rafał Fanselow<sup>1</sup>, Artem Yakovliev<sup>1</sup>, Jakub Szlachetko<sup>2</sup>

<sup>1</sup>*Institute of Nuclear Physics Polish Academy of Sciences, Radzikowskiego 152,  
31-342 Krakow, Poland,*

<sup>2</sup>*Solaris National Synchrotron Radiation Centre, Czerwone Maki 98, 30-392 Krakow,  
Poland*

\*E-mail: gabriela.imbir@ifj.edu.pl

Transition metal-based nanoparticles (NPs) such as gold, silver, and copper have attracted a lot of attention from nanotechnologists due to unique optical properties involving intense light absorption and scattering caused by the collective motion of conduction electrons, i.e., plasmons. Such excitation results in localization and enhancement of the electric field causing the simultaneous oscillations of the nanoparticle's free electron and corresponding electromagnetic field oscillations, named localized surface plasmon resonance (LSPR) [1]. Among plasmonic-based nanostructures, copper nanoparticles gathered interest as a cost-effective alternative to expensive silver or gold metals [2]. However, Cu NPs are challenging to analyze due to their affinity for rapid oxidation, particularly at sizes below 50 nm [2]. Their surface readily oxidizes in ambient atmospheres and at room temperature, requiring the application in core-shell type structures to prevent oxidation. While the encapsulation could inhibit oxidation, it can also alter the optical and electronic properties of the nanoparticles, hindering their physicochemical attributes [2]. The fundamental aspects of these nanomaterials, including the effect of Cu NPs surface oxide on LSPR strength and coupling the surface oxide to molecular linkers remain unknown and are still being investigated [2].

In the presented study, we aimed to investigate structural and physicochemical properties of Cu NPs at different oxidation conditions using mainly X-ray absorption spectroscopy technique at the POLYX beamline of the SOLARIS National Synchrotron Radiation Centre. The experiment was executed around the Cu K-absorption edge (8980 eV) on liquid samples with two different Cu NPs sizes to evaluate structural changes caused by oxidation.

The outcome of this research provided the basis for determining Cu-oxide/Cu-metal compositions in the obtained CuO<sub>x</sub>@Cu core-shell type structures. These findings will help to design and develop plasmonic Cu-based nanostructures for various applications, including electronics, biosensing, and the improvement of antibacterial properties.

**Acknowledgment:** This project was financed by the National Science Centre (Poland) under grant number 2020/37/B/ST3/00555

References:

- [1] V.G. Kravets et al., Chem. Rev. 118, 5912 (2018)
- [2] P. Kanninen et al., J. Coll. Inter. Scien. 318, 88-95 (2008)

### MOLECULAR INSIGHTS OF THE OXIDATION PROCESS OF IRON OXIDE AND COBALT FERRITES NANOPARTICLES INCORPORATED IN ALGINATE FIBERS

Paweł Winiarski<sup>1,2\*</sup>, Anna Rypel<sup>2</sup>, Marta Gajewska<sup>2</sup>, Marcin Sikora<sup>3</sup>, Katarzyna Berent<sup>2</sup>,  
Joanna Stępień<sup>2</sup>, Szczepan Zapotoczny<sup>2,4</sup>, Dorota Lachowicz<sup>2</sup>

<sup>1</sup> *AGH University of Krakow, Faculty of Materials Science and Ceramics,  
al.A.Mickiewicza 30, 30-059 Krakow*

<sup>2</sup> *AGH University of Krakow, Academic Centre for Materials and Nanotechnology,  
al.A.Mickiewicza 30, 30-059 Kraków, Poland*

<sup>3</sup> *Solaris National Synchrotron Radiation Centre, Jagiellonian University, Czerwone  
Maki 98, 30-392 Kraków, Poland*

<sup>4</sup> *Faculty of Chemistry, Jagiellonian University, Gronostajowa 2, 30-387 Kraków, Poland*

\*E-mail: winiarski@agh.edu.pl

Functional hybrid fibers based on biopolymers are becoming increasingly popular due to their unique properties[1]. Smart fibers have dual functions of sensing and reaction at the same time. They can sense changes in external environmental conditions (mechanical, thermal, chemical, light, humidity, electromagnetic, etc.), and adjust their internal structures to respond to external stimuli in an optimized way[2]. Iron oxide nanoparticles or mixed ferrites are most often used to obtain magnetic fibres due to their magnetic properties and lack of toxicity. Alginate is chosen for its mechanical properties and ability to act as a matrix for nanoparticles[3]. However, the interaction between the nanoparticle and the polymer significantly affects the durability of magnetic properties over time. The project's main goal was to investigate the influence of alginate (an anionic polysaccharide) on the magnetic properties and chemical structure of iron oxide and cobalt ferrite nanoparticles over time. For this purpose, X-ray absorption spectroscopy (XAS) measurements were used. The local structures around the Co, Fe, and O sites were investigated as reflected by the K-edge X-ray Absorption Spectra. The nanoparticle composition was determined based on a multivariate analysis supported by ICP-OES data. To further explore the structure of all obtained composite fibres, XPS spectra of all polymer fibres were analysed to determine the chemical states.

[1] Q. Shi, et al, *Advanced Fiber Materials*, 1, 3-31 (2019)

[2] L. Huang, et al, *Advanced Materials*, 32, e1902034 (2020)

[3] H. Xu, et al, *Chemical Engineering Journal*, 489, 151223 (2024)

## RESEARCH AT THE PIRX BEAMLIN

K. Pitala<sup>1,\*</sup>, E. Partyka-Jankowska<sup>1</sup>, J. Stępień<sup>2</sup>, T. Strączek<sup>1</sup> and M. Zając<sup>1</sup>

<sup>1</sup>*SOLARIS National Synchrotron Radiation Centre,*

*Czerwone Maki 98, 30-392 Kraków, Poland*

<sup>2</sup>*AGH University of Science and Technology, Academic Centre for Materials and*

*Nanotechnology, Al. Mickiewicza 30, 30-059 Kraków, Poland*

\*E-mail: [krzysztof.pitala@uj.edu.pl](mailto:krzysztof.pitala@uj.edu.pl)

The PIRX beamline [1] at SOLARIS National Synchrotron Radiation Centre [2] is an excellent example of infrastructure with sub-nanometer element sensitivity and selectivity. With absorption spectroscopy method in the soft X-ray range: 100-2000 eV (XAS), it is a powerful tool to study chemical and electronic properties, in particular the oxidation state or the local geometric arrangement of surrounding atoms. Furthermore, the PIRX beamline gives the possibility to study dichroism phenomena exploiting methods such as XMCD, XMLD and XNLD which provide a deep insight into the structural and magnetic features of the materials. The end station of the beamline is also equipped with a preparation chamber that allows to prepare or modify materials in-situ.

Possible applications range from spintronics, physics and materials science, through chemistry and catalysis to biological sciences and medicine. Examples of those applications and the research capabilities of the beamline will be outlined by this presentation.

### References

1. M. Zając, T. Giela, K. Freindl, K. Kollbek, J. Korecki, E. Madej, K. Pitala, A. Koziół-Rachwał, M. Sikora, N. Spiridis, J. Stępień, A. Szkudlarek, M. Ślęzak, T. Ślęzak, D. Wilgocka-Ślęzak; *Nuclear Instruments and Methods in Physics Research Section B*: 492, 43-48, (2021); <https://doi.org/10.1016/j.nimb.2020.12.024>
2. J. Szlachetko et al., *SOLARIS National Synchrotron Radiation Centre in Krakow, Poland*, *The European Physical Journal Plus* 138, 10 (2023). <https://doi.org/10.1140/epjp/s13360-022-03592-9>



### Spectroscopic Synergy at the ASTRA Beamline: Combining X-ray Absorption and Raman Spectroscopy for Advanced Analysis of Complex Materials

Lulu Alluhaibi<sup>1</sup>, Alexey Maximenko<sup>1</sup>, Grzegorz Gazdowicz<sup>1</sup>, Marcin Brzyski<sup>1</sup>, Marcel Piszak<sup>1</sup>, Henning Lichtenberg<sup>2</sup>, Alexander Prange<sup>2</sup> and Josef Hormes<sup>3</sup>

<sup>1</sup>*Solaris National Synchrotron Radiation Centre, Jagiellonian University, Czerwone Maki 98, 30-392 Kraków, Poland*

<sup>2</sup>*Hochschule Niederrhein University of Applied Sciences, Krefeld, Germany*

<sup>3</sup>*Institute of Physics, Rheinische Friedrich-Wilhelms-Universität, Bonn, Germany*

Email: lulu.alluhaibi@uj.edu.pl

Combining X-ray Absorption Spectroscopy (XAS) with vibrational spectroscopy techniques such as Raman spectroscopy offers a powerful approach for studying structural and chemical changes in materials, particularly catalysts. Simultaneously recording XAS and Raman spectroscopic data allows for the observation of structural changes in solid materials while also monitoring adsorbed species on their surfaces, providing a more complete picture of the entire process.

Raman spectroscopy is a versatile analytical method used under in situ conditions to study chemical structures and interactions of gases, liquids, solids and their interfaces. Combination with XAS can reveal detailed correlations between the local electronic structure (XAS) and the molecular vibrations and bonding environment (Raman). This is especially useful for investigating complex materials, where changes in the local structure can significantly impact overall properties. While XAS probes the oxidation state and coordination geometry of specific chemical elements, Raman spectroscopy provides information on bond types and the molecular framework. Together, these techniques offer comprehensive insights into the chemical state and bonding environment, allowing researchers to cross-validate and enrich their findings.

The installation of a Raman spectrometer with two laser sources (782 nm and 532 nm) at the XAS beamline ASTRA (SOLARIS synchrotron) was successfully completed in July 2024. The second part of the project involves the integration of the Raman probe into ASTRA's sample chamber for measurements under vacuum or in helium atmosphere and will be realized within a few months. We are optimistic that combined measurements will be feasible during beamtimes allocated based on the upcoming calls. This presentation will feature an overview of the infrastructure installed so far for the Raman probe, and the status of its integration at the ASTRA beamline. Furthermore, examples of a comprehensive investigation of P and S containing compounds by analyzing XAS and Raman spectra will be shown, along with the unique possibilities these new experimental capabilities offer ASTRA's user community.

### THE USE OF SYNCHROTRON RADIATION IN THE STUDY OF THORIUM COMPLEXES WITH P-DONOR LIGANDS

Ewelina Grabias-Blicharz<sup>1</sup>, Agnieszka Gładysz-Płaska<sup>2\*</sup>, Agnieszka Lipke, Marek Majdan,

Alexey Maximenko<sup>3</sup>

<sup>1</sup>*Medical University of Lublin, Faculty of Pharmacy, Lublin, Poland*

<sup>2</sup>*Maria Curie-Skłodowska University, Lublin, Poland*

<sup>3</sup>*Solaris National Synchrotron Radiation Centre, Jagiellonian University, Czerwone Maki 98,*

*30-392 Kraków, Poland*

\*e-mail: [agnieszka.gladysz-plaska@mail.umcs.pl](mailto:agnieszka.gladysz-plaska@mail.umcs.pl)

These studies are extremely important for understanding the influence of phosphorus on thorium binding, which is necessary to control the mobility of this element in the environment. Due to the fact that thorium can be used as fuel in nuclear power plants and in the situation of moving away from coal-fired electricity production, this issue is currently gaining more and more practical importance.

The mechanisms of Th binding and immobilization are of fundamental importance for determining and predicting both the stabilizing capacity and the migration potential or developing remedial strategies. XANES measurements are an excellent tool for analysis, because they allow for a deeper insight into the sample. Therefore, understanding the modification of composite materials by the Th(IV) sorption process requires XANES spectroscopy to study the local structure of complexes in the solid phase. Measurements performed on the ASTRA beamline allowed for recording XANES spectra of thorium measured at the M4 and M5 absorption edges, while the phosphorus spectrum at the K edge.

