18th SOLEIL USERS' MEETING

JANUARY 18th - 19th, 2024

Synchrotron SOLEIL (Saint-Aubin)

SCIENTIFIC COMITTEE

Pierre ASSELIN (De la Molécule aux Nano-objets : Réactivité, Interactions et Spectroscopies - Paris)
Amélie BORDAGE (Inst. de Chimie Moléculaire et des Matériaux d'Orsay - Orsay)
Florent CARN (Lab. de Matière et Systèmes Complexes - Paris)
Charlotte CATROUILLET (Institut de Physique du Globe de Paris - INSU - INEE – Paris)
Fabien CHEYNIS (Centre Interdisciplinaire de Nanoscience de Marseille - Marseille)
Héloïse DOSSMANN (Inst. Parisien de Chimie Moléculaire - Paris)
Paloma FERNANDEZ VARELA (Institut de Biologie Intégrative de la Cellule - INSB - Gif-Sur-Yvette)
Sara GONZALEZ (Institut de Nanotechnologies de Lyon - INSIS - INC – Villeurbanne)
Benoît MASQUIDA (Génétique Moléculaire Génomique Microbiologie - Strasbourg)
Debora PIERUCCI (Centre de Nanosciences et de Nanotechnologies - Palaiseau)
Simona RANERI (National Research Council - Institute of Chemistry of Organometallic Compounds – Sesto Fiorentino)
Asma TOUGERTI (Unité de Catalyse et de Chimie du Solide – Villeneuve d'Ascq)

Information and registration:
https://www.synchrotron-soleil.fr/fr/evenements/sum2024-0

SOLEIL SYNCHROTRON

SOLEIL Users' Meeting

January 18th - 19th, 2024

Synchrotron SOLEIL, Saint-Aubin - France

Summary

SUM2024

Welcome

The 18th SOLEIL Users' Meeting takes place on Thursday January 18th and Friday 19th, 2024 at SOLEIL.

This invaluable forum for the synchrotron radiation users' community provides the opportunity to exchange and learn about the evolution of the machine and the beamlines.

It is also the opportunity to share scientific, technical and practical issues about the synchrotron radiation use.

The plenary lecturer covers recent research highlights of SOLEIL in "Dynamic, Reactivity and Chemical analysis" areas.

Scientific communications are presented during three parallel sessions, selected from the submitted abstracts.

In the afternoon of January, 18th, a social time and scientific exchange are held at SOLEIL, including the poster session, stands from commercial exhibitors and the dinner buffet.

Tutorial is organised on site on Friday afternoon the 19th of January, 2024.

In parallel, a round table held on Friday 19th of January, 2024 at SOLEIL: TEA-BAG - Exchange about the BAG projects.

Bienvenue

Le 18ème Colloque des Utilisateurs de SOLEIL a lieu les jeudi 18 et vendredi 19 janvier 2024, à SOLEIL.

Ce rendez-vous incontournable pour la communauté des utilisateurs du rayonnement synchrotron est l'occasion d'échanges et d'informations sur l'évolution de la machine et des lignes de lumière.

Il est aussi le lieu pour échanger sur les aspects scientifiques, techniques et pratiques de l'utilisation du rayonnement synchrotron.

La conférence plénière couvre les thèmes de recherche de la communauté des utilisateurs de SOLEIL en « Dynamique, réactivité et analyse chimique »

Les sessions parallèles sont composées d'exposés scientifiques originaux, sélectionnées à partir des résumés soumis.

Un temps de convivialité et de discussion sont organisés à SOLEIL le jeudi 18 janvier après-midi avec la session posters, les stands d'entreprises et le buffet dînatoire.

Une formation est organisée le vendredi 19 janvier 2024 après-midi à SOLEIL.

En parallèle, une table ronde a lieu le vendredi 19 janvier 2024 à SOLEIL de 15H00 À 17H30 : TEA-BAG - Echanges Autour des projets BAG.

Programme

Thursday, January 18th, 2024

SOLEIL Auditorium - Main Building
(Broadcast in Phenix and Orion Rooms)

09:00 - 10:00	*Registration & coffee*
10:00 - 10:10	Welcome / Introduction, ORGUES Chair **– *Amélie Bordage***
10:10 - 10:50	The word of SOLEIL General Director – ***Jean Daillant***
10:50 - 11:35	**Dynamic, Reactivity and Chemical analysis** Electrochemical energy storage and Synchrotron Radiation ***Lorenzo Stievano -*** *Institut Charles Gerhardt, Montpellier, France*
11:35 - 12:00	Developments in robotic for process automation at SOLEIL ***Yves-Marie Abiven*** - *Synchrotron SOLEIL, Saint Aubin, France*
12:00 - 12:30	Event “20 Years of LUCIA” - ***Delphine Vantelon*** AFURS / ESUO / ORGUES Opened questions session ***Amélie Bordage & Roland Thissen***
12:30 - 13:45	*Lunch*
14:00 - 16:00	**Parallel sessions** – 3 different auditoriums (see the detailed programme below) • Advanced Materials (Structure / Electronic Properties /Surfaces & Interfaces) • Dynamic, Reactivity & Chemical analysis (Diluted Matter & Chemistry) • Health & well-being, Environment & Geosciences, Cultural Heritage
16:00 - 16:30	*Coffee break*
16:30 - 18:00	**Parallel sessions** – 3 different auditoriums (see the detailed programme below) • Advanced Materials (Structure / Electronic Properties /Surfaces & Interfaces) • Dynamic, Reactivity & Chemical analysis (Diluted Matter & Chemistry) • Health & well-being, Environment & Geosciences, Cultural Heritage
18:00 - 20:00	Posters session / Commercial Exhibitors
20:00 - 21:30	Dinner / **Award of the best student poster**

Programme

Friday, January 19th, 2024

09:00 -10:45 **Parallel sessions** – 3 different auditoriums (see the detailed programme below)

- Advanced Materials (Structure / Electronic Properties /Surfaces & Interfaces)
- Dynamic, Reactivity & Chemical analysis (Diluted Matter & Chemistry)
- Health & well-being, Environment & Geosciences, Cultural Heritage

10:45 - 11:15 *Coffee break* – Cafeteria Space near ***SOLEIL Auditorium - Main Building***

11:15 - 12:30 PRC Round Table "Proposal / Experimental Report" - ***SOLEIL Auditorium - Main Building***

12:30 - 13:45 *Lunch*

14:00 - 15:00 Visit of 3 Beamlines: ANTARES - CRISTAL - DEIMOS

14:00 - 17:00

SOLEIL Reception Building Auditorium - Ground Floor

Tutorial - On-site only

Data treatment and analysis on SIXS

15:00 - 17:00

SOLEIL Auditorium - Main Building

Round table

TEA-BAG - Exchange about the BAG projects

Parallel Session Schedule

Advanced Materials
(Structure / Electronic Properties / Surfaces & Interfaces)

Chairpersons: A. Bordage, D. Pierucci, F. Cheynis, S. Gonzalez

SOLEIL - Main Building

Thursday, January 18th, 2024

14:00 - 14:30 (25'+5')	10 years operations of the GALAXIES beamline: Status and perspectives ***Jean-Pascal Rueff*** *- Synchrotron SOLEIL, Saint Aubin, France*
14:30 - 14:55 (20'+5')	Combining Synchrotron single-crystal and powder diffraction data to tackle highly complex structures of MOFs ***Nathalie Guillou*** *- Institut Lavoisier de Versailles, France*
14:55 - 15:20 (20'+5')	Investigation of magneto-optical van der Waals magnet via correlative spectroscopic techniques ***Victor Porée*** *- Synchrotron SOLEIL, Saint Aubin, France*
15:20 - 15:45 (20'+5')	Two pathways of frosting on surfaces with varying wettability as seen by GIWAXS ***Patrick Kekicheff*** *- Institut Charles Sadron, Strasbourg, France*
15:45 - 16:15	*Coffee Break*
16 :15 - 16 :45 (25'+5')	Band engineering of earth abundant materials for efficient solar water splitting ***Dana Stanescu*** *- SPEC, CEA Saclay, Gif-sur-Yvette, France*
16:45 - 17:10 (20'+5')	Site occupancies in the quinary Co–Cr–Fe–Mn–Ni σ phase using resonant diffraction and EXAFS ***Jean-Marc Joubert*** *- Institut de Chimie et des Matériaux Paris-Est, Thiais, France*
17:10 - 17:35 (20'+5')	Influence of the crystal structure and nature of the ligands on the valence of uranium in chalcogenides compounds. ***Thomas Stephant*** *- Institut des Sciences Chimiques de Rennes, France*
17:35 - 18:05 (25'+5')	The electrodynamics properties of superconducting $Nd_{0.8}Sr_{0.2}NiO_2$ nickelate ***Stefano Lupi –*** *Department of Physics, La Sapienza University, Rome, Italy*

Parallel Session Schedule

Advanced Materials
(Structure / Electronic Properties / Surfaces & Interfaces)

Chairpersons: A. Bordage, D. Pierucci, F. Cheynis, S. Gonzalez

SOLEIL - Main Building

Friday, January 19th, 2024

09:00 - 09:30 (25'+5')	Spin crossover in self-assembler monolayers ***Patrick Rosa*** *- Institut de Chimie de la Matière Condensée de Bordeaux, France*
09:30 - 09:55 (20'+5')	Synchrotron-based infrared studies of transition metal dichalcogenides at high pressure ***Béatrice D'Alò*** *- Sapienza University of Rome, Italy*
09:55 - 10:20 (20'+5')	Electric field-driven phase transition in antiferroelectric PbZrO3 by in situ X-ray diffraction ***Alexandre Zing*** *- Centre de Nanosciences et Nanotechnologies, Palaiseau, France*
10:20 - 10:45 (20'+5')	Using Synchrotron Radiation for probing the energy landscape of nanocrystal-based optoelectronic devices in situ and operando ***Erwan Bossavit*** *- Institut des NanoSciences de Paris et Synchrotron SOLEIL, Saint-Aubin, France*
10:45 - 11:15	*Coffee break*

Parallel Session Schedule

Dynamic, reactivity and Chemical analysis (Dilluted Matter & Chemistry)