CAPABILITIES OF THE ASTRA BEAMLINE FOR X-RAY ABSORPTION SPECTROSCOPY  
IN LIFE SCIENCES AND AGRICULTURE: HIGHLIGHTS AND FUTURE PLANS

Grzegorz Gazdowicz<sup>1\*</sup>, Alexey Maximenko<sup>1</sup>, Henning Lichtenberg<sup>2</sup>, Lulu Alluhaibi<sup>1</sup>,  
Marcin Brzyski<sup>1</sup>, Marcel Piszak<sup>1</sup>, Alexander Prange<sup>2</sup> and Josef Hormes<sup>3</sup>

<sup>1</sup>*Solaris National Synchrotron Radiation Centre, Jagiellonian University,  
30-392 Kraków, Poland*

<sup>2</sup>*Hochschule Niederrhein University of Applied Sciences, 47805 Krefeld, Germany*

<sup>3</sup>*Institute of Physics, Rheinische Friedrich-Wilhelms-Universität, 53115 Bonn, Germany*

\*Email: grzegorz.gazdowicz@uj.edu.pl

The ASTRA beamline at the SOLARIS National Synchrotron Radiation Centre in Krakow is a handy and versatile tool for X-ray absorption spectroscopy (XAS). The available energy range of 1-15 keV is quite unique among other synchrotron X-ray spectroscopic beamlines. It encompasses the tender and part of the hard X-ray radiation and covers the K-edges of significant chemical elements like magnesium, silicon, sulfur, phosphorus, chlorine and 3d transition metals, which are important for many enzymes and other bioactive chemical compounds. Therefore, gathering information about their chemical state provides direct insights into biochemical processes in given specimens. L- absorption edges up to bismuth and M-edges of actinides can be investigated at ASTRA as well. The beamline's capabilities are especially valuable not only for material sciences and catalyst research but also for the life sciences, agriculture, and the food industry.

In this presentation, X-ray absorption spectra of samples measured in both solid and liquid phase, at reduced or ambient pressure, will be presented, highlighting ASTRA's research potential in the mentioned areas. Moreover, the current status of the reference spectra library of sulfur containing compounds commonly used in biomedical studies involving cell cultures or protein crystal growth will be discussed. Furthermore, the technical further development of ASTRA will be discussed, with a strong focus on the integration of a Raman probe into the XAS set-up. We believe that such a combination of two spectroscopic techniques will bring ASTRA even closer to topics in life science and agro-food industry. Also, combining two spectroscopies for *in-situ* and *operando* measurements will be highly attractive for chemists working in the fields of catalysis, nanoparticle research and electrochemistry.

**Acknowledgements:** The further development of the ASTRA beamline for measuring at low photon energies was supported within the EU Horizon2020 programme (952148-Sylinda).

ELECTRONIC STRUCTURE OF  $\text{ZnIn}_2\text{S}_4$   
REVEALED BY PHOTOEMISSION INVESTIGATIONSAgata Sabik,<sup>1,\*</sup> Wojciech M. Linhart,<sup>2</sup> Natalia Olszowska,<sup>3</sup> Marcin Rosmus,<sup>3</sup>  
Milosz Grodzicki,<sup>2</sup> Zdenek Sofer,<sup>4</sup> and Robert Kudrawiec<sup>2</sup><sup>1</sup>*Department of Physics and Astronomy, University of Wrocław, 50-204 Wrocław, Poland*<sup>2</sup>*Faculty of Fundamental Problems of Technology, Wrocław University of Science and  
Technology, 50-370 Wrocław, Poland*<sup>3</sup>*Solaris National Synchrotron Radiation Centre, Jagiellonian University,  
30-392 Kraków, Poland*<sup>4</sup>*Department of Inorganic Chemistry, University of Chemistry and Technology Prague,  
166 28 Prague 6, Czech Republic*

\*E-mail: agata.sabik2@uwr.edu.pl

Zinc indium sulphide ( $\text{ZnIn}_2\text{S}_4$ ) attracts interdisciplinary attention due to its appealing catalytic and photosensing activities, which can be used in photodetectors, solar cells or fuel cells [1-3]. Moreover, high physicochemical stability and durability, together with low toxicity, strengthen the  $\text{ZnIn}_2\text{S}_4$  candidature for its application in the next generation of environmentally friendly devices. For this purpose the fundamental knowledge about electronic properties of the material is required. Therefore, we probed the electronic structure of the hexagonal  $\text{ZnIn}_2\text{S}_4$  crystal by combination of photoemission measurements, i.e., synchrotron radiation-based angle-resolved photoelectron spectroscopy (ARPES) together with X-ray and UV photoelectron spectroscopies. The results are supported by optical studies carried out by transmission and photoluminescence techniques. We experimentally confirm, previous predictions from the calculations based on density functional theory [2], that  $\text{ZnIn}_2\text{S}_4$  is a n-type semiconductor wherein a valence band maximum is located at a  $\Gamma$  high-symmetry point in a Brillouin Zone. Furthermore, the data allows for determination of basic electronic parameters of the crystal such as width of band gap, electron affinity, and work function.

## References

- [1] L. Valdman et al., *Adv. Optical Mater.*, 9 2100845 (2021).
- [2] R. Yang et al., *Small Methods*, 5 2100887 (2021).
- [3] G. Yadav et al., *Inorg. Chem. Commun.*, 138 109288 (2022).

## Acknowledgments

This work has been supported by the Polish National Science Center (No. 2019/35/B/ST5/02819). The ARPES studies have been performed at the Solaris National Synchrotron Radiation Centre (Exp. no. 221911).

## Hydrostatic compression effects on metallic glasses -a combined XAFS and simulation study

Przemysław Dziegielewski,<sup>1</sup> Zuzanna Kostera,<sup>1</sup> and Jerzy Antonowicz<sup>1,\*</sup>

<sup>1</sup>Faculty of Physics, Warsaw University of Technology, Koszykowa 75, 00-662 Warsaw, Poland,

\*E-mail: jerzy.antonowicz@pw.edu.pl

Metallic glasses (MGs) are amorphous alloys that lack the regular atomic structure typical of crystalline metals. The stability of MGs against crystallization is attributed to their high atomic packing density, which, despite the absence of long-range periodicity, displays significant short- and medium-range order. The atomic packing efficiency of MGs can be further enhanced by applying external hydrostatic pressure. Recent findings suggest that, under compression, MGs adapt to external load through complex structural reorganization involving electronic effects.

In this study, we investigate the high-pressure atomic and electronic structures of binary Zr-Cu and Zr-Ni MGs using X-ray absorption spectroscopy and theoretical modeling. Our results show that compression induces the development of atomic icosahedral short-range order, involving crystallographically forbidden five-fold symmetry [1, 2]. This structural reconfiguration is primarily driven by the preferential straining of mechanically soft Zr-Zr pairs. Additionally, as suggested by molecular dynamics simulations [3] and confirmed experimentally by X-ray absorption data, an unexpected collapse in the Zr atomic radius occurs around 50 GPa. Density functional theory calculations indicate that this effect is related to a pressure-induced change in the electronic configuration of Zr [4].

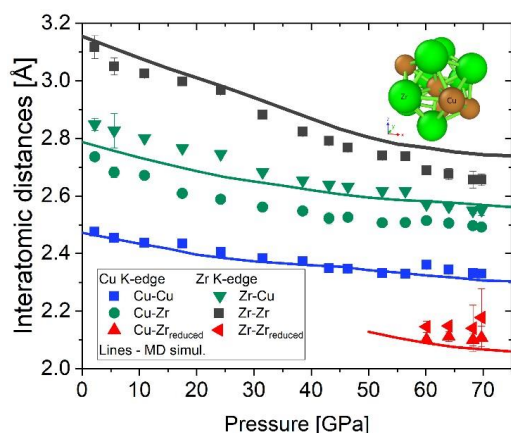


Figure 1. Pressure dependence of interatomic distances during hydrostatic compression of  $Zr_{67}Cu_{33}$  metallic glass derived from EXAFS fitting (symbols). Solid lines represent the results of the molecular dynamics simulations.

### References

- [1] J. Antonowicz *et al.*, *Phys. Rev. B* 93 (2016) 144115,
- [2] P. Dziegielewski *et al.*, *High Press. Res.* 40 (2020) 54, \
- [3] P. Dziegielewski, G. Evangelakis, J. Antonowicz, *Comput. Mater. Sci.* 208 (2022) 111345
- [4] Z. Kostera, J. Antonowicz, P. Dziegielewski, *New J. Phys.* 26 (2024) 073032.

## PHELIX - An advanced tool for complementary photoemission experiments

Edyta Beyer<sup>1</sup>, Barbara Wolanin<sup>1</sup>, Tomasz Sobol<sup>1</sup>

<sup>1</sup>*SOLARIS National Synchrotron Radiation Centre, Jagiellonian University, Krakow, Poland*

Email: edyta.beyer@uj.edu.pl

PHELIX is an undulator beamline[1] installed at the BM06 straight section of SOLARIS, a third-generation synchrotron light facility with an electron energy of 1.5 GeV. The beamline is designed to conduct experiments with ultra-high vacuum X-ray photoemission and X-ray absorption spectroscopy.

The beamline end station is intended to investigate the electronic structure of various materials, from highly ordered crystalline solids to amorphous phases like ceramics, glass, or minerals. Numerous available techniques make this station a powerful and unique tool for studying complex systems. The photoemission experiment can be carried out with techniques like angle resolved photoemission (ARPES), Circular-Dichroism-ARPES, Spin-Resolved-ARPES, and XPS. The SPECS PHOIBOS 225 energy analyzer with a deflector system and a CMOS camera, allow to collect photoemission data with an energy resolution better than 2 meV and an angle resolution of 0.1°. The combination of X-ray photoemission and absorption spectroscopy enables Resonant-PES (ResPES) measurements.

The source of PHELIX is an APPLE-II type undulator which delivers soft X-rays with following parameters:

- Photon energy range from 50 eV up to 2000 eV (horizontally polarized light),
- Linear (horizontal and vertical) and Circular (left and righthanded) polarized light,
- Flux:  $\sim 10^{12}$  ph/s.

The optical design of the PHELIX beamline is based on a classic plane-grating monochromator (PGM) setup operating with a collimated beam. The focusing and re-focusing mirrors system allows for obtaining a beam size spot on the sample of 120  $\mu\text{m}$  x 40  $\mu\text{m}$  (h x v).

### References

- [1] M. Szczepanik, T. Sobol, J. Szade, *Nuclear Instruments and Methods in Physics Research B* 492 (2021) 49–55

## On-site Coulomb energy in TMDC compounds by resonant Photoemission

Yashasvi Mehra<sup>1,2,3</sup>, Samuel Bealieu<sup>4</sup>, Mauro Faniculli<sup>1,2</sup>, Olivier Heckmann<sup>1,2</sup>,  
Karol Hrivoni<sup>1,2</sup>, Marchin Rosmos<sup>5</sup>, Natalia Olszowska<sup>5</sup>, Tomasz Sobol<sup>5</sup>, Edyta Beyer<sup>5</sup>,  
Aki I. O. Pulkkinen<sup>3</sup>, Jan Minar<sup>3</sup>, Maria Christine Richter<sup>1,2</sup>

<sup>1</sup>Université Paris-Saclay, CEA, LIDYL, Gif-sur-Yvette, France

<sup>2</sup>CY Cergy Paris Université, CEA, LIDYL, Gif-sur-Yvette, France

<sup>3</sup>University of West Bohemia, NTC, Pilsen, Czech Republic

<sup>4</sup>Université de Bordeaux, CNRS, CEA, CELIA, UMR 5107, Talence, France

<sup>5</sup>SOLARIS National Synchrotron Radiation Centre, Jagiellonian University, Krakow,  
Poland

\*E-mail: yashasvi@ntc.zcu.cz

The Coulomb interaction  $U$ , serves as a pivotal parameter influencing electron behavior, particularly accentuated within low-dimensional materials. Transition Metal Dichalcogenides, quasi-2-D systems, exhibit diverse electronic traits like CDW order, co-existing CDW with superconductivity, and topologically nontrivial phases. Their 2D nature intensifies coulomb interaction of electrons, leading to phenomena like Mott-Hubbard transitions. The on-site Coulomb energy for transition metal and chalcogenide atoms is determined through a method proposed by Cini and Sawatzky [1-3].

This approach is based on comparison of the energy of the correlation satellite linked to the two-valence-hole (VV) Auger final state in resonant photoemission with the uncorrelated two-valence-hole energies derived from a self-convolution of single hole states obtained from a non-resonant photoemission spectrum. The energy difference between the main peaks of the resonantly enhanced spectrum and the uncorrelated two-hole spectrum serves as a measure of the Coulomb energy. Here we aim to determine the on-site Coulomb interaction for each element within two series of TMDC materials ( $MX_2$ , where  $X = S, Se, Te$  and  $M = Nb, Ta$ ) by resonant ARPES.

[1] Sawatzky G. A., Phys. Rev. Lett. 39, 504 (1977).

[2] Cini M., Phys. Rev. B 17, 2788 (1978).

[3] Sawatzky G.A., et al PhysRevB.21.1790 (1980).

## CORRELATIVE FLUORESCENCE AND SOFT X-RAY MICROSCOPY IN THE WATER WINDOW IN AN INTEGRATED LABORATORY-BASED SETUP

Sophia Kaleta\*<sup>(1, 2)</sup>, J. Reinhard<sup>(2)</sup>, J. J. Abel<sup>(2)</sup>, F. Wiesner<sup>(2)</sup>, M. Wünsche<sup>(1, 2)</sup>, T. Weber<sup>(2)</sup>,  
F. Hillmann<sup>(3)</sup>, A. Iliou<sup>(3)</sup>, C. Eggeling<sup>(4, 5)</sup>, M. Westermann<sup>(6)</sup>, E. Seemann<sup>(7)</sup>,  
H. Fiedorowicz<sup>(8)</sup>, S. Fuchs<sup>(9)</sup>, G.G. Paulus<sup>(1, 2)</sup>

(1) *Helmholtz Institute Jena, Fraunhoferstr. 8, Jena, Germany*

(2) *Institute of Optics and Quantum Electronics, Max-Wien-Platz 1, Jena, Germany*

(3) *Leibniz Institute for Natural Product Research and Infection Biology, Hans Knöll Institute  
(Leibniz-HKI), AdolfReichwein-Str. 23, 07745 Jena, Germany*

(4) *Institute of Applied Optics and Biophysics, Friedrich Schiller University Jena, Max-Wien-  
Platz 1, 07743 Jena, Germany*

(5) *Leibniz Institute of Photonic Technology e.V., Albert-Einstein Strasse 9, 07745 Jena,  
Germany*

(6) *Electron Microscopy Center, Jena University Hospital, Ziegmühlenweg 1, 07743 Jena,  
Germany*

(7) *Institute of Biochemistry I, Jena University Hospital, Nonnenplan 2, 07743 Jena, Germany*

(8) *Institute of Optoelectronics, Military University of Technology, Kaliskiego 2, 00-908  
Warsaw, Poland*

(9) *Laserinstitut Hochschule Mittweida, University of Applied Science Mittweida,  
Technikumplatz 17, 09648 Mittweida, Germany*

*Helmholtz Institute Jena, Institute for Optics and Quantum Electronics, Friedrich  
Schiller University, Jena, Germany*

\*E-mail: sophia.kaleta@uni-jena.de

We present a correlative water window (WW) and visible light fluorescence microscope in an integrated lab-based setup [1]. The WW spectral range between the absorption edges of carbon and oxygen (280-530 eV) is particularly valuable for biological samples as it offers natural structural contrast due to the high absorption in carbon and high transmission in oxygen. Combining this with the functional contrast of fluorescence microscopy provides a holistic picture of the sample.

The wide-field zoneplate microscope is based on a laser plasma source, the gas puff target [2], while the fluorescence microscope operates in a wide-field epi configuration. By mounting the zoneplate and the fluorescence objective on a shared stage, it is possible to switch between the imaging modalities without alternation or moving of the sample.

With the WW microscope we achieve a resolution of 50nm half pitch, as demonstrated using a Siemens star test target. We present correlative imaging of different samples, ranging from simple test samples, such as fluorescent nanobeads, to biological specimens like cyanobacteria and critical-point dried NIH-3T3 and COS7 cells.

### References:

- [1] Reinhard, Julius, et al. "Laboratory-Based Correlative Soft X-ray and Fluorescence Microscopy in an Integrated Setup." *Microscopy and Microanalysis* 29.6: 2014-2025, 2023.
- [2] P. W. Wachulak, et al., "“water window” compact, table-top laser plasma soft x-ray sources based on a gas puff target," *Nucl. Instruments Methods Phys. Res. Sect. B: Beam Interactions with Mater. Atoms* 268, 1692–1700, 2010.



EXPLORING THE INFLUENCE OF VARIOUS NZFO CONTENT  
ON THE ELECTRONIC STRUCTURE IN NZFO/F-MWCNTS  
NANOCOMPOSITES FABRICATED VIA EX-SITU SYNTHESIS

A. Bajorek,<sup>1,\*</sup> J. Kubacki,<sup>1</sup> S. Lewińska,<sup>2</sup> B. Liszka,<sup>3</sup> M. Pawlyta,<sup>4</sup>  
A. Ślawska – Waniewska,<sup>2</sup> M. Szczepanik,<sup>5</sup> T. Sobol<sup>1,5</sup>

<sup>1</sup>*A. Chelkowski Institute of Physics, University of Silesia in Katowice, Chorzów, Poland,*

<sup>2</sup>*Institute of Physics, Polish Academy of Sciences, Warsaw, Poland*

<sup>3</sup>*Faculty of Natural Sciences, University of Silesia in Katowice, Sosnowiec, Poland*

<sup>3</sup>*Institute of Engineering Materials and Biomaterials, Silesian University of Technology, Gliwice, Poland* <sup>4</sup>*National Synchrotron Radiation Centre SOLARIS, Jagiellonian University, Kraków, Poland*

\*E-mail: anna.bajorek@us.edu.pl

In a couple of previous years, a new generation of advanced SF-NPs/CNTs hybrids with tailored magnetic properties and simultaneously retaining properties of individual components emphasizing the synergic effect began being investigated by our group [1-4]. Herein, the comparison between NZFO/f-MWCNTs composites based on Ni<sub>0.5</sub>Zn<sub>0.5</sub>Fe<sub>2</sub>O<sub>4</sub> (NFZO) nanoparticles with 2, 5 and 25 wt.% and functionalized multi-walled carbon nanotubes (fMWCNTs) synthesized via *ex-situ* method is shown. The structural and microstructural analysis confirms the efficiency of the synthesis process. The estimated crystallite size just slightly varies with the NZFO content. However, the presence of single particles, clusters and aggregates on the surface of the nanotubes is proven by Scanning-Transmission (S/TEM) electron microscopy in all analyzed composites. The dominant role of the f-MWCNTs building blocks was exposed by electronic structure analysis shown by XPS and XAS in all studied hybrids as designed. The slight redistribution of iron cations is noted in XPS, XAS, and ResPES studies. The redistribution of iron cations over tetrahedral and octahedral sites versus NZFO content is proved by studying Fe2p spectra. The magnetic properties analysis revealed the cluster-glass magnetic state of NZFO particles. The core-shell-like structure with a magnetic core and disordered layer is evidenced. The influence of Fe-based carbon matrix residues in all studied hybrids was detected.

References:

- [1] A. Bajorek, C. Berger, M. Dulski, et al., J. Phys. Chem. Solids **129** (2019) 1-21
- [2] A. Bajorek, B. Szostak, M. Dulski, J.M. Greneche, et al., Materials **15**(3) (2022) 977
- [3] A. Bajorek, B. Liszka, B. Szostak, M. Pawlyta, J. Magn. Magn. Mater. **503** (2020) 166634
- [4] A. Bajorek, B. Szostak, M. Dulski, J.M. Greneche, et al., J. Magn. Magn. Mater. **585** (2023) 171150

## MOLECULAR DYNAMICS SIMULATIONS OF THE STRUCTURE OF PROBUCOL PHARMACEUTICAL IN THE VITRIFIED AND PRESSURE-DENSIFIED PHASES

Anna Janowska,<sup>1,\*</sup> Joanna Grelska,<sup>1</sup> Taoufik Lamrani,<sup>1</sup> Ali Aminian,<sup>1</sup>  
and Karolina Jurkiewicz,<sup>1</sup>

<sup>1</sup>*Institute of Physics, University of Silesia in Katowice, 41-500 Chorzów, Poland*

\*E-mail: anjanowska@us.edu.pl

The research in amorphous pharmaceuticals is becoming more and more popular. Amorphous forms can exhibit better solubility and bioavailability in comparison to their crystalline counterparts. However, there are different methods of obtaining amorphous forms of pharmaceuticals, which leads to gaining structures with various properties. Even very subtle differences in the structure might be crucial in the context of applications and bioavailability. Therefore, understanding the connection between the preparation process and the final structure is essential for the development and commercialization of pharmaceuticals in an amorphous form.

A standard experimental method for the characterization of the atomic-scale structure, like laboratory X-ray diffraction, may provide insight into the organization of atoms and molecules, even in the case of amorphous-like phases. However, this method may not sufficiently identify subtle differences in various amorphous-like phases. In such cases, computer simulations of the structure are a highly desired tool enabling the interpretation of the experimental diffraction data. Moreover, high-resolution synchrotron diffraction combined with pair distribution function measurements is a game-changer for resolving the structure of amorphous pharmaceuticals.

Here, we examined the structure of probucol – a well-known active pharmaceutical ingredient applied in anti-hyperlipidemic formulations. Gromacs software was used to perform molecular dynamics simulations under various temperature and pressure conditions that mimic those applied during the preparation of ordinary probucol glass obtained by vitrification of melt and the so-called pressure-densified glass produced by compression of supercooled liquid. The obtained results indicate changes in the molecular conformations and hydrogen bonds under pressure-densification, which affects the local intermolecular structure and explains the variation in molecular relaxation processes observed under high pressure.

Authors acknowledge financial support from the National Science Centre (Poland), grant number: Opus 21 No. 2021/41/B/NZ7/01654.

### Achieving enhanced microwave shielding efficiency with absorption-dominant effect in electrospun carbon nanofibers by tailoring the addition of Co/Ni phase

Krystian Sokolowski<sup>1</sup>, Dorota Lachowicz<sup>1</sup>, Marcel Zambrzycki<sup>2</sup>, Anna Lapinska<sup>3</sup>,  
Ryszard Wielowski<sup>2</sup>, Marcin Sikora<sup>4</sup> and Andrzej Bernasik<sup>1</sup>

<sup>1</sup>*Academic Centre for Materials and Nanotechnology, AGH University of Krakow,  
Mickiewicza Av. 30, 30-059 Krakow, Poland*

<sup>2</sup>*Faculty of Materials Science and Ceramics, AGH University of Krakow, Mickiewicza  
Av. 30, 30-059 Krakow, Poland*

<sup>3</sup>*Faculty of Physics, Warsaw University of Technology, Koszykowa Av. 75, 00-662  
Warsaw, Poland*

<sup>4</sup>*National Synchrotron Radiation Centre Solaris, Jagiellonian University, Ul. Czerwone  
Maki 98, 30-392 Krakow, Poland*

Email: krysok@agh.edu.pl

Carbon nanofibers (CNF) obtained by electrospinning are reflected as promises filler candidate for designed high-performance polymer-based electromagnetic interference (EMI) shielding materials. However, although, CNF have high electrical conductivity, high modification possibilities, there are also have high reflection caused secondary EMI pollution. To the best of our knowledge, no research has explored the adjusted of CNF electromagnetic parameters by concentration tailoring the acetylacetonates-derived CoNi nanoparticles. For this reason, this work investigates the impact of CoNi concentration on shielding efficiency (SE) and shielding mechanism in the frequency range of 2-13.5 GHz. It was found that even a small content of CoNi improved EMI SE from 25.3 dB up to 56.7 dB at 5GHz and at 50  $\mu\text{m}$  thickness. The excellent EMI SE with absorption-dominant effect were achieved at 3%acac. With the greater concentration of acac, the EMI SE was inhibited due to the deterioration of individual CNF integrity greater susceptibility of CoNi to oxidation and loss of CoNi nanoparticles from the material.

[1] Bayat M, Yang H, Ko FK, Michelson D, Mei A. Electromagnetic interference shielding effectiveness of hybrid multifunctional Fe<sub>3</sub>O<sub>4</sub>/carbon nanofiber composite. *Polymer (Guildf)* 2014;55.

[2] Guan G, Yan L, Zhou Y, Xiang J, Gao G, Zhang H, et al. Composition design and performance regulation of three-dimensional interconnected FeNi@carbon nanofibers as ultralightweight and high efficiency electromagnetic wave absorbers. *Carbon N Y* 2022;197.

LINEARLY POLARIZED INFRARED MICROSPECTROSCOPY  
METHODS IN POLYMER SCIENCEKarolina Kosowska,<sup>1,\*</sup> Tomasz P. Wrobel<sup>1</sup><sup>1</sup>*Solaris National Synchrotron Radiation Centre, Jagiellonian University,  
Czerwone Maki 98, Krakow, Poland*

\*E-mail: karolina.kosowska@uj.edu.pl

So far, detailed studies of the structure and orientation of macromolecules in semicrystalline polymers have been fundamentally based on X-ray scattering and diffraction. High-energy sources are necessary for studies at the appropriate scale, but they are costly, as are other cost-related issues. The infrared microspectroscopy methods are less demanding, complementary techniques that shed new light on the organization of macromolecules. The spectra data relate to the vibrational motions of chemical bonds. In anisotropic materials, the orientation of specific bonds can be quantified by measuring absorbance dependent on linear polarization. Calculating the orientation of the molecular chain in three dimensions assumes that the first transition dipole moment is aligned along the geometric axis of the molecule and the second perpendicularly to it [1].

The visualization of macromolecular orientation in 3D allows the tracking and discussion of structural changes in a non-uniform sample. Local anisotropy in polymers with partial crystallization is associated with the arrangement of molecules into superstructures like spherulites, shish-kebabs, and transcrystalline formations. Studying nanostructures requires super-resolution below the diffraction limit of infrared light. One such method is O-PTIR microscopy, which utilizes the effect of photothermal expansion in the infrared. The end station on the CIRI beamline has been specially equipped with an automated linear polarizer for rapid imaging of materials exhibiting local anisotropy.