Chairpersons: A. Tougerti, F. Carn, H. Dossmann, P. Asselin

SOLEIL - Reception Building Auditorium
Ground Floor & PA.1.12 Rooms

Thursday, January 18th, 2024

14:00 - 14:30 (25'+5')	Weakly bound systems of chemical and biological relevance probed by double imaging photoelectron photoion coincidence spectroscopy ***Sebastien Hartweg*** *- Institute of Physics, University of Freiburg, Germany*
14:30 - 14:55 (20'+5')	Induced photoelectron circular dichroism onto an achiral chromophore ***Etienne Rouquet*** *- Synchrotron SOLEIL, Saint Aubin et Institut des Sciences Moléculaires d'Orsay, France*
14:55 - 15:20 (20'+5')	Experimental study of polarization-dependent PCI effect in neon and water following K-shell photoionization ***Abhishek Verma*** *- Laboratoire de Chimie Physique Matière et Rayonnement, Paris, France*
15:20 - 15:45 (20+5')	A time-resolved mechanistic study into the effects of a partially-hydroxylated surface during atomic layer deposition of HfO_2 on Si(111) ***Rosemary Jones*** *- Department of Physics, Lund University, Sweden*
15:45 - 16:15	*Coffee break*
16:15 - 16:40 (20'+5')	Rovibrational spectroscopy of gas phase precursors of secondary organic aerosols from high resolution synchrotron-base Fourier transform and QCL infrared measurements ***Arnaud Cuisset*** *- Laboratoire de Physico-Chimie de l'Atmosphère, Dunkerque, France*
16:40 - 17:05 (20+5')	Carburization, passivation and re-activation of Mo- and Ni/Cu-Mo-based catalysts for the upgrading of furfural: A time-resolved, in-situ XAS study ***Eric Marceau*** *- Unité de Catalyse et Chimie du Solide, Lille, France*
17:05 - 17:30 (20'+5')	Application of photoelectron spectroscopy to uracil and bromouracil molecules in liquids ***Marine Fournier*** *- Laboratoire de Chimie Physique Matière et Rayonnement, Paris et Synchrotron SOLEIL, Saint-Aubin, France*
17:30 - 17:55 (20'+5')	Evidencing an elusive conical intersection in the dissociative photoionization of methyl iodide

***Sonia Marggi Poullain** - Departamento de Química Física, Universidad Complutense de Madrid, Spain*

Parallel Session Schedule

Dynamic, reactivity and Chemical analysis (Dilluted Matter & Chemistry)

Chairpersons: A. Tougerti, F. Carn, H. Dossmann, P. Asselin

SOLEIL - Reception Building Auditorium
Ground Floor & PA.1.12 Rooms

Friday, January 19th, 2024

09:00 - 09:30 (25'+5')	XAS hyperspectral imaging at the ROCK beamline: Adding micrometer spatial resolution to second time resolution for chemical transformation monitoring ***Valerie Briois –** Synchrotron SOLEIL, Saint Aubin, France*
09:30 - 09:55 (20'+5')	Electrochemical and structural study of NiRux heterofunctional catalysts for the alkaline HER ***Marie-Sophie Dias Fernandes** - Synchrotron SOLEIL, Saint-Aubin et Institut Polytechnique de Paris, Palaiseau, France*
09:55 - 10:20 (20'+5')	Spectroscopic and kinetic studies of X-ray and UV induced desorption from molecular ices ***Daniela Torres-Díaz** - Institut des Sciences Moléculaires d'Orsay et LERMA, Paris, France*
10:20 - 10:45 (20'+5')	THz spectroscopy of radical species using the heterodyne receiver of the AILES beamline ***Luan Juppet -** Institut des Sciences Moléculaires d'Orsay, France*
10:45 - 11:15	*Coffee break*

Parallel Session Schedule

Health & Well-being, Environment & Geosciences, Cultural Heritage

Chairpersons: B. Masquida, C. Catrouillet, P. Fernandez Varela, S. Raneri

CEA Bloch Auditorium

Thursday, January 18th, 2024

14:00 - 14:30 (25'+5')	Extracting information on ancient manufacturing techniques and exchange networks from metallic artefacts: A case study on arms and armour ***Emilie Berard -*** *Laboratoire Archéomatériaux et Prévision de l'Altération, Gif-sur-Yvette, France*
14:30 - 14:55 (20'+5')	Early alterations of diabetic mouse aortas revealed by X-ray micro-CT ***Sébastien Almagro*** *- MEDyC, Université de Reims Champagne-Ardenne, France*
14:55 - 15:20 (20'+5')	Play it again – Recovering archived music from degraded recordings with RIXS-MCD ***Sebastian Gliga*** *- Paul Scherrer Institute, Villigen, Switzerland*
15:20 - 15:45 (20'+5')	A New model of niobium (Nb) enrichment in laterites revealed by X-ray absorption spectroscopies and Synchrotron diffraction ***Quentin Bollaert*** *- Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie, Paris, France et CEDON, KU Leuven, Belgium*
15:45 - 16:15	*Coffee Break*
16:15 - 16:45 (25'+5')	Analysis of arsenic speciation in environmental samples using different Synchrotron-based techniques ***Pierre Le Pape –*** *Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie, Paris, France*
16:45 - 17:10 (20'+5')	In-depth 3D analysis of iron age mineralised textiles using Synchrotron-based techniques ***Clémence Iacconi*** *- ENS Paris-Saclay, Gif-sur-Yvette, France*
17:10 - 17:35 (20'+5')	Stability field of FeO_2H_x in the Earth's mantle from in situ X-ray diffraction at extreme conditions ***Anne-Elisabeth. Marceline*** *- Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie, Paris, France*
17:35 - 18:00 (20'+5')	Hommage à Yann Gohon ***Frédéric Jamme -*** *Synchrotron SOLEIL, Saint-Aubin, France*

Parallel Session Schedule

Health & Well-being, Environment & Geosciences, Cultural Heritage

Chairpersons: B. Masquida, R. Le Hir, R. Marsac, S. Raneri

CEA Bloch Auditorium

Friday, January 19th, 2024

09:00 - 09:30 (25'+5')	Peptides inspired by the left-handed β–helix: Structural characterization by circular dichroïsm and X-ray diffraction ***Vincent Lebrun** - Institut de Chimie, Université de Strasbourg, France*
09:30 - 09:55 (20'+5')	Effects of environmental factors on Co speciation at the surface of magnetite ***Laura Fablet** - Géosciences Rennes, France et Synchrotron SOLEIL, Saint-Aubin, France*
09:55 - 10:20 (20'+5')	Structural resolution of the metabolic activation pathway of the antiviral drug bemnifosbuvir : From pro-drug to target ***François Ferron** - Aix-Marseille Université, France et European Virus Bioinformatics Center, Jena, Germany*
10:20 - 10:45 (20'+5')	Synchrotron radiation techniques for the characterization and conservation of painted metal objects of industrial heritage (The CoPaiM Project) ***Julie Gordon** - Musée du quai Branly - Jacques Chirac, Paris, France*
10:45 - 11:15	*Coffee Break*

PLENARY SESSION

PLENARY SESSION

Amélie BORDAGE, Chairperson

SOLEIL Auditorium - Main Building

Thursday, January 18th, 2024

10:00 – 10:10	**Welcome / Introduction, ORGUES Chair – *Amélie Bordage***
10:10 – 10:50	The word of SOLEIL General Director – ***Jean Daillant***
10:50 – 11:35	**Dynamic, Reactivity and Chemical analysis** Electrochemical energy storage and Synchrotron Radiation ***Lorenzo Stievano*** *- Institut Charles Gerhardt, Montpellier, France*
11:35 – 12:30	Developments in robotic for process automation at SOLEIL - ***Yves-Marie Abiven*** *Event "20 YEARS OF LUCIA" -* ***Delphine Vantelon*** *AFURS / ESUO / ORGUES* *Opened questions session*

Electrochemical Energy Storage and Synchrotron Radiation

Lorenzo Stievano

ICGM, Univ. Montpellier, CNRS, ENSCM, Montpellier, France.
Réseau sur le Stockage Electrochimique de l'Energie (RS2E), CNRS, Amiens, France

ABSTRACT

The exploration of advanced materials and technologies in battery research is crucial in the pursuit of sustainable and high-performance energy storage solutions. Synchrotron-based spectroscopies have emerged as powerful and versatile tools, playing a significant role in unravelling the complex features of battery materials and their electrochemical processes.

Synchrotron sources, known for their high photon flux and energy resolution, provide researchers with a unique capability to delve into the atomic and molecular intricacies of battery materials. Techniques such as X-ray absorption spectroscopy (XAS) and X-ray photoelectron spectroscopy (XPS) offer unparalleled elemental and chemical sensitivity, enabling precise analysis of the chemical state and electronic structure of individual elements within battery components and interfaces. This high resolution is crucial for understanding redox reactions, chemical transformations, structural changes, and evolutions occurring during battery operation. These insights are essential for understanding and preventing degradation processes that can decrease battery lifetime.

A distinctive feature of synchrotron-based spectroscopies is their ability to go beyond conventional analytical methods, allowing in situ and operando studies. By enabling researchers to monitor dynamic changes in real-time during electrochemical cycling processes, synchrotron techniques provide crucial insights into the evolving electrochemical processes within the battery. This dynamic perspective is essential for designing materials with enhanced stability, efficiency, and cycling performance.

Furthermore, synchrotron sources facilitate advanced imaging techniques such as X-ray tomography, providing three-dimensional visualization of the internal structure of batteries. This capability is instrumental in studying electrode morphology, particle distribution, and the impact of cycling on the microstructure.

The surface sensitivity of techniques like XPS contributes to a nuanced understanding of surface chemistry, electrode-electrolyte interactions, and the formation of passivation layers. Such insights are essential for mitigating issues related to capacity fading, impedance growth, and overall degradation in battery performance.

In this presentation, an overview of the main advances achieved through synchrotron-based spectroscopies will be given, underscoring their pivotal role in advancing battery research. The combination of high resolution, in situ/operando capabilities, non-destructive nature, imaging, and surface sensitivity, coupled with advanced data analysis methods, positions synchrotron techniques as indispensable tools for unravelling the complexities of battery materials and accelerating the development of next-generation energy storage technologies.

LUCIA a 20 Ans

P. Lagarde, B. Lassalle, A. Pradas, C. Rivard, D. Roy,
N. Trcera, D. Vantelon

Synchrotron SOLEIL, L'orme des merisiers, départementale 128, 91190 Saint Aubin, France

ABSTRACT

We are pleased to announce the workshop "**LUCIA a 20 ans**"

LUCIA is the SOLEIL beamline dedicated to X-ray micro-absorption, µXANES & µEXAFS, and X-ray micro-fluorescence experiments in the "soft" X-ray range (0.5 - 8.5 keV).
Thanks to its characteristics, the beamline finds applications in a wide range of scientific fields such as surface and materials sciences, chemistry, biology, geosciences and cultural heritage.

LUCIA saw its first photons in 2004 at SLS in Switzerland, 2024 will mark 20 years of scientific activity.
The aim of this workshop is to gather scientists from the various communities using LUCIA's capabilities, so that we can share our experiences together.
It will include scientific presentations (invited and contributed) from users and a poster session. Presentations from the beamline staff followed by a round table will foster discussions on the beamline's future prospects in the context of the upgrade of SOLEIL.

The workshop will be held at the SOLEIL synchrotron, Saint Aubin, on June 20-21, 2024.