**Acknowledgment:**

This research was funded in whole by the National Science Centre, Poland (SONATINA, Grant No. 2023/48/C/ST4/00176). FT-IR and O-PTIR measurements were performed at the CIRI beamline under the provision of the Polish Ministry and Higher Education project “Support for research and development with the use of research infrastructure of the National Synchrotron Radiation Centre SOLARIS” under contract nr 1/SOL/2021/2.

**Reference:**

1. K. Kosowska, *et al.* *Macromolecules* 2024, 57, 9, 335-43, doi.org/10.1021/acs.macromol.3c01593.

## A Multitechnique Integrated Approach for Unveiling the Monoatomic Nature and Properties of Active Centers in Single-Atom Catalysts

Nicolò Allasia<sup>1</sup>, Lulu Alluhaibi<sup>2</sup>, Alexey Maximenko<sup>2</sup>, Sean M. Collins<sup>3</sup>,  
Quantin M. Ramasse<sup>3</sup>, and Gianvito Vilé<sup>1\*</sup>

<sup>1</sup>*Department of Chemistry, Materials and Chemical Engineering “Giulio Natta”,  
Politecnico di Milano, Piazza Leonardo 32, 20133 Milano, Italy*

<sup>2</sup>*Solaris National Synchrotron Radiation Centre, Jagiellonian University,  
Czerwone Maki 98, 30-392 Kraków, Poland*

<sup>3</sup>*SuperSTEM Laboratory, SciTech Daresbury Campus, Keckwick Lane, WA4 4AD  
Daresbury, United Kingdom*

\*e-mail: nicolo.allasia@polimi.it

Single-atom catalysts (SACs) on carbon nitride have attracted significant attention due to their unique properties, such as enhanced reactivity, selectivity, and stability compared to nanoparticle counterparts [1]. These catalysts feature isolated active metal atoms on a nitrogen-rich carbon-based matrix, offering maximized atomic efficiency and superior catalytic performance [2]. Evaluating the monoatomic nature of active sites in SACs is essential for confirming successful synthesis, characterized by homogeneously and singly dispersed metal centers. High-angle annular dark-field scanning transmission electron microscopy (HAADF-STEM) is commonly used for this purpose. Additionally, novel single-atom level spectroscopic methods, though often time-consuming and costly, have been developed [3]. X-ray absorption spectroscopy (XAS), particularly the extended X-ray absorption fine structure (EXAFS) region, is the preferred method to confirm the absence of metal-metal interactions in SACs, ensuring monoatomic active metal centers. This study explores the structural and electronic properties of nickel SACs through HAADF-imaging, Fourier-transform infrared (FT-IR) spectroscopy, XAS, and advanced STEM imaging. Nickel catalysts were synthesized through a wet impregnation method, with each synthesis step optimized *via* a one-variable-at-a-time approach. The catalytic activity was validated by performing amination reactions on various aryl halides, achieving up to 80% yields of anilines, essential intermediates for pharmaceuticals.

[1] M. A. Bajada, et al, *Chemical Society Reviews*, **51**, 3898-3925 (2022).

[2] M. B. Gawande, et al, *ACS Catalysis*, **10**, 2231-2259 (2020).

[3] N. Allasia, et al, *Angewandte Chemie International Edition*, e202404883 (2024).

## Examining the electronic structure of zinc selenide quantum dots for the development of novel hybrid plasmonic materials

Rafał Fanselow<sup>1</sup>, Gabriela Imbir<sup>1</sup>, Joanna Czapla-Masztafiak<sup>1</sup>, Jakub Szlachetko<sup>2</sup>

<sup>1</sup>*Institute of Nuclear Physics Polish Academy of Sciences, Radzikowskiego 152,  
31-342 Kraków, Poland*

<sup>2</sup>*SOLARIS National Synchrotron Radiation Centre, Jagiellonian University,  
Czerwone Maki 98, 30-392 Kraków, Poland*

Email: rafal.fanselow@ifj.edu.pl

Semiconductor quantum dots (QDs) constitute a unique group of nanostructures, exhibiting size-dependent optical and electronic properties that could be potentially exploited in high-performance hybrid optoelectronic devices for energy conversion applications. Among various explored QD compounds, zinc selenide (ZnSe) emerged as one of the top candidates for the development of next-generation QDs-based technologies. However, QD electronic properties are highly influenced by the surface and defect effects, which are inadequately understood in the case of ZnSe.

In the presented work, we show the application of combined UV-Vis and X-ray spectroscopy approaches to investigate defect states in ZnSe QDs. A series of synthesized ZnSe QDs suspensions with varying particle mean sizes were examined with a laboratory-based X-ray spectrometer [1, 2] equipped with a dedicated sample liquid cell [2], allowing simultaneous acquisition of Zn K-edge absorption and Zn K $\alpha$  emission spectra. Additionally, the Zn K-edge XAS measurements were conducted using a much more intense X-ray source at the ASTRA beamline of the SOLARIS National Synchrotron Radiation Centre. The obtained data was supported with theoretical calculations and complementary femtosecond optical transient absorption spectroscopy experiments.

The acquired results revealed the presence of zinc vacancies and their role in the electronic structure of the investigated materials, contributing to the current attempts directed toward ZnSe QDs' real-life applications. Such a goal could be achieved by integrating the QDs materials into more advanced structures. Future work will focus on the preparation of a QD-plasmonic nanoparticle hybrid system to take advantage of the localized surface plasmon resonance phenomenon, boosting the performance of optoelectronic devices.

**Acknowledgment:** This project was financed by the National Science Centre (Poland) under grant number 2020/37/B/ST3/00555

[1] R. Fanselow et al., *X-ray Spectrometry* 52 (5), 2022, 247-253

[2] R. Fanselow et al., *Spectrochimica Acta Part B: Atomic Spectroscopy* 189, 2022, 106367

## X-ray absorption spectroscopy of advanced aerogel/liquid metal composites

Klaudia Trembecka-Wojciga<sup>1,2</sup>, Dorota Lachowicz<sup>3</sup>, Sylwia Terlicka<sup>1</sup>, Anna Korniewa<sup>1</sup>,  
Marcin Sikora<sup>3,4</sup>, Angelika Kmita<sup>3\*</sup>, Natalia Sobczak<sup>1\*</sup>

<sup>1</sup>Polish Academy of Sciences, Reymonta 25 St., 30-059 Krakow, Poland

<sup>2</sup>Cracow University of Technology, Warszawska 24 St., 30-155 Cracow, Poland

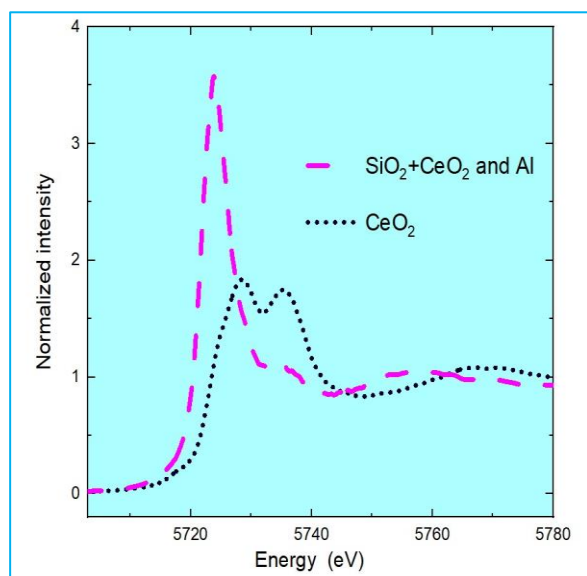
<sup>3</sup>AGH University of Krakow, al. Mickiewicza 30 St., 30-059 Krakow, Poland

<sup>4</sup>National Synchrotron Radiation Centre SOLARIS, Jagiellonian University, Czerwone Maki  
98 St., 30-392, Krakow, Poland

\*E-mail: akmita@agh.edu.pl

\*E-mail:n.sobczak@imim.pl

X-ray absorption spectroscopy provides element selective information on the electronic structure of unoccupied states. It can be considered as a fingerprint of local atomic environment and charge state of the absorbing element. The former is represented in the shape of the spectra, while the latter is in the energy position of the absorption edge. XAS probed in transmission



may be considered as volume averaging probe, which results from atomic concentration weighted contribution of the characteristic spectral shapes of crystal sites and atomic species of the probed element, which are present in the system studied. A comparison of XAS collected at the CeL<sub>3</sub> edge from SiO<sub>2</sub>/CeO<sub>2</sub> aerogel and CeO<sub>2</sub> reference powder is shown in Figure 1. It reveals striking differences, which indicate that local symmetry and charge of the dominant fraction of Ce atoms are significantly dissimilar in both systems.

Figure 1. Ce L<sub>3</sub>-edge XAS for SiO<sub>2</sub>/CeO<sub>2</sub> aerogel/Al and reference powder of CeO<sub>2</sub>.

### Acknowledgements

This publication was partially developed under the provision of the Polish Ministry and Higher Education project "Support for research and development with the use of research infrastructure of the National Synchrotron Radiation Centre SOLARIS" under contract nr 1/SOL/2021/2. We acknowledge SOLARIS Centre for the access to the Beamline ASTRA, where the measurements were performed. We would like to thank Dr. A. Maximenko for his kind assistance. Authors acknowledge stimulating discussion and exchanges in the frame of COST Action "CA 18125 AERoGELS: Advanced Engineering and Research of aeroGels for Environment and Life Sciences".

## MORPHOLOGICAL ANALYSIS OF 3D PRINTED CARBON DOT-BASED HYDROGELS USING SEM/AFM/NANO-FTIR/s-SNOM

Agnieszka Sysło,<sup>1</sup> Dominika Krok-Janiszewska,<sup>1</sup> Wiktor Kasprzyk,<sup>1</sup> and Joanna Ortyl<sup>1,2,3</sup>

<sup>1</sup>*Cracow University of Technology, Warszawska 24, 31-155 Cracow, Poland*

<sup>2</sup>*Photo HiTech Ltd., Bobrzyńskiego 14, 30-348 Cracow, Poland*

<sup>3</sup>*Photo4Chem, Warszawska 24, 31-155 Cracow, Poland*

\*E-mail: agnieszka.syslo1@gmail.com

A promising technique for creating highly individualized and detailed objects is additive manufacturing, commonly referred to as 3D printing. This approach offers significant advantages, including the capacity to create complex and customized designs, rapid prototyping, and reduced waste production. 3D printing is widely used across various sectors, such as electronics, robotics, and the military, as well as in numerous fields of tissue engineering and medicine. A one-pot, solvent-free synthesis is one of the most common and straightforward forms of obtaining carbon dots from citric acid. To acquire a greater understanding of the photoluminescence phenomenon of carbon dots and the materials produced using them, extensive spectroscopic and kinetic research are required. Investigating their surface and particle distribution within samples is crucial for understanding their impact on the adjacent environment. Surface characterization may be obtained with high precision by using s-SNOM technique. s-SNOM measurements, which are sensitive to optical properties like refractive index and absorption, have the ability to confirm the location of the nanoparticles present in the tested sample. This work demonstrates citric acid-based carbon dots and carbon dot materials spectroscopic and kinetic characterization, which provides a complex profile with potential applications in biomedicine. The performed studies indicate intriguing characteristics of the synthesized carbon dot materials and imply their potential application in photopolymerization processes for 3D printing and they might significantly improve the understanding of using carbon sources in photoinitiating systems.

This research was funded by the NCN project OPUS (“Emerging strategy approaches for the design and functionalization of carbon dots as multifunctional, dynamic, green systems photoinitiators and photocatalysts involved in photopolymerisation processes”),

Grant No. UMO-2021/41/B/ST5/04533



## NANOCOMPOSITE FILTERS BASED ON CARBON NANOFIBERS AND TiO<sub>2</sub> NANOPARTICLES FOR WATER PURIFICATION USING PHOTOCATALYTIC PROCESS AND SOLAR ENERGY

Elżbieta Tądel<sup>1,2\*</sup>, Paweł Winiarski<sup>2</sup>, Krystian Sokołowski<sup>2</sup>, Marcin Sikora<sup>3</sup>, Katarzyna Berent<sup>2</sup>, Piotr Jabłoński<sup>2</sup>, Szczepan Zapotoczny<sup>2,4</sup>, Dorota Lachowicz<sup>2</sup>

<sup>1</sup>*AGH University of Krakow, Faculty of Metals Engineering and Industrial Computer Science, al.A.Mickiewicza 30, 30-059 Krakow, Poland*

<sup>2</sup>*AGH University of Krakow, Academic Centre for Materials and Nanotechnology, al.A.Mickiewicza 30, 30-059 Kraków, Poland*

<sup>3</sup>*Solaris National Synchrotron Radiation Centre, Jagiellonian University, Czerwone Maki 98, 30-392 Kraków, Poland*

<sup>4</sup>*Faculty of Chemistry, Jagiellonian University, Gronostajowa 2, 30-387 Kraków, Poland*

\*Email: tadel@student.agh.edu.pl

The problem of water pollution caused by, among other things, poor waste management is a major challenge, especially in regions of the world with limited access to clean and safe drinking water[1]. In recent years, intensive research has been underway on photocatalytic water purification using nano- and micro-particles of titanium dioxide (TiO<sub>2</sub>)[2]. TiO<sub>2</sub> is one of the most promising materials used for photocatalysis due to its high oxidation capacity, chemical stability and large specific surface area. Although titanium dioxide (TiO<sub>2</sub>) is generally considered safe, many works are reporting the toxic effects of TiO<sub>2</sub>, especially in nanoparticle form[3]. The increase in TiO<sub>2</sub> toxicity is known to be influenced by the nanoparticle size and its form. Therefore, in this work, we propose to create composite systems with TiO<sub>2</sub> nanoparticles that retain their photocatalytic properties while limiting the release of nanoparticles into the environment. In this paper, we present two methods for obtaining composites based on carbon nanofibers and titanium dioxide nanoparticles (TiO<sub>2</sub>/CNF): 1) TiO<sub>2</sub> nanoparticles were prepared by physical vapor deposition(PVD) technique on CNFmats 2) nanocomposite was formed by electrospinning and heat treatment of polyacrylonitrile fibers containing a precursor TiO(acac)<sub>2</sub>

Titanium dioxides are polymorphic materials with rutile, anatase and brookite structure. The method of obtaining nanocomposite can influence the structure of produced TiO<sub>2</sub> nanoparticles. In this project, the influence of the composite production technique and annealing process on TiO<sub>2</sub> nanoparticles was assessed. For this purpose, X-ray absorption spectroscopy (XAS) measurements were used. The local structures around the Ti and O sites were investigated as reflected by K-edge X-ray Absorption Spectra.

[1] <https://www.unicef.org/reports/progress-drinking-water-sanitation-and-hygiene> (2017)

[2] E. Horváth, et al, Clean Water, 5, 10 (2022).

[3] S. Shabbir, et al, BioNanoSci. 11, 621–632 (2021). [4] O.Kose, Chem. Res. Toxicol. 33, 9, 2324–2337(2020)

## EVALUATION OF THE EFFECT OF POLYMER ON THE STRUCTURE AND STABILITY OF COPPER-ZINC FERRITE NANOPARTICLES

Polymer Layer.

Dorota Lachowicz<sup>1\*</sup>, Angelika Kmita<sup>1</sup>, Marta Gajewska<sup>1</sup>, Marcin Sikora<sup>2</sup>,  
Jan Żukrowski<sup>1</sup>, Joanna Stępień<sup>1</sup>, Andrzej Bernasik<sup>1,3</sup>, Szczepan Zapotoczny<sup>1,4</sup>

<sup>1</sup>*AGH University of Krakow, Academic Centre for Materials and Nanotechnology, al.A.Mickiewicza 30, 30-059 Kraków, Poland*

<sup>2</sup>*Solaris National Synchrotron Radiation Centre, Jagiellonian University, Czerwone Maki 98, 30-392 Kraków, Poland*

<sup>3</sup>*Solaris 2AGH University of Science and Technology, Faculty of Physics and Applied Computer Science, al. A. Mickiewicza 30, 30-059 Krakow, Poland*

<sup>4</sup>*Faculty of Chemistry, Jagiellonian University, Gronostajowa 2, 30-387 Kraków, Poland*

\*E-mail: dorota.bielska@agh.edu.pl

Iron oxides and ferrite nanoparticles have been intensively researched as alternative MRI contrast agents[1]. However, the biomedical application of magnetic nanoparticles is limited by aggregation [2]. The use of polymer coatings can prevent this negative phenomenon[3,4]. We showed that the coatings based on ionic derivatives of chitosan [5,6] ensured the stability and biocompatibility of the SPIONs aqueous suspension. Furthermore, the applied derivatives can form durable metal-polymer connections by chelating relevant metal ions. However, there are reports that the attachment of ligands via anchor groups to nanoparticles may cause changes on the particle surface, such as oxidation or surface degradation [7]. Oxidation processes reduce the saturation magnetization of iron nanoparticles[8], but the appropriate ligands can reduce spin slanting in the surface region.

The project's main goal was to investigate the influence of the polymer layer (a cationic derivative of chitosan and dextran, PEG) on the magnetic structure of copper-zinc ferrite nanoparticles. For the application of copper-zinc ferrite nanoparticles as contrast agents in magnetic resonance imaging (MRI) or in magnetic hyperthermia, their surface has to be coated by a polymer or surfactant layer. This modification can influence the surface oxidation state and the magnetic properties of the particles. In this work, we evaluated the effect presence of the layer of three polymers, cationic chitosan, cationic dextran, and polyethene glycol on copperzinc ferrite nanoparticles. For this purpose, X-ray absorption spectroscopy (XAS) and X-ray magnetic circular dichroism (XMCD) measurements were used, thanks to which the local magnetic and electronic properties of the particles' surface area were examined with and without surface modification.

- [1] Monitor. Sci. Rep.. 2019 (9),
- [2] Adv Coll. Interface Sci. 2019 (265), 29-44.
- [3] J. Nanoparticle Res.2014(16), 1–11.
- [4] Coll. Surf. B, 2017 (150), 402–407 .

- [5] J. Mater. Chem. B, 2019 (7), 2962–2973
- [6] Soft Matter 2009(5), 4726–4732.
- [7] Zeitschrift fur Phys.Chemie,2018(232), 819–844.
- [8] J.Phys.Chem.C,2015(119),19404-19414.

Enhanced electrochemical performance of partially amorphous  
 $\text{La}_{0.6}\text{Sr}_{0.4}\text{CoO}_{3-\delta}$  oxygen electrode materials for low-temperature solid oxide cells  
operating at 400 °C

Bartłomiej Lemieszek<sup>a</sup>, Mindaugas Ilickas<sup>b</sup>, Jan Jamroz<sup>c</sup>, Asta Tamulevičienė<sup>b</sup>,  
Jakub Karczewski<sup>d</sup>, Patryk Błaszczak<sup>d</sup>, Alexey Maximenko<sup>e</sup>, Brigita Abakevičienė<sup>b</sup>,  
Marcin Małys<sup>c</sup>, Sigita Tamulevičiūtė<sup>b</sup>, Piotr Jasiński<sup>a</sup>, Sebastian Molin<sup>a</sup>

<sup>a</sup>Advanced Materials Centre, Faculty of Electronics, Telecommunications and Informatics,  
Gdańsk University of Technology, ul. G. Narutowicza 11/12, 80-233 Gdańsk, Poland

<sup>b</sup>Institute of Materials Science of Kaunas University of Technology,  
K. Baršausko str. 59, Kaunas LT-51423, Lithuania

<sup>c</sup>Warsaw University of Technology, Faculty of Physics, Koszykowa 75,  
00-662 Warsaw, Poland

<sup>d</sup>Advanced Materials Centre, Faculty of Applied Physics and Mathematics, Gdańsk  
University of Technology, ul. G. Narutowicza 11/12, 80-233 Gdańsk, Poland

<sup>e</sup>National Synchrotron Radiation Centre SOLARIS, Jagiellonian University,  
Czerwone Maki 98, 30-392, Kraków, Poland

Corresponding Author: bartlomiej.lemieszek@pg.edu.pl

Solid oxide cells (SOCs) represent a promising prospective source of energy. This potentially zeroemission solution has the potential to contribute to an efficient transformation of energy. Nevertheless, one of the most significant obstacles to be surmounted is the considerable polarization resistance exhibited by the oxygen electrode. This has created a need for innovative oxygen electrode materials to meet the demand for high-performance solid oxide cells (SOCs) operating at lower temperatures.

Electrochemical impedance measurements indicated an enhanced electrochemical efficiency of the partially amorphous material compared to that of the crystalline form. A comprehensive examination of the impedance spectra enabled the identification of the underlying mechanisms impeding the effective electrochemical reaction. Analysis of partially amorphous materials presents a significant challenge due to the structural complexity of such materials. The application of XAS (X-ray Absorption Spectroscopy) enabled the establishment of a correlation between the enhanced electrochemical efficiency of the LSC material ( $\text{La}_{0.6}\text{Sr}_{0.4}\text{CoO}_{3-\delta}$ ) and its partially amorphous form. The average oxidation state of cobalt within the material was shown to be diminished from  $3.4^+$  to  $2.9^+$ . The use of EXAFS (Extended X-Ray Absorption Fine Structure) analysis and Wavelet Transform allowed for a comprehensive characterization of the material properties. In addition, EXAFS analysis revealed a noticeable decrease in the coordination number for oxygen in the Co-O shell of the partially amorphous material in comparison to the crystalline form. In addition, changes in the position of the oxygen atom near the central cobalt atom were observed.

#### Acknowledgements

This research has been supported by National Science Centre (NCN) DAINA 2 project number UMO-2020/38/L/ST8/00513; “Porous metal supported micro-scale solid oxide fuel cells: fundamentals, fabrication and testing”.

## OPERANDO OBSERVATION OF ELECTROCATALYST ACTIVE SPECIES DURING THE GLUCOSE ELECTROOXIDATION REACTION

K. Ostrowska<sup>1\*</sup>, K. Lankauf<sup>1</sup>, A. Maximenko<sup>2</sup>, B. Lemieszek<sup>1</sup>, P. Jasiński<sup>1</sup>, S. Molin<sup>1</sup>

<sup>1</sup> *Gdansk University of Technology, Faculty of Electronics, Telecommunications and Informatics, Narutowicza 11/12, 80-233, Gdańsk, Poland*

<sup>2</sup> *National Synchrotron Radiation Center SOLARIS, Czerwone Maki 98, 30-392 Kraków, Poland*

\*E-mail: katarzyna.ostrowska@pg.edu.pl

Diabetes is one of the civilization diseases of the 21st century. Effective glucose monitoring is an important diagnostic test for active prevention and treatment of diabetes. In addition to widely used enzyme-based sensors, solutions based on non-enzymatic sensors are actively developed. The highest sensing performance has been reported for cobalt-containing compounds (i.e.  $\text{Co}_3\text{O}_4$ ), but certain challenges related to carcinogenicity, high cost and toxicity necessities the search for new materials. Our study develops novel materials based on abundant element  $(\text{Cu},\text{Mn})_3\text{O}_4$  oxide spinels.

The research presents the electrocatalytic capabilities of modified manganese-copper spinel oxides in relation to the detection of glucose in solutions. The spinel oxides were doped with nickel in various mass ratios. For the purposes of this work, 4 powders were prepared:  $\text{CuMn}_2\text{O}_4$ ,  $\text{CuMn}_{2-x}\text{Ni}_{(x=0,0.3,0.6,0.9)}\text{O}_4$ . Structural analysis was performed to determine the crystalline properties. The influence of nickel content on the electrocatalytic activity was investigated. It was found that the amount of nickel had a significant impact on the sensing properties of the prepared sensors. The sensitivity of the most active samples was determined to be  $\sim 470 \mu\text{AmM}^{-1}\text{cm}^{-2}$ . Electrochemical studies have also been extended to determine selectivity for selected compounds.

To further investigate the effect of nickel doping on catalytic properties toward glucose oxidation, electrochemical results were compared with XAS analysis. An operando study was conducted to determine changes at operating conditions. A special measuring cell was also designed for this purpose. As a result, it was possible to determine the active sites of the tested compounds.

## POLYX@SOLARIS: LAYOUT, SPECIFICATION &amp; FIRST RESULTS

Tomasz S. Kołodziej,<sup>1,\*</sup> Katarzyna Sowa,<sup>1</sup> Paweł Wróbel,<sup>1,2</sup> and Paweł Korecki<sup>1,3</sup><sup>1</sup>SOLARIS National Synchrotron Radiation Centre, Czerwone Maki 98, 30-392 Kraków, Poland<sup>2</sup>Faculty of Physics and Applied Computer Science, AGH University of Science and Technology, al. Mickiewicza 30, 30-059 Kraków, Poland<sup>3</sup>Institute of Physics, Jagiellonian University, ul. Łojasiewicza 11, 30-348 Kraków, Poland

\*E-mail: t.kolodziej@uj.edu.pl

**PolyX** (polychromatic X-rays and polycapillary X-ray optics) is a newly developed bending magnet beamline at SOLARIS National Synchrotron Radiation Centre in Kraków, Poland. SOLARIS is a 1.5 GeV synchrotron build with unique collaboration between MAX IV Laboratory and Jagiellonian University [1]. The beamline is dedicated to X-ray microimaging and X-ray spectromicroscopy [2] and is open for user access since **1<sup>st</sup> March 2024**.