More information is available in the web page
https://intranet.synchrotron-soleil.fr/fr/evenements/lucia-20-ans

PARALLEL SESSIONS

PARALLEL SESSION

Advanced Materials

(Structure / Electronic Properties /Surfaces & Interfaces)

SOLEIL - Main Building

Thursday, January 18th

Chairpersons:

A. Bordage, D. Pierucci, F. Cheynis, S. Gonzalez

IT-01	10 years operations of the GALAXIES beamline: Status and perspectives ***Jean-Pascal Rueff***
OC-01	Combining Synchrotron single-crystal and powder diffraction data to tackle highly complex structures of MOFs ***Nathalie Guillou***
OC-02	Investigation of magneto-optical van der Waals magnet via correlative spectroscopic techniques ***Victor Porée***
OC-03	Two pathways of frosting on surfaces with varying wettability as seen by GIWAXS ***Patrick Kekicheff***
IT-02	Band engineering of earth abundant materials for efficient solar water splitting ***Dana Stanescu***
OC-04	Site occupancies in the quinary Co–Cr–Fe–Mn–Ni σ phase using resonant diffraction and EXAFS ***Jean-Marc Joubert***
OC-05	Influence of the crystal structure and nature of the ligands on the valence of uranium in chalcogenides compounds. ***Thomas Stephant***
IT-03	The electrodynamics properties of superconducting $Nd_{0.8}Sr_{0.2}NiO_2$ nickelate ***Stefano Lupi***

PARALLEL SESSION

Advanced Materials
(Structure / Electronic Properties /Surfaces & Interfaces)

SOLEIL - Main Building

Friday, January 19th

Chairpersons:

A. Bordage, D. Pierucci, F. Cheynis, S. Gonzalez

IT-04	Spin crossover in self-assembler monolayers ***Patrick Rosa***
OC-06	Synchrotron-based infrared studies of transition metal dichalcogenides at high pressure ***Béatrice D'Alò***
OC-07	Electric field-driven phase transition in antiferroelectric PbZrO3 by in situ X-ray diffraction ***Alexandre Zing***
OC-08	Using Synchrotron Radiation for probing the energy landscape of nanocrystal-based optoelectronic devices in situ and operando ***Erwan Bossavit***

10 Years Operations of the GALAXIES Beamline: Status and Perspectives

J-P. Rueff[1], J. Ablett[1], D. Céolin[1]

1. Synchrotron SOLEIL, L'Orme des Merisiers, Départementale 128, 91190 Saint-Aubin

ABSTRACT

The GALAXIES beamline is dedicated to RIXS and HAXPES x-ray spectroscopic techniques in 2-12 keV energy range [1]. The beamline has been successfully operated for 10 years, hosting more than 200 experiments in various fields of research including quantum materials, high pressure phenomena, chemistry and battery science, fundamental processes and cultural heritage. The beamline instrumentation has been continuously improved since the beginning to provide new monochromators, spectrometers, and samples environments, thus enlarging the beamline experimental capabilities. We will review here the present status of the GALAXIES beamline and discuss about future perspectives specially in connection to SOLEIL II.

REFERENCES

1. J.-P. Rueff et al., J. Synchrotron Rad. 22 (2015), 175

Combining Synchrotron Single-crystal and Powder Diffraction Data to Tackle Highly Complex Structures of MOFs

S. De[a], G. Mouchaham[b], F. Liu[a], M. Affram[b], B. Abeykoon[a], E. Janneau[a], N. Guillou[b], A Fateeva[a] and T. Devic[c]

[a]*LMI, UMR CNRS 5615, Université Claude Bernard Lyon 1, Villeurbanne, France*
[b]*ILV, UMR CNRS 8180, UVSQ, Université Paris-Saclay, Versailles, France*
[c]*IMN, UMR CNRS 6502, Université de Nantes, Nantes, France*

ABSTRACT

Because of guest adsorption/desorption properties combined to light absorption and electron transfer, porphyrin based Metal–Organic Frameworks (MOFs) have generated a growing interest.[1] This study deals with the structural investigation of two new porous MOFs based on trivalent cations (Al, Ga, In) and the H_{10}TcatPP and NiH_8TcatPP porphyrin ligands, functionalized with tetracatecholate coordinating groups.[2] Synchrotron single-crystal and powder diffraction data analyses were all undertaken on the CRISTAL Beamline at SOLEIL. The MOF obtained with Ga^{3+} and Al^{3+} crystalizes in an orthorhombic unit cell [*S.G.* $P2_12_12_1$, a = 21.7828(2), b = 21.7555(2), c = 39.3019(2) Å, V = 18625.0(2) Å^3 for GaNiTcatPP], whereas that obtained with In^{3+} crystallizes in a trigonal one [*S.G.* $P3c1$, a = 28.5321(3), c = 29.1054(2) Å, V = 20519.7(4) Å^3 for InNiTcatPP]. They present both 3-D structures, with **cds** and **stp** topologies, for Al^{3+}/Ga^{3+} and In^{3+} MOFs, respectively. The two materials present original redox properties and accessible porosity (BET surface area larger than 2000 $m^2.g^{-1}$ for the In^{3+} compound), which could be further exploited, despite the modest chemical stability of the compounds.

Structural characterization of these two new porphyrinic phases was non-trivial and presented significant challenges. Indeed, it was necessary to use a comprehensive approach that integrates both single crystal and powder diffraction techniques complemented by spectroscopic analysis (NMR, EPR, UV-vis). In particular, the structural determination of Al^{3+}/Ga^{3+} MOFs, which crystallize in a pseudo tetragonal unit cell, relied on powder diffraction to accurately determine the unit cell parameters and detect the orthorhombic symmetry, without which the single crystal data could never have led to the structural model, even with synchrotron data. On the other hand, the major impact of the pore content on powder data hindered the achievement of a complete structural model through this technique alone, requiring information gained from single crystal diffraction and spectroscopy.

REFERENCES

1. S. De, T. Devic and F. Fateeva, *Dalton Trans*, 1166-1188 (2021).
2. S. De *et al., J Mater Chem. A.*, in press, DOI: 10.1039/D3TA04490D (2023).

Investigation of Magneto-optical van der Waals Magnet via Correlative Spectroscopic Techniques

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ABSTRACT

Magnetic van der Waals (vdW) materials have attracted significant attention over the last decade. Thanks to their quasi-2D behavior, the possibility to control the number of layers and to construct vertical heterostructures, these systems offer vast possibilities to explore new physics and design advanced spintronic devices.

In this context, Cr-based vdW magnets display a great potential thanks to their optical and magnetic characteristics [1,2]. We focus here on the vdW antiferromagnet CrSBr. Its stability in air, together with its unique magnetoelectric coupling properties, makes this system one of the most promising materials for future optoelectronic applications. At low temperature CrSBr show a transition from a paramagnetic to an anti-ferromagnetic (AFM) phase, composed by anti-ferromagnetically coupled ferromagnetic (FM) layers stacked along the **c**-axis. Moreover, this system was shown to support optically active Wannier exciton resonances near 1.35 eV. The associated photo-luminescence (PL) can be tuned in energy and shape by strain [3], number of layers and by driving the system from AFM to FM phase upon the application of a relatively weak magnetic field of a few hundreds of mT [4,5].

In order to gain further insights into the mechanisms involved in CrSBr's PL and to correlate it to the electronic structure of the system, we combined Resonant Inelastic X-ray scattering (RIXS) with X-ray excited optical luminescence (XEOL). We will show how the linear dichroism observed in RIXS and modeled by mean of crystal field calculations allowed us to determine the chromium crystal field scheme. Aiming to correlate magnetic properties and the PL behavior we have measured both RIXS and PL under the application of a magnetic field and were able to observe the AFM to FM transitions with both spectroscopies. Finally, this work underlines the usefulness of combining excitation and recombination spectroscopy techniques as well as the capabilities of the newly installed MAGELEC sample environment.

REFERENCES

1. Seyler, K.L., Zhong, D., Klein, D.R. et al. Nature Phys 14, 277–281 (2018).
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Two Pathways of Frosting on Surfaces with Varying Wettability as seen by GIWAXS

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ABSTRACT

Ice accretion on surfaces have significant implications: it can cause hazardous road conditions, induce stall aircraft engines, weight down power lines, add challenges on ships and off-shore platforms, reduce the performance of energy generation by wind turbines, etc. Surface icing and frost / rime formation are common sources for such occurrences in cold regions. The need of protecting outdoors equipment and infrastructure elements has stimulated the development of anti-icing systems and coatings in the last decade.[1-4] It has been noted in the literature that one of the most effective anti-icing methods is the use of passive superhydrophobic coatings because of the synergetic action of several mechanisms which minimize the accumulation of supercooled water and ice on the surface.[5]

Despite their significance, the processes of water condensation and desublimation on solid surfaces under supersaturation are not well understood due to the lack of methods that can provide insight into the first stages of phase transitions. Taking advantage of synchrotron Grazing-Incidence Wide-Angle X-ray Scattering (GIWAXS) on SIRIUS, two pathways of the frosting process are studied in real time for substrates with different wetting properties from highly hydrophilic to hydrophobic and superhydrophobic, in supersaturated vapors at −18 °C. A fully quantitative structural and orientational characterization of the undergoing phase transition reveals the information on the very first stages of direct condensation or nucleation from vapor onto the substrates. The diversity of frosting scenarios, including direct desublimation from the vapor and two-stage condensation–freezing processes are observed for different combinations of substrates wettability and vapor supersaturations. To explain this diversity, the nucleation theory is called for. Our analysis shows that the classical theory with the usual approximation setting equality of contact angles for liquid and solid nucleus can be successfully applied to accurately predict the type of phase transition for the systems, where the change in Gibbs free energy required for nucleating a critical embryo $\Delta G(\text{water/ice})^*$ essentially exceeds the k_BT. Thus, the theory correctly predicts the phase transitions for hydrophobic and superhydrophobic substrates. In contrast, for hydrophilic substrates, when $\Delta G(\text{water/ice})^*/k_BT < 1$, the nucleus contact angle for water must be smaller than that for ice to get the correct prediction.

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Band Engineering of Earth Abundant Materials for Efficient Solar Water Splitting

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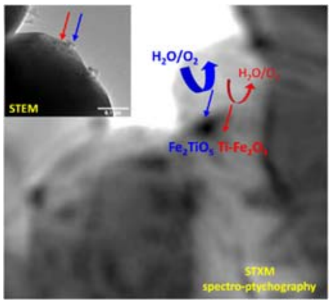
ABSTRACT

Hydrogen production by solar water splitting is a very attractive idea because it allows storing solar energy in the H_2 molecules using a clean method. First demonstration of solar water splitting was reported in 1972 using TiO_2 as photoanode[1]. Since then, plethora of studies were reported, owing to materials chemists' infinite imagination, addressing different classes of photosensitive materials including semiconducting oxides, III-V semiconductors[2], MOF (metal-organic framework) architectures[3], ferroelectric materials[4], etc. Band engineering is often employed targeting the same single aim: enhance the efficiency of the photoelectrochemical reactions, increasing thus hydrogen production efficiency in a solar water splitting process.