PolyX offers several techniques:  $\mu$ CT ( $\sim 0.7\mu\text{m}$  resolution),  $\mu$ XRF,  $\mu$ XAS and  $\mu$ XES [3]. Imaging resolution  $\sim 200$  nm will be possible via recently developed X-ray tomography with multiple ultranarrow cone beams [4]. The end station can be easily reconfigured; therefore, in addition to implementing other experimental methods at short notice, PolyX will also work as a test station for innovative hard X-ray methods as well as new solutions of X-ray optics, new imaging geometries or detection systems. PolyX can also provide a dedicated area for user experiments and/or user end-stations. The scheme of PolyX optics layout and a photo of the experimental setup are presented in Fig. 1. The beamline operates in three modes: high flux (DMM, bandwidth 2%), high resolution (DCM, Si(111), bandwidth 0.02%) and a white beam mode. Polycapillary and monocrapillary optics are used to generate hard X-ray beam in the energy range of 5-15keV with spot sizes in range  $\sim 5\mu\text{m}$ -100 $\mu\text{m}$ .

In this contribution the current status of the beamline will be presented as well as the beamline layout (optical, acquisition and detection systems). Additionally, first, commissioning results will be presented, to give an overall view on the beamline capability.

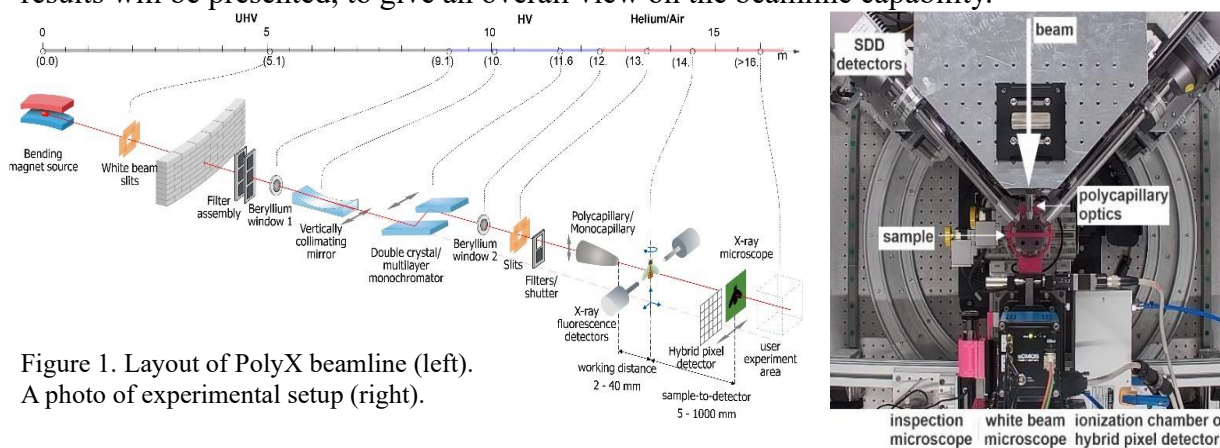


Figure 1. Layout of PolyX beamline (left).  
A photo of experimental setup (right).

**Acknowledgements:** The construction of PolyX was financed by Ministry of Polish Ministry of Science and Higher Education (6991/IA/SP/0010/2019). The work is supported under the Polish Ministry and Higher Education project: “Support for research and development with the use of research infrastructure of the National Synchrotron Radiation Centre SOLARIS” under contract nr 1/SOL/2021/2.

#### References:

- [1] J. Szlachetko et al., (2023). SOLARIS national synchrotron radiation centre in Krakow, Poland. *The European Physical Journal Plus*. 138. 10.
- [2] K.M. Sowa, P. Wróbel, T. Kołodziej, W. Błachucki, F. Kosiorowski, M. Zajac, P. Korecki (2023). *PolyX beamline at SOLARIS—Concept and first white beam commissioning results*. *NIMB*, **538** (131–137).
- [3] [https://synchrotron.uj.edu.pl/en\\_GB/linie-badawcze/polyx](https://synchrotron.uj.edu.pl/en_GB/linie-badawcze/polyx)
- [4] K.M. Sowa, P. Korecki (2020). *X-ray tomography with multiple ultra narrow cone beams*. *Optics Express* **28**, 23223.

## DEVELOPMENT OF URANOS BEAMLIN INFRASTRUCTURE

N. Olszowska<sup>1,\*</sup>, M. Rosmus<sup>1,2</sup>, D. Wutke<sup>1,2</sup>, P. Nowak<sup>1</sup>, J. J. Kołodziej<sup>2</sup>

<sup>1</sup>*Solaris National Synchrotron Radiation Centre, Jagiellonian University, Czerwone Maki 98,  
30-392 Kraków, Poland*

<sup>2</sup>*Marian Smoluchowski Institute of Physics, Jagiellonian University, Prof. S. Łojasiewicza 11,  
30-348 Kraków, Poland*

\*E-mail: Natalia.olszowska@uj.edu.pl

The URANOS (Ultra Resolved ANgular phOtoelectron Spectroscopy) beamline is designed for studying the band structure of solids, primarily utilizing the angle-resolved photoelectron spectroscopy (ARPES) technique, which has been available to users for six years at the SOLARIS National Synchrotron Radiation Center [1]. The beamline brings together a group of users who use the highly monochromatic and spectrally pure photon beams in the range of 8 - 160 eV with fully controlled polarization throughout the available energy range.

The end station is equipped with a DA30L (SCIENITA) electron spectrometer with deflection mode and offers low temperatures (6-500K) of samples during measurements. In response to user demand and following trends in solid state physics research, work has begun on the installation of 3D VLEED spin detectors, i.e. two spin filters in orthogonal geometry. This enables the measurement of the complete dispersion relation  $E(k_x, k_y, k_z)$  along with information on all spin components ( $S_x, S_y, S_z$ ). Additionally, by using variable light polarization, it is possible to gather information about the orbital geometry. The spin detectors are now installed, and the initial system tests are currently underway.

Concurrently, in collaboration with PREVAC, a new 6-axis cryogenic manipulator is under construction for work at low temperatures (2.5-500K), and it will soon undergo preliminary cryogenic tests.

In addition to the extension of the end station, a mirror guiding low-energy radiation perpendicular to the beam axis has recently been installed, which can be used for other studies than standard measurements at the end station. The mirror chamber is equipped with a MgF2 viewport transmitting VUV radiation in the produced range. Both low- and high-pressure chambers can be connected to the mirror chamber, depending on the needs of the users.

More information about URANOS beamline you can find her:  
[https://synchrotron.uj.edu.pl/en\\_GB/linie-badawcze/uranos](https://synchrotron.uj.edu.pl/en_GB/linie-badawcze/uranos).

## OPTICAL DESIGN AND NUMERICAL SIMULATION OF THE UPCOMING BEAMLINES AT SOLARIS CENTRE

Tomasz S. Kołodziej<sup>1</sup>

<sup>1</sup>SOLARIS National Synchrotron Radiation Centre, Jagiellonian University, 30-007 Kraków

\*E-mail: t.kolodziej@uj.edu.pl

The initial project of the new beamline to be built at any synchrotron radiation source requires certain considerations to be taken. Optical setup of the synchrotron beamline has to be matched to: given synchrotron radiation source, required photon energy range, end-user requirements (focusing, flux, resolution etc.), and, last but not least, geometrical constrains of the beamline development area. In vast majority of the cases the distances, dimensions, shapes and angles of the optical elements can be calculated analytically, together even with expected shape errors. However, precise determination of the performance efficiency requires numerical analysis of the whole setup with the ray-tracing procedure made with certain code of choice. In this presentation the results are obtained with ShadowVUI within XOP package [1] and ShadowOUI within the OASYS environment [2].

The projects and results for few upcoming beamlines at NSRC SOLARIS will be presented: SMAUG (bending magnet, small angle x-ray scattering beamline), SOLCRYSS (3-pole wiggler, macromolecular crystallography), BM-03 beamline (bending magnet, microdiffraction and x-ray absorption spectroscopy), NAP-XPS (elliptically polarizing undulator, side branch for the PHELIX beamline for near ambient pressure x-ray photoemission spectroscopy).

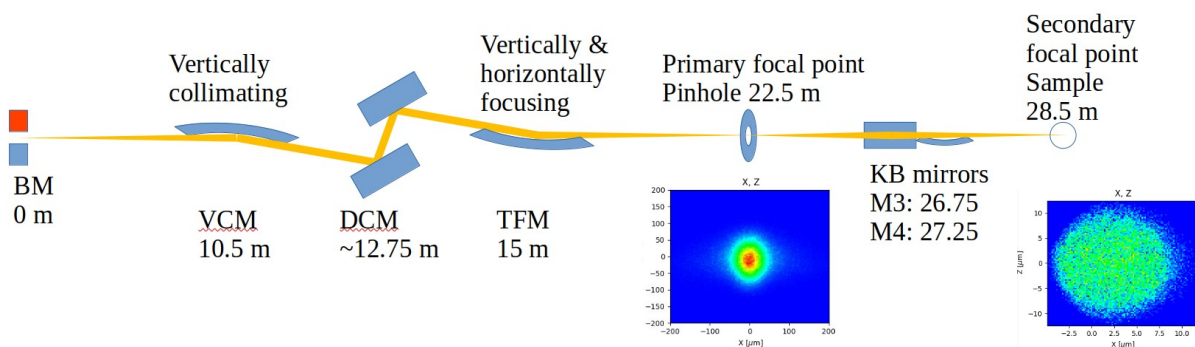


Fig. 1. Initial optical design of the future BM-03 beamline with example of beam spot results in primary and secondary focal points.

### References:

- [1] Manuel Sanchez del Rio, Niccolo Canestrari, Fan Jiang, and Franco Cerrina, "SHADOW3: a new version of the synchrotron X-ray optics modelling package," *Journal of Synchrotron Radiation* **18**, 708–716 (2011)
- [2] Luca Rebuffi and Manuel Sánchez del Río, "ShadowOui: a new visual environment for X-ray optics and synchrotron beamline simulations," *Journal of Synchrotron Radiation* **23**, 1357–1367 (2016)

HIGH RESOLUTION X-RAY EMISSION SPECTROSCOPY  
AT THE POLYX BEAMLINE OF SOLARIS

W. Błachucki<sup>1,\*</sup>, K. M. Sowa<sup>2</sup>, T. Kołodziej<sup>2</sup>, P. Wróbel<sup>3</sup>, J. Czapla-Masztafiak<sup>1</sup>,  
P. Korecki<sup>2,4</sup>, J. Szlachetko<sup>2</sup>

<sup>1</sup>*Institute of Nuclear Physics, Polish Academy of Sciences, Kraków, Poland*

<sup>2</sup>*National Synchrotron Radiation Centre SOLARIS, Jagiellonian University, Kraków,  
Poland*

<sup>3</sup>*AGH University of Science and Technology, Kraków, Poland*

<sup>4</sup>*Marian Smoluchowski Institute of Physics, Jagiellonian University, Kraków, Poland*

\*E-mail: wojciech.blachucki@ifj.edu.pl

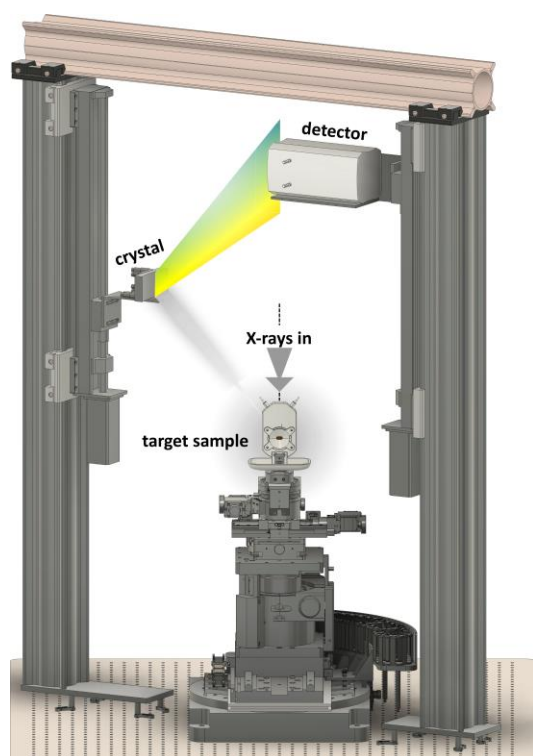


Figure 1. Design of the X-ray emission spectrometer at the PolyX beamline.

Following the development of a high resolution spectrometer for X-ray absorption spectroscopy (XAS) at the PolyX beamline of SOLARIS [1,2], the beamline is currently being equipped with another spectrometer for X-ray emission spectroscopy (XES) studies. Similar to the XAS spectrometer, the XES spectrometer will be based on the von Hámos geometry, providing high energy resolution ( $\Delta E/E \approx 2 \times 10^{-4}$ ) without moving the spectrometer components and maintaining high multimodality of the beamline. The X-ray fluorescence radiation induced in the target sample with the synchrotron beam will be Bragg-diffracted on a cylindrically bent crystal which will lead to spatial sorting of photons of different energies. The sorting will allow spectral analysis of the diffracted radiation using a position-sensitive detector, such as a charge-coupled device (CCD) camera. The spectrometer will be oriented in the vertical direction (see Fig. 1) to mitigate the

influence of sample mispositioning and sample instability (e.g. liquid jets) on the detected X-ray lines energies. The spectrometer will allow detection of the X-ray lines in the energy range 4 – 11 keV and above. The commissioning is scheduled for February 2025.

[1] W. Błachucki, K. M. Sowa, T. Kołodziej, P. Wróbel, P. Korecki, J. Szlachetko, *Nucl. Instrum. Methods Phys. Res., B.* **542**, 133 (2023).

[2] K. M. Sowa, P. Wróbel, T. Kołodziej, W. Błachucki, F. Kosiorowski, M. Zając, P. Korecki, *Nucl. Instrum. Methods Phys. Res., B.* **538**, 131 (2023).



### Development of in situ/operando spectroscopy at SOLARIS synchrotron: a powerful approach towards understanding catalysts and electrocatalysts

A. Wach,<sup>1,\*</sup> M. Śliwa,<sup>1,2</sup> M. Brzyski,<sup>1</sup> M. Zając,<sup>1</sup> J. Szlachetko,<sup>1</sup> and Z. Sojka<sup>2</sup>

<sup>1</sup> *SOLARIS National Synchrotron Radiation Centre, Jagiellonian University, Poland*

<sup>2</sup> *Faculty of Chemistry, Jagiellonian University, Poland*

Email: anna.wach@uj.edu.pl

With increasing consumption of fossil fuels and growing concern over global environmental issues, the pursuit of new materials and catalytic/electrocatalytic processes has become a key goal in sustainable development. Over the last two decades, researchers have increasingly focused on using the operando approach, which involves studying materials directly under working conditions and allows for the direct correlation of their physicochemical properties with electronic and structural changes [1].

In the present work, the future perspectives of the in situ/operando project at SOLARIS synchrotron will be discussed. Specifically, the development of an in situ/operando end-station that enables synchrotron-based multitechnique studies at hard X-ray energies will be presented. In a single experiment, penetrating properties and site-selectivity of X-ray absorption spectroscopy (XAS) will be combined with diffuse reflectance infrared Fourier transform spectroscopy (DRIFT) and mass spectrometry (MS), all conducted under material's working conditions (temperature, gas flow, etc.). The operando end station will provide significant experimental evidence to address the most important key issues in the field of catalysis/electrocatalysis: (1) stability of material's electronic and structural configuration under working conditions; (2) identity and changes of electronic and structural active sites; (3) identity and configuration of key intermediates; (4) preferred transformation paths.

Further, the parallel development of the NAP-XPS end-station, dedicated to in situ investigations of catalysts in gaseous environments within the mbar pressure range by X-ray photoelectron spectroscopy (XPS), will be described. We will present the possibilities of conducting research with NAP-XPS end-station in the soft X-ray energy range. The constructed end-station will be an ideal operando measurement method for investigating the electronic structure of materials at gas/solid interfaces while simultaneously monitoring the material's functions.

Acknowledgements: This work was partially supported by the National Science Centre (Poland) under grant number 2020/37/B/ST3/00555.

[1] L. Cao, et al, *Accounts of Chemical Research*, **55**, 2594-2603 (2022).

## NAP-XPS INSTRUMENTATION AND APPLICATIONS

Liana Socaciu-Siebert

*SPECS Surface Nano Analysis GmbH, Voltastr. 5, 13355 Berlin, Germany*

E-mail: [liana.socaciu-siebert@specs.com](mailto:liana.socaciu-siebert@specs.com)

Over the last decades it has been possible to develop XPS systems that can work far beyond the standard conditions of high or ultrahigh vacuum. Thus, Near Ambient Pressure (NAP) - XPS has become a rapidly growing field and has demonstrated its capability in a wide variety of applications. Starting from operando studies of surface reactions in catalysis, the applications soon have been extended towards studies of processes at liquid/solid or liquid/gas interfaces. Nowadays, the NAP-XPS analysis technique has become a standard analysis tool not only at synchrotrons, but also in laboratories. The availability of different optimized sample environments (gases, liquids, electrochemical cells) as well as the combination of various analysis methods (NAP-SPM, IRRAS, NAP-HAXPES etc.) allow for gaining insights into the fundamental processes that take place during a chemical reaction.

We present existing solutions for NAP-XPS analysis with an emphasis on SPECS latest developments of instruments and material analysis methods. Examples and results from existing NAP-XPS systems will be shown as well as future perspective of applications and scientific contributions of routine operando NAP-XPS.

## The inaugural Crosscarpatian Synchrotron School (CSS2024)

The inaugural Crosscarpatian Synchrotron School (CSS2024) was held at the SOLARIS Centre from June 10-14, 2024, and devoted to students, PhD students, and senior researchers with little to no experience in synchrotron radiation. The school offered a mix of theoretical lectures and hands-on workshops focusing on the diverse applications of synchrotron research. Participants, chosen from 100 applicants, received in-depth training at chosen two different experimental stations, covering experiment design, sample preparation, measurements, and data processing.

The school featured access to advanced beamlines and cryo-electron microscopy infrastructure, providing 37 selected scientists with a unique opportunity to enhance their expertise. The school also sought to address the "brain drain" issue by empowering young researchers in Central and Eastern Europe to engage with high-level research facilities locally. In addition to skill development, the event encouraged networking and sparked discussions that may lead to future scientific collaborations and innovative research projects.



## Lecture Series on Basics of Accelerator Physics

We are pleased to announce the upcoming lecture series, "Basics of Accelerator Physics," which offers a comprehensive overview of the principles, design, and applications of particle accelerators. This course is dedicated mainly for PhD students interested in gaining a deep understanding of accelerator physics.

### Course Highlights:

- ✚ Historical Perspective: An introduction to the development and types of accelerators.
- ✚ Beam Dynamics: In-depth exploration of transverse and longitudinal dynamics, linear imperfections, and correction methods, with an introduction to nonlinear dynamics.
- ✚ Interactive Tutorials: Hands-on experience with industry-standard tools, MADX and XSuite, through practical exercises on accelerator design and simulation.

**Advanced Topics:** Coverage of diagnostics, beam cleaning, collimation techniques, and the use of synchrotron light sources, as well as specialized applications in medical and industrial fields. Participants will gain a solid understanding of the physics behind particle accelerators, proficiency in using computational tools for accelerator design, insights into the diverse applications of accelerators in science and industry.

The course is led by Dr. Marcin Patecki from Warsaw University of Technology, an expert with extensive experience in Accelerator Physics.

**Schedule:** The course will be held online every Thursday from 10:15 to 11:45, starting on October 10, 2024, and concluding on January 30, 2025.

## INTERNSHIP OPPORTUNITIES AT THE EUROPEAN XFEL

A short-term (up to 6 weeks) and medium-term (up to 3 months) internships at the European X-ray Free-Electron Laser (EuXFEL) research stations is offered within the XFEL project funded by the Ministry of Science and Higher Education (MNiSW). These internships provide a unique opportunity for participants to familiarize themselves with the research topics and experimental techniques employed at EuXFEL. The goal is to equip young Polish scientists with the skills to leverage EuXFEL in their own research.

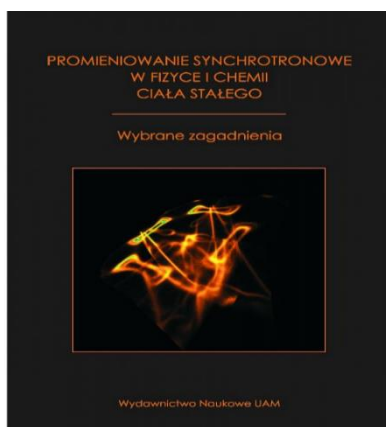
The first internships are scheduled to take place between October 1 and December 15, 2024, with costs covered by the project funds.

Detailed information, including the list of research topics, application form, and regulations, can be found on website: <http://www.ifpan.edu.pl/cd-xfel/staze-w-euxfel/>.

**The application deadline is September 15, 2024.** For further information, please contact [cd-xfel@ifpan.edu.pl](mailto:cd-xfel@ifpan.edu.pl).

Don't miss this chance to advance your research with cutting-edge tools at EuXFEL!

## BOOK



The book *Promieniowanie synchrotronowe w fizyce i chemii ciała stałego* (Synchrotron radiation in solid state physics and chemistry), written by

members of the PTPS, has been published under the editorship of Bogdan Kowalski and Wojciech Paszkowicz. An electronic version of the book is also available on the Adam Mickiewicz University Press website:

[https://press.amu.edu.pl/pl/promieniowanie-synchrotronowe-w-fizyce-i-chemii-ciala-stalego-wybrane-zagadnienia\\_oa.html](https://press.amu.edu.pl/pl/promieniowanie-synchrotronowe-w-fizyce-i-chemii-ciala-stalego-wybrane-zagadnienia_oa.html).

By the decision of the PTPS Board, the Society has purchased open access to the electronic version.

## RIANA

The RIANA project (Research Infrastructure Access in Nanoscience & Nanotechnology) has been running from March 1, 2024. As part of this project, the National Synchrotron Radiation Centre SOLARIS and 10 other LEAPS-affiliated European synchrotron sources, together with 58 other large research infrastructures from EU countries, are providing beamtime and offering assistance in preparing applications for measurement time through an ongoing call for proposals. Details can be found on the project's official website: <https://riana-project.eu/>.

## International Symposium Sylinda at the SOLARIS Centre

For two days (7-8 March 2024), the SOLARIS Centre was transformed into the capital of the world of X-ray absorption spectroscopy (XAS), thanks to outstanding specialists who accepted an invitation from the Krakow synchrotron. The event was held in a hybrid mode and gathered about 300 participants who had the opportunity to participate in the symposium via the Zoom platform.

“Sylinda” is an international project, whose leader is SOLARIS, while the partners are the ALBA synchrotron (Spain) and two universities: Hochschule Niederrhein and the University of Bonn. The consortium's activities aim

to encourage industry to use the SOLARIS research infrastructure and increase its capabilities. The project goals also include expanding the group of scientists that visit SOLARIS.

### SOLARIS Centre hosted the LEAPS-INNOV annual meeting and LEAPS General Assembly

SOLARIS Centre as a member of the League of European Accelerator-based Photon Sources (LEAPS), was organizer the LEAPS-INNOV annual meeting which took place from 8<sup>th</sup> to 10<sup>th</sup> April 2024. The conference was held in a hybrid format and was attended by a total of 120 participants. Than was followed by a scheduled meeting of the Consortium's Board of Directors, which deliberated on the strategic directions of development during the LEAPS General Assembly. The meeting with leading representatives of the European synchrotron community was also joined by the Director of the Department of Innovation and Development (DIR) of the Ministry of Science and Higher Education, Michał Doligalski.

### Infrared Nanoscopy Workshop at the SOLARIS Centre

Scientists from the CIRI beamline at the SOLARIS Center, together with Attocube system AG and COMEF, were the organizers of the Infrared Nanoscopy Workshop on Biological and Polymer Nanomaterials, which took place on April 24-26, 2024, at the Solaris Center and in the Auditorium of the Jagiellonian Innovation Centre. The event gathered over a hundred participants who had the opportunity to participate in lectures and poster sessions and make test measurements.

Lectures conducted by leading experts in infrared nanospectroscopy taught participants the basics of the above-

mentioned techniques and their selected applications in studying biological and polymer samples.

### ESRF

Scientists affiliated with Polish institutions can apply for the beamtime at the European Synchrotron Radiation Facility (ESRF) as part of Poland's 1% contribution paid with the grant from the Ministry of Science and Higher Education obtained by the National Consortium of Scientific Institutions interested in using the European Synchrotron Radiation Facility in Grenoble and coordinated by the Institute of Physics of the Polish Academy of Sciences. Anna Wolska is a Polish observer at the ESRF Council, while Anna Reszka is a representative at the Administrative and Financial Committee. Moreover, the MNiSW grant gives funding opportunities for participation in conferences, provided that the ESRF based research is presented. More information can be found on the grant website: <https://esrf.ifpan.edu.pl/>

### KEYWORD

At the initiative of the Council of Scientific Societies at the Presidium of the Polish Academy of Sciences, a new edition of the "Dictionary of Polish Scientific Societies" is being developed. Anna Wolska, Agnieszka Witkowska, and Edyta Piskorska-Hommel have prepared an updated keyword for the new edition.