We report here a simple band engineering approach applied to one of the most Earth abundant materials, the hematite, using Ti doping[3-6] and controlled annealing atmosphere. Enhanced photocurrent was obtained, mediated by surface states, as evidenced using electrochemical impedance spectroscopy. We found strongly enhanced photocurrent, of more than 200 %, for Ti-doped hematite photoanodes annealed under Nitrogen compared to equivalent photoanodes annealed in air[6]. The nanoscale origin of the increased photocurrent was addressed using combined XPEEM, STXM, X-rays spectro-ptychography and STEM. Shadow XPEEM alone can be used to discriminate surface and bulk contributions of the chemistry and chemical coordination. STXM complement successfully these results evidencing formation of Ti-rich clusters for photoanodes annealed in O_2-free atmosphere. Spectro-ptychography allows to better identify and isolate both spatially and chemically Ti-rich clusters. X-ray spectromicroscopies altogether were confronted with STEM measurements and DFT calculations, the results suggesting formation of pseudo-brookite clusters at the surface of the Ti-doped hematite.



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Site Occupancies in the Quinary Co–Cr–Fe–Mn–Ni σ Phase using Resonant Diffraction and EXAFS

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ABSTRACT

The σ phase [1] forms in many systems of technological interest, e.g., in steels, nickel-based superalloys and high entropy alloys [2-3] with negative effects related to its extremely fragile nature. The prediction of its stability and properties is therefore very much relevant and goes through the determination of its fine crystallographic properties. The phase crystallizes in the space group *P*4$_2$/*mnm* with 30 atoms distributed on 5 different sites on which a very high degree of occupancy disorder exists [1]: all sites can be occupied by all elements, each in different proportions. For a multi-component σ phase such as $Cr_{46.0}Mn_{15.2}Fe_{16.3}Co_{17.0}Ni_{5.5}$, the experimental determination of site occupancies is extremely challenging because of the large number of sites (5) and elements (5), which, additionally, show very low contrast in X-ray diffraction. We have used three different techniques:

- a crystallographic technique: joint Rietveld refinement of resonant diffraction data measured at CRISTAL-SOLEIL and collected at the 5 K-edges of the 5 respective elements
- a spectroscopic technique: XANES and EXAFS measured at LISA-ESRF
- a calculation technique: DFT coupled with machine learning [4].

The results [5] obtained from the three techniques are in very good agreement and show an atomic site distribution consistent with what is observed in the σ phase present in some of the binary systems.

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Influence of the Crystal Structure and Nature of the Ligands on the Valence of Uranium in Chalcogenides Compounds

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ABSTRACT

Thanks to its 5*f* orbitals, uranium benefits from several valence states, from U^{3+} to U^{6+}, in inorganic compounds and possesses a wide crystal-chemistry. The radial expansion of these orbitals leads to energetically close crystal field (dominating in the case of 3*d* elements) and spin-orbit (dominating in the case of 4*f* rare earths) interactions, and subsequent rich and exotic physical properties [1] (e.g. coexistence of superconductivity and ferromagnetism). Associated with a chalcogen element (Q = S, Se, Te), uranium forms inorganic compounds characterized by various crystallographic structures leading to unique uranium polyhedral structures [2] with e.g. the presence of $(S^2)^{2-}$ dimers.

However, due to the limited number of known uranium chalcogenides, practically no experimental information on the nature of the U-Q bond is available in the literature. As a consequence, understanding the localization of 5*f* electrons of actinides in solid-state, a great challenge for theoretical physicists, remain limited to the study of oxides [3] and intermetallic materials.

To increase the field of investigation, some binary uranium chalcogenides (S, Se, Te) have been characterized and studied by HERFD-XANES and RIXS spectroscopies at the U M4 edge. These preliminary measurements enabled us to determine the oxidation states of uranium for these binary compounds. Moreover, in the case of sulfide compounds, the study has been extended to ternary compounds from U-M-S systems (M = 3*d* metal) [4] with the aim to investigate their physical properties and to have a more general understanding of the chemistry of such class of materials.

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The Electrodynamics Properties of Superconducting $Nd_{0.8}Sr_{0.2}NiO_2$ Nickelate

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ABSTRACT

The intensive search for alternative non-cuprate high-transition-temperature (Tc) superconductors has taken a positive turn recently with the discovery of superconductivity in infinite-layer nickelates. This discovery is expected to be the basis for disentangling the puzzle behind the physics of high Tc in oxides. In the unsolved quest for the physical conditions necessary for inducing superconductivity, we report on a broad-band optical study of a $Nd_{0.8}Sr_{0.2}NiO_2$ film measured using optical and Terahertz spectroscopy, at temperatures above and below the critical temperature Tc ~ 13 K. The normal-state electrodynamics of $Nd_{0.8}Sr_{0.2}NiO_2$, can be described by a scattering time at room-T (t=1.3 × 10−14 s) and a plasma frequency (ωp =5500 cm−1) in combination with an absorption band in the Mid-Infrared (MIR), characteristics of transition metal oxides, located around ω0 ~ 2500 cm−1 and with an amplitude ωMIR of about 8000 cm−1 . The degree of electronic correlation can be estimated using the ratio ω2 p /(ω2 p + ω2 MIR). In the present system, this value is about 0.32 indicating a strong electron correlation in the NiO2 plane with a similar strength as cuprates. From 300 K to 20 K, we observe a spectral weight transfer between the Drude and MIR band, together with a strong increase in the Drude scattering time, in agreement with DC resistivity measurements. Below Tc, a superconducting energy gap 2Δ ~ 3.3 meV can be extracted from the Terahertz reflectivity using the Mattis-Bardeen model at finite temperature

Spin Crossover in Self-assembler Monolayers

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ABSTRACT

Spin crossover complexes (SCOs) are transition metal complexes that exhibit reversible state switching, often at ambient conditions. In iron (II) complexes, switching occurs between a diamagnetic low spin state ($S=0$) and a paramagnetic high spin state ($S=2$). The switching is accompanied by a change in the electronic properties, such that molecular junctions of these SCOs exhibit a change in conductance with the spin state[1].

Preparing ultrathin films of SCO complexes has been performed so far mainly through PVD techniques[2], limiting thus seriously the potential molecules (neutral, low-weight,…) and offering limited control on the films morphology, when transport measurements require continuous films[3]. We aim to circumvent this issue by using complexes enabling chemical grafting, in order to prepare Self-Assembled Monolayers (SAMs). Indeed SAMs enable chemically specific modifications of a surface and find increasing application in standard electronics.

We have thus prepared a library of functionalised iron (II) SCO complexes with different spin crossover behaviours in the bulks. With these SCOs we have prepared SAMs that were characterized physically and chemically by a variety of surface techniques (ToF-SIMS, PM-IRRAS, XPS). We used the excellent sensitivity of the DEIMOS beamline to measure XANES and XMCD at the Fe $L_{2,3}$ edges to evidence temperature- and photo-induced switching for those SAMs on Au and Cu substrates. We are now fabricating molecular junctions using eutectic gallium indium (EGaIn) as a conforming top electrode, thus with hopes to bring SCOs closer to applications in molecule-based electronics.

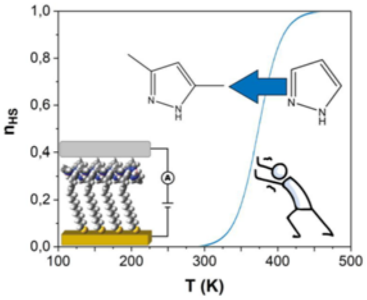

Fig. 1 Tuning the SCO temperature is possible by playing upon steric hindrance around the transition metal

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Synchrotron-based Infrared Studies of Transition Metal Dichalcogenides at High Pressure

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ABSTRACT

Semiconducting Transition Metal Dichalcogenides (TMDs) are constituted by three-atom-thick layers held together by weak inter-layer van der Waals (vdW) interactions. Despite their feeble intensity, vdW forces highly influence the electronic properties of TMDs, such as the direct/indirect nature of the bandgap and its energy [1, 2]. High-pressure (HP) represents a clean and direct tool to enhance the vdW inter-layer interactions in TMDs, enabling to tune their electronic properties: pressure reduces the gap energy, even inducing the metallization of these systems.

In the last few years, we investigated the HP evolution of different semiconducting TMDs by performing synchrotron-based infrared (IR) spectroscopy at the SMIS and AILES beamlines of synchrotron SOLEIL [3-5]. Due to the micrometric size of the TMD single crystals required for HP experiments, the high brightness and the micrometric spot of the synchrotron radiation represented a key element in collecting the IR spectra of our samples. The resulting data provided us with novel insights into the pressure-driven metallization of TMDs. Transmission measurements allowed us to identify not only the gap closure but also new spectral indicators for the onset of the metallic state. Among them, the pressure-evolution of the Fano asymmetric lineshape of the IR-active E1u phonon suggested that the electrons in the metallic state originate from n-type doping levels, revealing the fundamental role played by intrinsic doping in the metallization process of TMD crystals. Combining our results with those reported in the literature, we hypothesized a two-step mechanism is at work in the TMD metallization process, in which the pressure-induced hybridization between doping and conduction band states drives an early metallic behaviour, while the band gap closes at higher pressures [4,5]. Finally, some recent results concerning a HP broadband IR investigation of tin-based TMD single crystals will be presented, which was recently suggested to host periodic lattice modulations in the HP regime.

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Electric Field-driven Phase Transition in Antiferroelectric PbZrO3 by *in situ* X-ray Diffraction

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ABSTRACT

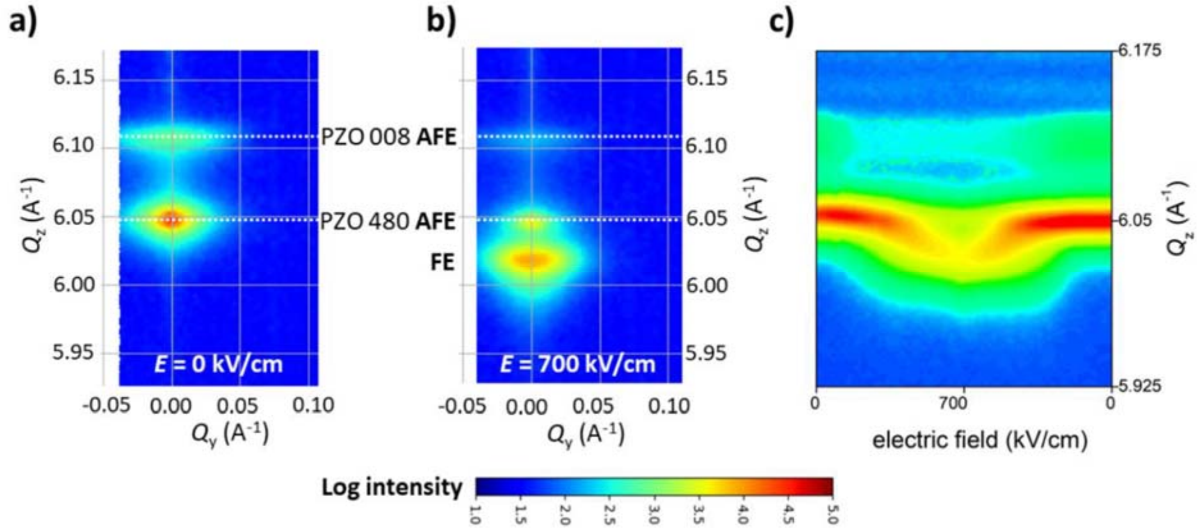

Figure: Reciprocal space maps around PZO 480 and 008 at a) 0 kV/cm and b) 700 kV/cm applied E-field, and c) Qy = 0 cut as a function of E-field from 0 to 700 kV/cm and back to 0.

Antiferroelectric (AFE) materials are electronic materials actively studied for their potential applications such as in high energy storage capacitors, high-strain transducers and actuators, and electrocaloric devices [1]. A microscopic picture for the AFE behavior proposed by Kittel [2] involves an antiparallel dipole alignment in adjacent cells, which yields zero net polarization in the absence of an applied electric field E and no piezoelectric activity. Transition to the ferroelectric (FE) phase under E-field application is a result of dipoles aligning in one direction, accompanied by a sharp change in volume and strain. Up to now, this transition has mainly been investigated at the macroscopic scale, without any structural information.

In this work, we present the first *in situ* synchrotron X-ray diffraction of the structural evolution and induced strain of the E-field-driven AFE/FE phase transition in PbZrO3 (PZO) thin films. 3D reciprocal space maps were recorded in the vicinity of the PZO 480 and 008 Bragg reflections during the application of E up to 700 kV/cm in steps of 20 kV/cm (Figure). Intrinsic strain values of up to 0.3% in the ferroelectric phase were determined at highest E, with a hysteretic behavior of the transformation process, and we observed an unexpected effect on the antiferroelectric phase under electric stimulus.

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Using Synchrotron Radiation for Probing the Energy Landscape of Nanocrystal-based Optoelectronic Devices *in Situ* and *Operando*

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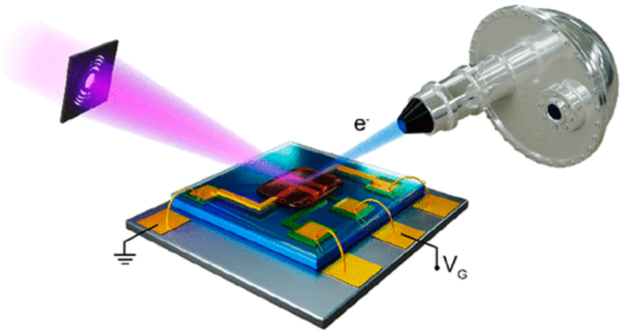
ABSTRACT

In the span of the last few years, significant progress has been made toward the integration of nanocrystal-based materials into efficient and high-performance optoelectronic devices. However, up to now most of the progress made toward these goals has been based on trial-and-error approaches. The new generation of optoelectronic devices will thus require a deeper understanding of the internal mechanisms at play during operation, to enable a rational approach of device optimization. To further this goal, we tested and demonstrated, through a series of experiments, the strong potential of soft X-ray photoemission microscopy as a probing tool for the energy landscape of nanocrystal-based device.

Using this technique, we were able to unveil *in situ*[1] the effect of differently doped materials on nanocrystal films, and to investigate *operando* the changes in the energy landscape of several device geometries, including field effect transistors[2] and photoconductor sensors[3]. To further demonstrate the applicability of this technique we also probed several different materials this way.



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PARALLEL SESSION

Dynamic, Reactivity & Chemical analysis
(Diluted Matter & Chemistry)

SOLEIL - Reception Building Auditorium
Ground Floor & PA.1.12 Rooms

Thursday, January 18th

Chairpersons:

A. Tougerti, F. Carn, H. Dossmann, P. Asselin

IT-05	Weakly bound systems of chemical and biological relevance probed by double imaging photoelectron photoion coincidence spectroscopy ***Sebastien Hartweg***
OC-09	Induced photoelectron circular dichroism onto an achiral chromophore ***Etienne Rouquet***
OC-10	Experimental study of polarization-dependent PCI effect in neon and water following K-shell photoionization ***Abhishek Verma***
OC-11	A time-resolved mechanistic study into the effects of a partially-hydroxylated surface during atomic layer deposition of HfO_2 on Si(111) ***Rosemary Jones***
OC-12	Rovibrational spectroscopy of gas phase precursors of secondary organic aerosols from high resolution synchrotron-base Fourier transform and QCL infrared measurements ***Arnaud Cuisset***
OC-13	Carburization, passivation and re-activation of Mo- and Ni/Cu-Mo-based catalysts for the upgrading of furfural: A time-resolved, in-situ XAS study ***Eric Marceau***
OC-14	Application of photoelectron spectroscopy to uracil and bromouracil molecules in liquids ***Marine Fournier***
OC-15	Evidencing an elusive conical intersection in the dissociative photoionization of methyl iodide ***Sonia Marggi Poullain***

PARALLEL SESSION

Dynamic, Reactivity & Chemical analysis

(Diluted Matter & Chemistry)

SOLEIL - Reception Building Auditorium
Ground Floor & PA.1.12 Rooms

Friday, January 19th

Chairpersons:

A. Tougerti, F. Carn, H. Dossmann, P. Asselin

IT-06	XAS Hyperspectral Imaging at the ROCK beamline: Adding micrometer spatial resolution to second time resolution for chemical transformation monitoring. ***Valérie Briois***
OC-16	Electrochemical and structural study of NiRux heterofunctional catalysts for the alkaline HER **Marie-Sophie Dias Fernandes**
OC-17	Spectroscopic and kinetic studies of X-ray and UV induced desorption from molecular ices ***Daniela Torres-Díaz***
OC-18	THz spectroscopy of radical species using the heterodyne receiver of the AILES beamline ***Luan Juppet***

Weakly Bound Systems of Chemical and Biological Relevance Probed by Double Imaging Photoelectron Photoin Coincidence Spectroscopy

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ABSTRACT

Many sample systems of chemical or biological relevance occur naturally in the solution phase, imposing challenges to the application of photoelectron spectroscopy and other techniques typically used on gas phase samples to obtain deep physical insights. Experiments on small non-covalently bound clusters can in principle be used to bridge this gap between the gas phase and condensed phases. This approach, however, requires a method to obtain cluster size resolved photoelectron and photoion data. Double imaging photoelectron photoion coincidence (i2PEPICO) spectroscopy has been successfully used on the DESIRS beamline of SOLEIL synchrotron to obtain such cluster size resolved data.

After briefly introducing the DELICIOUS III spectrometer, available on the DESIRS beamline, I will cover the requirements that need to be fulfilled in order to obtain cluster size resolved data. Subsequently, I will present our recent work on the dissociative photoionization of the hydrogen-bonded nucleobase pair Adenine-Thymine [1], emphasizing the possibilities created by the kinetic energy resolved detection of photoions in coincidence with photoelectrons. As a second example, I will present the identification of dynamic processes of solvated electrons in sodium ammonia clusters. These processes, triggered by the absorption of VUV photons, include the formation of spin-paired solvated electron pairs and their subsequent decay as well as the transfer of a solvated electron to the ammonia valence shell.

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Induced Photoelectron Circular Dichroism onto an Achiral Chromophore

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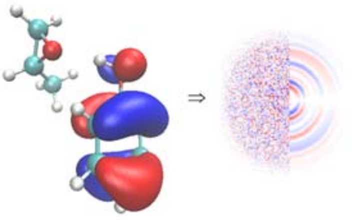
ABSTRACT



Ionisation of achiral phenol ⇒ Induced PECD

Photoelectron Circular Dichroism (PECD), the forward/backward asymmetry in the angular distribution of the electrons resulting from the ionization of a chiral molecule by circularly polarized light [1], is a very sensitive probe of molecular structures [2, 3, 4]. While PECD has been historically studied using synchrotron radiation, the field of fs and ns[5] laser-based PECD is now blooming. By using a ns-laser and a resonance-enhanced multiphoton ionization energy scheme, it is possible to selectively ionize different conformers of the same molecule in the gas phase, which enhances the analytical potential of PECD. However, one major drawback of this approach is the need for an accessible excited electronic state, *i.e.* the presence of a chromophore within the molecule.

To tackle this challenge, we complexed the chiral species to be studied, which does not bear a chromophore, with a non-chiral moiety with a chromophore. In this context, we could demonstrate a induced PECD from methyloxirane (MOx) *onto* the achiral chromophore phenol (PhOH)[6] . Indeed the formed PhOH-MOx complexes whose structure and orbitals were previously calculated, exhibits a non-chiral HOMO located solely on the PhOH moiety. However, we recorded a non-zero chiroptical response originating from the ionization of such a non-chiral HOMO of the complex, due to the electron scattering off offered by the chiral molecular potential of MOx to the PhOH departing electron. Such a method enlarges the scope of PECD as an analytical tool, allowing to gain extensive molecular information of chiral molecule, as well as conformer-specific chiroptical response for virtually any system in the gas phase. On a more fundamental point of view, our results demonstrate the very long range of PECD across inter-molecular distances, here of ~ 5 Å.

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Experimental Study of Polarization-dependent PCI Effect in Neon and Water following K-shell Photoionization

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ABSTRACT

***Keywords**: Photoelectron, post-collision interaction, polarization, recapture of photoelectron*

Photoionization of an atom near the ionization threshold of an inner shell induces the emission of a slow photoelectron, followed by the emission of a high kinetic energy Auger electron during the subsequent relaxation process, leading to the atom acquiring a doubly positive charge [1]. The three-body interaction between the emitted electrons and the ion involves energy and angular momentum exchange [2]. This phenomenon is termed post-collision interaction (PCI). Despite more than three decades of study [3], a comprehensive understanding of PCI remains elusive. In a pursuit to refine our understanding of PCI, our experimental investigation focuses on delineating various aspects of this interaction, particularly the exchange of energy and angular momentum. The study is specifically conducted on neon atoms and water molecules, two isoelectronic species in the gas phase, examining the O 1s edge for water and the 1s edge in neon. Slow photoelectron spectra, recorded using polarized light at energies above the ionization thresholds, were analyzed. The experimental setup utilized the PLEIADES beamline at SOLEIL, providing access to the relevant soft X-ray energy range with high energy resolution and variable polarization. A SCIENTA analyzer permitted the recording of spectra at high resolution. Our observations reveal a significant PCI shift for both neon and water, depending on the photon energy. Moreover, a more pronounced effect was observed with horizontally polarized X-rays compared to vertically polarized X-rays at identical photon energies. Notably, the considerable energy exchange in neon 1s ionization led to the recapture of photoelectrons in higher Rydberg states.

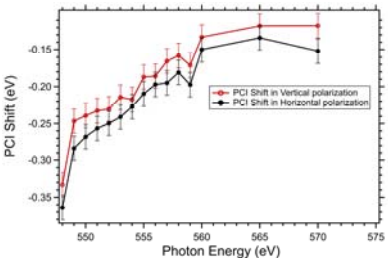

Figure 1: Energy shift observed for water vapor above the Oxygen 1s edge. The graphical representation is asfollows: The X-axis denotes the post-collision interaction (PCI) shifts, while the Y-axis shows the photon energy. The red curve, marked with circles, shows the PCI shift under vertical polarization, and the black curve, annotated with dots, shows the PCI shift under horizontal polarization.