### XFEL-Project website

**A new website related to the XFEL-project funded by the Ministry of Science and Higher Education (MNiSW) is now available:** <https://www.ifpan.edu.pl/cd-xfel/>

It contains information on (1) scientific opportunities offered by EuXFEL and Polish participation in it; (2) the network of XFEL Centers of Excellence, its tasks and

current activities, (3) opportunities for financial and substantive support to Polish scientists - potential users of EuXFEL; (4) upcoming events (conferences and workshops, internships, seminars, lectures etc.) related to XFEL science; (5) research projects implemented at EuXFEL by Polish scientists. The website also includes important documents: regulations for applying for support under the project, application templates, etc.

## ISSRNS conference 2025

The next, XVI ISSRNS conference will take place from 25<sup>th</sup> to 30<sup>th</sup> May 2025 in the mountains of Silesian Beskids. The chair is Anna Wolska. The latest information can be found at the conference website: <https://issrns.pl/>

## Summary of the twelfth and thirteenth call for proposals

The twelfth call for proposals for beamtime at the SOLARIS Centre closed on October 2, 2023. The International Evaluation Committee will once again have the opportunity to examine a record number of applications.

For the first time in this call, requesting beamtime on the CIRI and POLYX beamlines was possible. Beamtime, on these lines, was the subject of over 20 proposals. Decisions on the allocation of beamtime will be known before the end of the year, in mid-December.

169 applications were received in the twelfth call for beamtime on the SOLARIS infrastructure.

The thirteenth call for proposals at the SOLARIS Centre was ended on April 3. A total of 171 applications were received in this call.

This result confirms an upward trend in the number of researchers interested in experiments performed at SOLARIS.

A total of seven beamlines and a cryomicroscope are available to users.

The ASTRA beamline and Cryo-EM were the most popular techniques used in the applications submitted. 40 and 43 applications were submitted for research time, respectively.

80% represent national projects, and 20% constitute applications submitted by scientists from other countries, i.e., Germany, the Czech Republic, and Spain.

## The Autumn call for proposals is already open in SOLARIS

**The SOLARIS 2024 autumn call for proposals is now open! The deadline for submitting proposals is the 1<sup>st</sup> of October 2024 at 23:59 CET.**

Before submitting proposals, interested researchers are encouraged to contact our scientists:

Alexey Maximenko  
([alexey.maximenko@uj.edu.pl](mailto:alexey.maximenko@uj.edu.pl))  
for proposals related to ASTRA beamline;

Tomasz Wróbel ([tomek.wrobel@uj.edu.pl](mailto:tomek.wrobel@uj.edu.pl))  
for proposals related to CIRI beamline;

Marcin Zajac ([mar.zajac@uj.edu.pl](mailto:mar.zajac@uj.edu.pl))  
for proposals related to DEMETER beamline;

Tomasz Sobol ([t.sobol@uj.edu.pl](mailto:t.sobol@uj.edu.pl))  
for proposals related to PHELIX beamline;

Marcin Zajac ([mar.zajac@uj.edu.pl](mailto:mar.zajac@uj.edu.pl))  
for proposals related to PIRX beamline;

Katarzyna Sowa ([k.sowa@uj.edu.pl](mailto:k.sowa@uj.edu.pl))  
for proposals related to POLYX beamline;

Natalia Olszowska  
([natalia.olszowska@uj.edu.pl](mailto:natalia.olszowska@uj.edu.pl))

for proposals related to URANOS beamline;

Michał Rawski (michal.rawski@uj.edu.pl) for proposals related to Cryo-EM microscope,

who can advise on the technical possibilities of the instruments available at SOLARIS.

More information can be found on our website:

[https://synchrotron.uj.edu.pl/en\\_GB/dla-uzytownikow](https://synchrotron.uj.edu.pl/en_GB/dla-uzytownikow).

### Support available through the NEPHEWS Project

The Solaris Centre participates in the NEPHEWS project, which is dedicated to supporting users. We offer support through the following three programs:

#### **TNA Programme -**

<https://beamtime.eu/programmes-support/tna/>

This programme covers travel and accommodation costs for up to two research team members conducting measurements at Solaris.

#### **Twinning Programme -**

<https://beamtime.eu/programmes-support/twinning/>

This programme covers travel and accommodation expenses for a new user who joins a research team conducting measurements at Solaris.

#### **ESR Programme -**

<https://beamtime.eu/programmes-support/esrs/>

We offer a one-week internship at Solaris, including coverage of travel and accommodation costs.

Please note that these programmes are also available through other project partners.

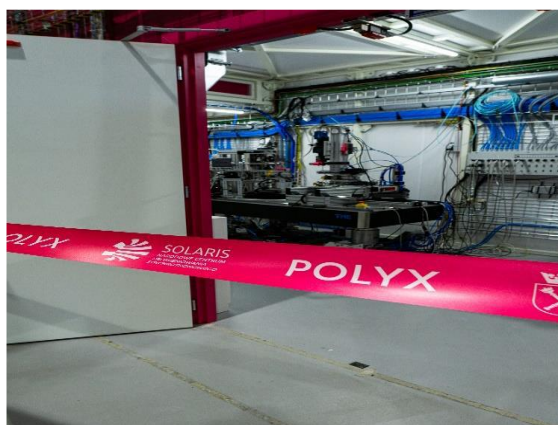
We encourage you to review the detailed information available on [www.beamtime.eu](http://www.beamtime.eu) and to make use of the support programmes offered.

For any enquiries regarding the NEPHEWS project, please contact: [nephews@uj.edu.pl](mailto:nephews@uj.edu.pl).

## New beamlines are open at the SOLARIS

### POLYX

POLYX is a compact beamline designed for X-ray microimaging and microspectroscopy in the 5-15 keV energy range. The name POLYX derives from the polycapillary X-ray optics used for focusing, as well as the capability to use polychromatic X-rays to enhance the X-ray flux from the SOLARIS bending magnet in the hard X-ray energy range.



The POLYX beamline allows for imaging 2D and 3D structures, elemental distribution, and chemical phases within the samples under investigation. The main experimental techniques available at POLYX include micro X-ray fluorescence imaging, micro X-ray absorption spectroscopy, and microtomography. The experimental geometry at POLYX can be easily reconfigured, and the beamline features a dedicated area for user setups, facilitating non-standard experiments and tests. Beamline tests in expert commissioning mode began in the winter of 2024, with regular user operations scheduled to start in September 2024.

The infrastructure was created in close cooperation with scientists from the

Jagiellonian University, the AGH University of Science and Technology and the Institute of Nuclear Physics, Polish Academy of Sciences.

### CIRI

A year and a half of work on the CIRI research line has reached its culmination. On August 27, 2024, the line's team announced the closure of CIRI's constitution stage. The beamline commissioning and opening ceremony are scheduled for the last quarter of this year.

CIRI (Chemical Infrared Imaging) is a beamline dedicated to IR imaging in the mid-to far-infrared ranges. It consists of 3 endstations that cover 3 spatial imaging scales: micrometric (FT-IR microscope), submicrometric (O-PTIR microscope), and nanoscale (s-SNOM/AFM-IR microscope). These modalities enable measurements of a wide range of samples, from tissue sections, cells, cosmetics and 2D materials to cultural heritage objects. The main contrast is based on chemical composition probed by vibrational spectroscopy, which requires covalent bonds present in the sample, but at the same time being sensitive to conformation of the probed molecule. The beamline in expert commissioning mode with laboratory sources began in 2023, and in the summer of 2024, the final parts of the beamline were installed, allowing for regular operation with synchrotron light to begin in 2025.



## Cooperation with international organizations

### ESUO - Towards Even Brighter European Photon Science (The ESUO Manifesto, 2014)

ESUO (the European Synchrotron and Free Electron Laser User Organization) is an international non-profit association which represents the interests and needs of all users of synchrotron and FEL facilities in Europe. The main vision of ESUO is to support the European synchrotron and FEL user community, ensuring equal opportunities for access and participation for all scientists, based solely on the scientific merit of their ideas.

ESUO was founded in 2010 and since July 12, 2021 possess a legal entity (A.I.S.B.L. in accordance with the Belgium Code of Companies and Associations). The form and scope of ESUO activities are regulated by the association's statute available on the website: <https://www.esuo.eu/>.

At present, users from 32 European member states and European associated countries are represented in ESUO by 45 national delegates/representatives. The main authority in the association is held by the General Assembly of the national delegates. The association is managed by the Executive Board consisting of seven members and the President. Since October 19, 2021, the President of ESUO is Cormac McGuinness, delegate from Ireland and Trinity College Dublin.

Poland has been an active member of ESUO from the very beginning of its existence. Until 2019, Polish photon users and PSRS (Polish Synchrotron Radiation Society) in ESUO were represented by Krystyna Jabłońska (Institute of Physics PAS), who was also a member of the ESUO Executive Board. Currently, Poland is represented by two delegates:

Agnieszka Witkowska (Gdansk University of Technology) and Ryszard Sobierajski (Institute of Physics PAS).

ESUO realizes its mission by ensuring scientists with equal Trans-National Access (TNA) to the relevant synchrotron and FEL facilities (CALIPSO, CALIPSOplus, NEPHEWS projects), supporting the facilities in creating equal opportunities for scientists, promoting advanced techniques and beamlines in SR and FEL facilities, fostering contacts between users and sharing knowledge and expertise, strengthening cooperation with national synchrotron and FEL user organizations.

### SOLARIS Centre hosted the LEAPS-INNOV annual meeting and LEAPS General Assembly

The LEAPS-INNOV pilot project is dedicated to advancing collaboration between European light sources, including synchrotrons, free-electron lasers, and industry. LEAPS-INNOV seeks to establish long-term partnerships that benefit both parties by implementing new strategies and activities.

SOLARIS Centre, as a member of the League of European Accelerator-based Photon Sources (LEAPS), was the organizer of the LEAPS-INNOV annual meeting, which took place from 8<sup>th</sup> to 10<sup>th</sup> April 2024—in the conference hybrid format, attended a total of 120 participants. The Consortium's Board of Directors deliberated on the strategic directions of development during the LEAPS General Assembly. The meeting with leading representatives of the European synchrotron community was also joined by the Director of the Department of Innovation and Development (DIR) of the Ministry of Science and Higher Education, Michał Doligalski.

## Cooperation between Poland, Ukraine, and Switzerland

As a center integrating three international scientific communities, SOLARIS is leading a unique project to construct a research beamline through collaboration between Poland, Ukraine, and Switzerland. Coordinated by the League of European Accelerator-based Photon Sources (LEAPS), the initiative supports Ukrainian researchers and strengthens scientific cooperation in Central and Eastern Europe.

Since 2022, SOLARIS and the Ukrainian Synchrotron Radiation Users Society have engaged over 500 scientists in workshops, shaping the research priorities and design of the beamline, which will be housed at the SOLARIS synchrotron in Krakow.

This project is driven by a unique trilateral partnership, with significant financial and technical support from the Paul Scherrer Institute and the Swiss National Science Foundation. Despite these contributions, additional funding is sought to complete the beamline, with SOLARIS actively pursuing support from the European Union and other regional partners.

The new beamline, designed to operate with moderate and hard X-rays, will enable groundbreaking research in agriculture, energy, metallurgy, biotechnology, and more. It will support critical advancements like improving food quality, promoting sustainable agricultural practices, enhancing energy efficiency, and developing advanced biomedical technologies. This infrastructure will not only boost innovation across crucial industries but also foster knowledge exchange, scientific mobility, and regional integration, advancing the strategic goals of the European Union.

SOLARIS remains committed to expanding international cooperation, particularly with Baltic and Transcarpathian countries, reinforcing its mission to strengthen Europe's scientific community and research capabilities.



# nephews

Neutrons and Photons  
Elevating Worldwide Science

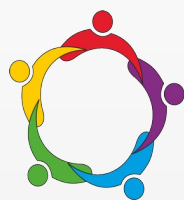


nephews@uj.edu.pl  
www.beamtime.eu



Co-funded by  
the European Union

Co-funded by the European Union. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or European Research Executive Agency. Neither the European Union nor the granting authority can be held responsible for them.



polish synchrotron  
radiation society



**SOLARIS**  
NATIONAL SYNCHROTRON  
RADIATION CENTRE

---

SYNCHROTRON RADIATION IN NATURAL SCIENCE

Bulletin of Polish Synchrotron Radiation Society

vol. 24, September 2024

ISSN 1644-7190