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A Time-resolved Mechanistic Study into the Effects of a Partially-hydroxylated Surface during Atomic Layer Deposition of HfO_2 on Si(111)

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ABSTRACT

The introduction of atomic layer deposition, ALD, to the microelectronics industry has introduced a large number of new possible materials, able to be deposited in layers with atomic thickness control. One such material is the high-κ oxide HfO_2; thermally stable and ultrathin HfO_2 films deposited by ALD are a significant contender to replace SiO_2 as the gate oxide in capacitor applications. In such a device the typical support remains Si, and thus the HfO_2 gate oxide/Si interface is an integral part of the device. The characteristics of this interface can dramatically affect the overall performance of the device itself. We present a mechanistic study of the first deposition cycle of HfO_2 on the Si(111) surface using tetrakis(dimethylamido) hafnium (TDMA-Hf) and water as precursors using operando ambient pressure x-ray photoelectron spectroscopy (APXPS). This methodology allows to observe the chemical reactions in a time-resolved manner, giving details of mechanism and kinetics of the reaction. It is found that even low levels of moisture contamination at the 1×10^{-6} mbar level can dramatically affect the substrate and therefore the initial ALD cycle. Here, we show that the hydroxylation of the clean Si(111) surface by residual water vapour, resulting in a 0.3 monolayer coverage of hydroxyls, leads to instantaneous full surface coverage of TDMA-Hf. The change in the atomic ratio of Hf to C/N found during the first deposition half-cycle, however, does not match the assumed immediate ligand loss through reaction with surface hydroxyls. One would expect an immediate loss of ligands, indicated by a Hf:N ratio of approx. 1:3 as TDMA-Hf deposits onto the surface, however, a Hf:N ratio of 1:3.6 is observed. The partial hydroxylation on the Si(111) surface leads to binding through the TDMAHf ligand N atoms resulting in both N and CH_3 being found remaining on the surface post water half cycle. Although there is evidence of ligand exchange reactions occurring at Si-OH sites it also seems that N binding can occur on bare Si, highlighting the complexity of the substrate/precursor reaction even when hydroxyls are present. Moreover, the initial low coverage of Si-OH/Si-H appears to severely limit the amount of Hf deposited which we hypothesise is due to the specific geometry of the initial arrangement of Si-OH/Si-H on the rest and ad atoms.

Considering the majority of Metal/H_2O ALD reactions start with a hydroxylation step, this study brings attention to the importance of the hydroxylation itself. That even with fast pulse regimes there is no guarantee of only reaction at hydroxyl sites. How surfaces react with a water pulse is of utmost importance to the properties of the deposited film.

Rovibrational Spectroscopy of Gas Phase Precursors of Secondary Organic Aerosols from High Resolution Synchrotron-base Fourier Transform and QCL Infrared Measurements

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ABSTRACT

Oxygenated Volatile Organics Compounds (OVOCs) are a significant component of biomass burning emissions which mainly exists in our atmosphere in the gas phase where they contribute to the formation of secondary organic aerosols (SOAs). Rovibrational spectroscopy is a promising tool to monitor atmospheric OVOCs and infer their role in SOA formation.

In this presentation we will report extensive jet-cooled rovibrational studies in the mid-IR region using two complementary set-ups, a continuous supersonic jet coupled to a high resolution Fourier transform spectrometer on the IR beamline of the SOLEIL synchrotron (JET-AILES)[1] and a pulsed jet coupled to a mid-IR tunable quantum cascade laser spectrometer (SPIRALES)[2].

In the case of methoxyphenol (MP) study[3], based on Q-branch frequency positions measured in the Jet-AILES FTIR spectra and guided by quantum chemistry calculations, we propose an extended vibrational and conformational analysis of the different MP isomers in their fingerprint region. Some modes such as far-IR out-of-plane –OH bending or mid-IR in-plane –CH bending allow us to assign individually all the stable conformers. Finally, using the SPIRALES setup with three different external cavity quantum cascade laser sources centered on the 930–990 cm−1 and the 1580–1690 cm−1 ranges, it was possible to proceed to the rovibrational analysis of the ring in-plane bending mode of the MP meta isomer providing a set of reliable excited state parameters, which confirms the correct assignment of two conformers.

In the case of furfural (FF) study[4], jet-cooled spectra recorded at rotational temperatures ranging between 20 and 50 K have been exploited to derive reliable excited state molecular parameters for tens of vibrational bands in the fingerprint region (700-1750 cm^{-1}). These parameters allow reproducing the mid-IR spectra at any temperature and any instrumental resolution at the experimental accuracy. Such an approach evidenced the major contribution of hot bands in the room temperature mid-IR FF spectra, which represents about 50% of the fundamental bands.

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Carburization, Passivation and Re-activation of Mo- and Ni/Cu-Mo-based Catalysts for the Upgrading of Furfural: A Time-resolved, *in-situ* XAS Study

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ABSTRACT

Unsupported molybdenum carbides catalyze the hydrodeoxygenation (HDO) of furfural, and the addition of metal promoters, such as Ni or Cu, has been expected to orientate the reaction towards specific products. However, little work has been dedicated to their *supported* analogues. The nature of the phases exposed to reactants, not only after the carburization of Mo, but also after passivation in oxygen, a necessary step for the safe storage of the catalysts, and subsequent re-activation in H_2, has been undisclosed so far.

In the present work,[1,2] characterization by XAS of Mo_2C/SiO_2, $Ni\text{-}Mo_xC_y/SiO_2$ and $Cu\text{-}Mo_xC_y/SiO_2$ catalysts was carried out in a quartz capillary, in the transmission mode, at the ROCK Quick-XAS beamline, upon carburization in CH_4/H_2 (30-650°C) and re-activation of passivated catalysts in H_2 (30-400°C), in *in situ* and time-resolved conditions (recording frequency: 2 Hz), either at the Mo K-edge (20000 eV) for the monometallic system, or alternatively at the Ni (8333 eV) / Cu (8979 eV) and Mo K-edges for the bimetallic systems.

XAS applied to the calcined precursors evidenced MoO_3 in all cases; $\alpha\text{-NiMoO}_4$ was also identified on the Ni-Mo system (Ni K-edge: Ni at 2.97 Å, Mo at 3.17 Å). MCR-ALS analysis showed that carburization involved four successive groups of Mo species: (i) Mo(VI) oxides; (ii) Mo(IV to VI) suboxides; (iii) above 300 °C, weakly carburized $MoO_{2-x}C_x$; (iv) above 500°C, Mo_2C. Ni formed highly dispersed metallic particles (about 1 nm; N(Ni) = 6.8) in strong interaction with Mo_2C. Cu metallic particles formed at 200 °C, vs. 300 °C for Ni, and were larger in size than Ni (N(Cu) = 9.0). The presence of Ni did not change the reduction and carburization temperatures, but Cu lowered the reduction temperature of Mo(VI) by 100°C.

Upon passivation, a severe oxidation of Mo was evidenced, while Ni and Cu were oxidized to Ni^{2+} and Cu^{2+}. The fraction of Mo(VI) was evaluated by linear combinations of standard spectra: 27% on Mo_2C/SiO_2, 41% on $Ni\text{-}Mo_xC_y/SiO_2$, 62% on $Cu\text{-}Mo_xC_y/SiO_2$.

The reactivation under H_2 of the passivated catalysts was interpreted by a MCR-ALS analysis based on the spectral components extracted during carburization: Ni and Cu were reduced between 120 and 300°C, Mo_2C was restored between 200 and 400°C. However, $Cu\text{-}Mo_xC_y/SiO_2$ appeared as strongly decarburized (the best fit involves metallic Mo), and a Ni-Mo alloy was suggested for $Ni\text{-}Mo_xC_y/SiO_2$. This relates to the low selectivity of $Cu\text{-}Mo_xC_y/SiO_2$ in furfural HDO, and the high activity of $Ni\text{-}Mo_xC_y/SiO_2$ compared to Mo_2C/SiO_2.

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Application of Photoelectron Spectroscopy to Uracil and Bromouracil Molecules in Liquids

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ABSTRACT

The knowledge of the electronic structure and the ionization energy are shaping the behaviours of molecules. Our study aimed to determine the influence of solvation on the electronic structure of uracil, a RNA nucleobase and one of its derivatives, the 5-bromouracil. For this, soft X-rays electron spectroscopy has been used. The measurements have been performed using synchrotron radiation (synchrotron SOLEIL) and an under-vacuum liquid jet, coupled with and electron spectrometer, available on PLEIADES beamline[1]. With this configuration, it is possible to probe about three molecular layers at the surface of the liquid, which means that our measurements are very are surface-sensitive. The 1s electronic core level of carbon and nitrogen have been probed in two different pH conditions (basic and neutral). The recorded photoelectrons spectra of solvated uracil in neutral condition are closely similar to the ones obtained on water-uracil clusters[2]. The comparison between photoelectrons spectra at each pH condition reveals some binding energies differences of the peaks in the photoelectron spectra that could illustrate a modification of the chemical environment. Additionally, information on the Lowest Unoccupied Molecular Orbital (LUMO) electronic level has also been retrieved. A tentative of deciphering the different de-excitation pathways following a photoexcitation of a 1s electron, from carbon or nitrogen, to the LUMO, highlighted the complexity to interpret such data obtained in liquid phase.

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Evidencing an Elusive Conical Intersection in the Dissociative Photoionization of Methyl Iodide

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ABSTRACT

Radiationless transitions between electronic states of the same multiplicity, referred to as internal conversion (IC), constitute a universal first step in the photo-induced dynamics of polyatomic systems leading afterwards to a variety of outcomes including dissociation or isomerization. The topology characterizing the potential energy surfaces of the electronic states involved directly determines the efficiency and the associated timescale of this type of process. For instance, IC in prebiotic molecules1 is often mediated by the presence of conical intersections leading to an efficient fast decay back into the ground state in a subpicosecond timescale, preventing thus any photodamage. In contrast, IC in other molecular systems, such as alkyl radicals2, occurs between bound electronic states where no curve crossing is located leading to a remarkably slow transfer of population. Here, in a joint experimental and theoretical investigation3, an elusive conical intersection is revealed to mediate IC from the first excited state into the ground state of ionic methyl iodide (CH3I+).

The valence-shell dissociative photoionization of methyl iodide (CH3I) is studied using double imaging photoelectron photoion coincidence (i2 PEPICO) spectroscopy in combination with highly-tunable synchrotron radiation from SOLEIL. The experimental results are complemented by new high-level *ab initio* calculations of the potential energy curves of the relevant electronic states of the methyl iodide cation (CH3I+).

An elusive conical intersection is found to mediate internal conversion from the initially populated first excited state, CH3I+(Ã 2*A*1), into the ground cationic state, leading to the formation of methyl ions (CH3+). The reported threshold photoelectron spectrum for CH3+ reveals that the □5 scissors vibrational mode promotes the access to this conical intersection and hence, the transfer of population. An intramolecular charge transfer takes place simultaneously, prior to dissociation. Upon photoionization into the second excited cationic state, CH3I+(B 2*E*), a predissociative mechanism is shown to lead to the formation of atomic I+.

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XAS Hyperspectral Imaging at the ROCK Beamline: Adding Micrometer Spatial Resolution to Second Time Resolution for Chemical Transformation Monitoring

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ABSTRACT

The high time-resolution provided by Quick-EXAFS beamlines operating on third generation synchrotron radiation facilities makes the technique powerful for revealing reaction pathways followed by catalysts and battery electrodes in working conditions. However, it is not rare to observe non-uniform spectroscopic responses - *e.g*. induced by reactant gradients within the catalytic reactor [1] or resulting from different ion transport rates during charge/discharge of the battery [2] - with side-effect to lead to inconsistency between the spectroscopic results and the global online analysis of materials performances. This explains the recent appealing for the developments made at some Quick-EXAFS beamlines [3-5] to offer micrometer-scale spatial resolution in addition to the second-scale time resolution and chemical speciation offered by X-ray Absorption Spectroscopy for *operando* characterization of such heterogeneous systems.

In this presentation, we will present the implementation at the ROCK-SOLEIL beamline of the Quick-EXAFS hyperspectral Full Field (FF) Imaging [6] based on the recording of the visible light emitted by a scintillator imaging the sample absorption by a pixelated CMOS camera (ORCA Flash 4.0 V3, Hamamatsu). The pixel size and Field of View (FoV) can range from 0.65 µm to 1.625 µm and 1.3 mm to 3.3 mm, respectively, with intrinsic beamline spatial resolution of ca. 5 µm. Around 600 images at different energies of the XAS spectrum are collected during the Quick-EXAFS monochromator energy scan yielding to one complete hyperspectral cube every 11 s. Post-processing for spectra normalization, spatial pixel binning or cube binning is based on Jupyter notebooks. Speciation in each cube is determined by Multivariate Curve Resolution with Alternating Least Square (MCR-ALS) analysis.

We will illustrate the capability of the full-field hyperspectral spatio-temporal technique implemented at ROCK for monitoring the preparation of catalysts [7], the regeneration of spent bimetallic catalysts [8], and the charge and discharge of $LiFePO_4$ electrodes.

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Electrochemical and Structural Study of $NiRu_x$ Heterofunctional Catalysts for the Alkaline HER

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ABSTRACT

The alkaline water electrolysis is a promising method to store intermittent energy sources while producing green hydrogen efficiently. Among the different technologies available, anion exchange membrane (AEM) electrolyzers has the advantage of functioning with catalysts based on non-noble metals. Indeed, the use of alkaline medium provides suitable chemical stability for a large range of materials such as transition metals, which significantly reduces the AEM cost and allows a large-scale use. However, the performances and stability observed for AEM catalytic films are lower due to the sluggish water dissociation step occurring during the hydrogen evolution reaction (HER). Therefore, the concept of heterofunctional catalysts emerged as an efficient approach to combine the properties of active materials and create a synergy between them in order to promote the dissociation of water. To do so, members of our team developed a new family of heterofunctional catalysts based on large particles of nickel decorated by ruthenium nanoparticles. XPS results indicate that ruthenium is mostly observed on the nickel surface (see figure 1.a), which supports a heterogeneous structure. We carried out electrochemical characterizations (cyclic voltammetry measurements and electrolyzer test) and the results showed very high efficiencies for this family of materials (see figure 1.b), with performances similar to the platinum ones (60% Pt/C). The materials structure was also analyzed by *operando* X-Ray Absorption Spectroscopy (XAS) at the Ni and Ru K-edges to identify which metals are involved in the catalysis at low and high ruthenium content (see figure 1.c). In this presentation, the electrochemical and XAS results will be presented as well as the relationship between the structure and activity of these materials.

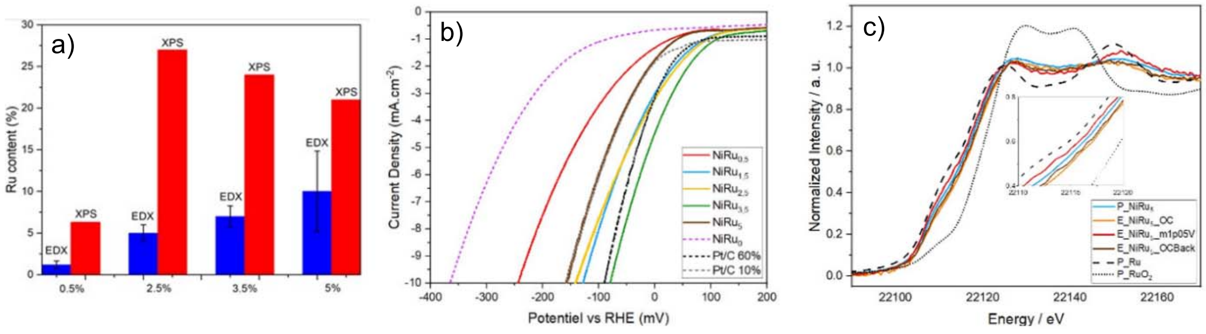

Figure 1: (a) The Ru content measured for the $NiRu_x$ samples by XPS and EDX; (b) cyclic voltammograms of the $NiRu_x$ and Pt/C 10% and 60% wt. references in 0.1 M KOH; (c) Operando XANES spectra registered for the NiRu5 and the references.

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Spectroscopic and Kinetic Studies of X-ray and UV Induced Desorption from Molecular Ices

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ABSTRACT

In the coldest regions (10 K – 100 K) of the interstellar medium, where stars and planets are formed, molecular matter exists mainly in the solid phase, forming ices on the surface of dust grains. However, several molecules have been detected in the gas phase in quantities that cannot be explained without considering non-thermal desorption mechanisms [1,2]. Among these mechanisms, photon-induced desorption has been widely studied, especially UV-induced desorption and, more recently, X-ray-induced desorption. However, most of the experimental data is not quantitative and, when yields are available, there are discrepancies in the literature regarding the efficiency of the process. Aiming to characterise the mechanisms involved and their efficiency, we have carried out irradiation experiments using the SPICES setup coupled to two SOLEIL synchrotron beamlines: (i) DESIRS, UV photons of 6 – 14 eV and (ii) SEXTANTS, soft X-rays of 395 – 420 eV (N 1s edge) or 525 – 570 eV (O 1s edge). The ices are formed by vapor deposition (50 – 100 molecular layers) on a cold substrate (15K – 100K), and the desorption of neutral species is probed and quantified by mass spectrometry. Temperature-programmed desorption (TPD) is used to calibrate the desorption signal and the ice thickness, and as a post-irradiation analysis of the ice. The ice composition changes are followed in situ by FT-RAIRS during UV irradiation, or by photo-absorption during X-ray irradiation. The systems we have studied previously include CO, N_2 [3], CH_3OH [4], CH_3CN [5], and HCOOH [6] both as pure ices and in mixtures with water. This talk will focus on the most recent and complete set of results obtained on ammonia NH_3 ices, comparing the inner- and valence-shell excitation regions. We derived desorption yields as a function of the incident energy in the low-fluence regime (spectroscopic study) or as a function of the fluence at fixed energy (kinetic study). We also focus on identifying chemical changes in the ice composition during irradiation and on quantifying the desorption of irradiation products. The mechanisms leading to desorption after photon absorption will be discussed, including the role of secondary electrons created in the ice [7], as well as the (in)dependence of the desorption yields on different parameters such as photon flux, ice morphology, irradiation temperature, and ice thickness.

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THz spectroscopy of radical species using the heterodyne receiver of the AILES beamline

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ABSTRACT

Spectroscopic data of gas phase molecules in the THz domain (1-10 THz) are of significant interest for molecular physics, laboratory astrophysics[1], and atmosphere physics[2]. However, due to the lack of powerful and tunable sources in this domain[3], spectroscopic measurements remain scarce. Thanks to its large spectral coverage and brilliance, synchrotron radiation[4] constitutes a highly suitable THz sources for spectroscopic applications. Nevertheless, commonplace Fourier transform spectrometers, which are well-adapted instruments to analyze the spectral composition of such broadband sources, possess an inherently limited spectral resolution of tens of MHz. Even for light species, this ultimate resolution (30MHz for the FTS of the AILES beamline) is much larger than the Doppler broadening at room temperature. This strong limitation of the spectroscopic capabilities leads some of us to develop a new THz high-resolution spectrometer[5] in the past years. This new spectrometer exploits the heterodyne mixing of the THz continuum extracted by the AILES beamline with laser lines produced by a QCL-based optically pumped molecular laser[6] acting as the THz local oscillator. With an ultimate resolution of 80 kHz, the spectrometer allows to resolve fine structures in the THz spectra of numerous species. This HR-spectrometer already provided some promising results on methanol[5], a well-known molecule with intense absorption lines and displaying a torsion large amplitude motion inducing several line splitting unresolved previously. In the present work, we will present the recent improvements of this new experimental station, and we demonstrate its association with a pulsed discharge absorption cell to record the THz spectra of radical species with sub-MHz resolution. Several NH_2 rotational transitions have been observed and hyperfine structures yet unresolved were revealed thanks to the improved resolution.

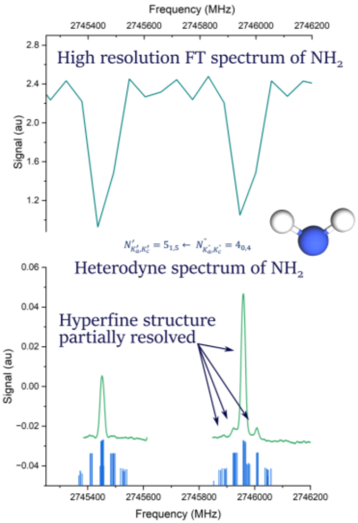

Figure 1: Comparison of NH_2 spectra recorded with a FT spectrometer at the top and the HR-spectrometer at the bottom, both installed on the AILES beamline. Blue lines correspond to the predicted spectra.

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PARALLEL SESSION

Health & Well-being, Environment & Geosciences, Cultural Heritage

CEA Bloch Auditorium

Thursday, January 18th

Chairpersons:

B. Masquida, C. Catrouillet, P. Fernandez Varela, S. Raneri

IT-07	Extracting information on ancient manufacturing techniques and exchange networks from metallic artefacts: A case study on arms and armour ***Emilie Berard***
OC-19	Early alterations of diabetic mouse aortas revealed by X-ray micro-CT ***Sébastien Almagro***
OC-20	Play it again – Recovering archived music from degraded recordings with RIXS-MCD ***Sebastian Gliga***
OC-21	A New model of niobium (Nb) enrichment in laterites revealed by X-ray absorption spectroscopies and Synchrotron diffraction ***Quentin Bollaert***
IT-08	Analysis of arsenic speciation in environmental samples using different Synchrotron-based techniques ***Pierre Le Pape***
OC-22	In-depth 3D analysis of iron age mineralised textiles using Synchrotron-based techniques ***Clémence Iacconi***
OC-23	Stability field of FeO_2H_x in the Earth's mantle from in situ X-ray diffraction at extreme conditions ***Anne-Elisabeth. Marceline***

Hommage à Yann Gohon

Frédéric Jamme - *Synchrotron SOLEIL, Saint-Aubin, France*

PARALLEL SESSION

Health & Well-being, Environment & Geosciences, Cultural Heritage

CEA Bloch Auditorium

Friday, January 19th

Chairpersons:

B. Masquida, C. Catrouillet, P. Fernandez Varela, S. Raneri

IT-09	Peptides inspired by the left-handed β–helix: Structural characterization by circular dichroïsm and X-ray diffraction ***Vincent Lebrun***
OC-24	Effects of environmental factors on Co speciation at the surface of magnetite ***Laura Fablet***
OC-25	Structural resolution of the metabolic activation pathway of the antiviral drug bemnifosbuvir : From pro-drug to target ***François Ferron***
OC-26	Synchrotron radiation techniques for the characterization and conservation of painted metal objects of industrial heritage (The CoPaiM Project) ***Julie Gordon***

Extracting Information on Ancient Manufacturing Techniques and Exchange Networks from Metallic Artefacts: A Case Study on Arms and Armour

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I. Guillot (6), P. Dillmann (3)

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ABSTRACT

The metal study of medieval arms and armour is of great interest to document ancient manufacturing techniques and exchanges networks of both raw material and finished products. However, for such artefact sampling size and location are very limited and only give access to a localized information. Non or minimally invasive approaches constitute important tool to assess the heterogeneity of the ferrous alloys in a representative manner. Furthermore, crucial information on the metal provenance can be also deduced by studying the chemical compositions of Slag inclusions (SI) entrapped in the metal matrix, in particular lithophile trace elements such as rare earth elements (REE).

This contribution will present the methodology used to study the nature and origin of the ferrous alloys in complete museum artefact by various techniques (metallographic examinations, LA-ICP-MS measurement, SR-XRD at the DiffAbs beamline, SR-XRF at the PUMA beamline, SOLEIL Synchrotron) [1]. Ancient ferrous alloys being often heterogeneous, the methodology involved also the fabrication and characterization of model alloys in laboratory at targeted carbon concentration, representative of medieval ferrous alloys.

The nature of mineral phases and the presence of a crystallographic texture was investigated at the DiffAbs beamline, thanks to the available rotation carrying the CirPAD detector [2]. To shed light on the metal provenance, the composition of small SI (< 30µm) entrapped in the metal was further investigated by SR-XRF at the PUMA beamline. However, the detection of targeted trace elements (several dozen of ppm), at the micrometer scale presented analytical difficulties due to the fluorescence emission of iron, which generates a background noise that can mask the emission lines of targeted elements [3]. Such measurements were coupled and discussed with Laser Ablation Inductively Coupled Plasma Mass Spectrometry (LA-ICP-MS) analysis on a dozen of SI.

We will show how the combination of all these approaches allowed to shed new light on the manufacturing techniques implemented by the craftsmen, but also on the medieval metal supply networks.

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Early Alterations of Diabetic Mouse Aortas Revealed by X-ray Micro-CT

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ABSTRACT

Background. Diabetes is a chronic pathology affecting about 10% of the world population. It increases the probability of cardiovascular diseases and accelerates arterial stiffness. The effect of diabetes on the stiffness of the vascular system has been broadly estimated to correspond to 6–15 years of chronological aging. This pathology is mainly characterized by an important level of blood glucose leading to the formation of cross-links within elastin fibers and collagens, resulting in a decrease of arterial wall distensibility.

Large arteries such as the aorta contain, in their extracellular matrix, an amorphous elastic hydrophobic polymer named elastin, which is the major component of elastic fibers. Its entropic elasticity and its concentric lamellar organization within the aortic wall allow the aorta to remain in a reversible deformation domain during the cardiac cycle, which alternates phases of overpressure and contraction. Alterations to elastin due to a pathological situation or aging permanently affect the arterial mechanics.

Materials & Methods. X-ray microtomography enables imaging of large sample volumes with sub-micrometric resolution associated to millimeter field size [1]. We have developed a method to harvest, with a limited collapse, the aorta from 6-month-old mice for X-ray µ-CT imaging in pathophysiological conditions [2]. We are then able to image large aortic segment with a 0.65 µm/voxel resolution, from the heart to the iliac bifurcation.

Results. Our work demonstrates a drastic change in the appearance of elastic structures. The control presents a wavy aspect indicating that this elastic tissue still contains a reserve length such like the coils of a spring. Conversely, the diabetic condition exhibits a smoother aspect suggesting an overstretched structure. We have measured a loss of 30% of the reserve length in diabetic condition. We have previously shown [3] that an inner lattice-like network is present inside the elastic structure. This network supposedly contributes to flexibility and resistance. 6-month-old diabetic mice exhibit a drastic destruction of this network in comparison of normal mice of the same age.

Conclusions. Our results show that the reserve length of elastic lamellae is significantly reduced in diabetic mice together with the loss of filaments that support the wall. This suggests that elasticity is correlated to the existence of this lattice-like network that has disappeared from mouse aortic wall after 6 months of diabetes.

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Play it Again – Recovering Archived Music from Degraded Recordings with RIXS-MCD

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ABSTRACT

A significant fraction of twentieth century audio-visual heritage is stored on magnetic tape.
Between the 1930s and the late 2000s, audio and video recordings were predominantly made on tape. However, magnetic tapes deteriorate over time from wear and chemical degradation [1]. This can prevent their playback, where the read head is in physical contact with the tensioned tape. While large digitisation efforts have taken place over the past decades, millions of unique recordings could not be digitised due to chemical decay and are becoming irrecoverable [2]. Compounding the issue of tape degradation, original playback machines and spare parts are becoming significantly harder to find. This equipment obsolescence means that it will no longer be possible to play back an increasing number of tapes.

Our goal is to develop a non-destructive technique for the recovery of information from such heavily damaged magnetic media in a contactless way, minimizing the risk of further damaging the tape. To that effect, we performed proof-of-concept RIXS-MCD [3-5] measurements at GALAXIES to readout the analogue magnetic waveform recorded on reel-to-reel audio tapes (Fig. 1a), including heavily degraded tapes. RIXS-MCD has proven to be an excellent technique for reading out analogue waveforms from segments of audio recordings (Fig. 1b). Optimal signal on a ¼-inch $Fe2O3$-based magnetic tape was obtained at the K edge. The Fe Kα emission line from the inelastically scattered photons was detected using a set of spherically bent Ge(440) crystal analyzers arranged in a vertical Rowland geometry. The signal was as high as 6% in saturation and 4% at remanence owing to the enhanced magnetic contrast provided by 1s2p RIXS-MCD (Fig. 1c). As an example, we successfully measured separate tracks containing audio frequency sweeps (50 Hz – 1000 Hz). The RIXS-MCD signal is in very good agreement with the signal readout by a Studer A820 player. Slight differences between the two signals are explained by the signal processing electronics of the player. We also Measured a segment of physically damaged tape with folds and cracks, where the audio signal showed amplitude variations when readout with a conventional player. Using RIXS-MCD, we recovered the signal without any amplitude variation, since the magnetic signal is normalized by the total counts (left- and right- circularly polarized X-ray counts).

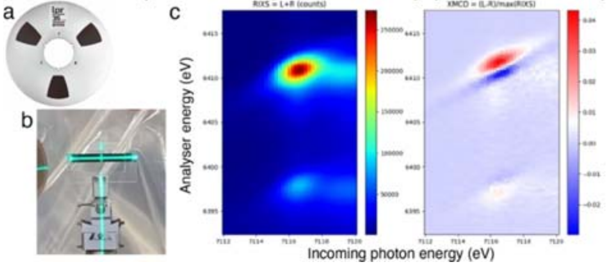

Figure 1: a) ¼" audio tape and b) a measured prerecorded tape segment. The green laser is used for positioning. c) 1s2p RIXS map (left) and RIXS-MCD map (right) measured at remanence.

These results are very exciting for the development of a contactless recovery method. While several attempts have been made to retrieve data from damaged magnetic media [6,7], none has shown the potential of RIXS-MCD, which allows accessing information throughout the thickness of the tape and measuring the magnetic state itself, rather than stray fields, which can be complex in damaged tapes. Therefore, we believe that RIXS-MCD has the potential to enable the recovery of tapes damaged or decayed beyond the reach of other traditional digitization technologies. Moreover, the microfocussing capabilities at the GALAXIES beamline provide the flexibility to digitize any track format, potentially offering a solution to equipment obsolescence.

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A New Model of Niobium (Nb) Enrichment in Laterites Revealed by X-ray Absorption Spectroscopies and Synchrotron Diffraction

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ABSTRACT

Niobium (Nb) is a quintessential critical element used to manufacture superalloys, superconducting magnets, and catalysts **[1]**. Niobium concentrates in alkaline granites and in carbonatites in which Nb minerals, such as pyrochlore ($A_2Nb_2O_7$), crystallize, or in which Nb incorporates more common minerals such as rutile. When such rocks are exposed to weathering, the relative resistance of primary Nb minerals to alteration limits Nb leaching **[2]**, making it one of the most immobile elements **[3]**. The formation of the largest Nb deposits is a consequence of this geochemical behavior, which leads to a significant residual enrichment during lateritic weathering of primary deposits **[2]**. Although the alteration of primary Nb carriers during intense weathering has been evidenced in several studies, the fate of Nb is hindered by (1) equivocal identification of secondary Nb minerals due to their smaller grain size than the resolution of conventional microscopic techniques; and (2) scarcity of Nb hosts in the profiles which render them challenging to track along the profiles using conventional XRD techniques.

For the first time, synchrotron radiation was used to study the geochemical behavior of Nb in two thick lateritic profiles from the Amazonas region. Micro-XANES spectroscopy was used to identify the main Nb minerals occurring as micrometric crystals in the profiles by comparing their spectra with those from a set of reference Nb-rich materials, indicating that Fe and Ti oxides are the main Nb hosts in the profiles **[4,5]**. The distinct spectral signatures of Nb-rich oxides resulting from the sensitivity of XAS to the electronic environment of Nb **[6,7]** indicates that Nb incorporation is eased into goethite compared to hematite. The evolution of the average Nb speciation along the profile was then quantitatively monitored by linear combination fitting of bulk XAS spectra with reference spectra showing increasing contribution of Fe and Ti oxides along with increasing degree of weathering **[4,5]**. The sensibility of synchrotron XRD shows that the weathering of the primary Nb carriers is consistent with their decreasing contribution to the average speciation in the profiles **[5]**. Finally, the modeling of XANES and EXAFS spectra of Nb-bearing Fe and Ti oxide demonstrate the capacity of Nb^{5+} to substitute for Fe^{3+} and Ti^{4+} in common oxides formed from weathering processes **[4,5]**.

Using synchrotron-radiation techniques, we highlight a new model of concentration of Nb in laterites. Residual Nb enrichment will thus depend on (1) the chemistry of the parent rock, which must provides Fe and Ti for secondary oxides precipitation, and on (2) the physico-chemical conditions of formation of the laterite, which must favor the precipitation of goethite and Ti oxides **[5]**.

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Analysis of Arsenic Speciation in Environmental Samples using Different Synchrotron-based Techniques

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L. Fernandez-Rojo[4], E. Resongles[4], S. Delpoux[4], A. Desoeuvre[4], M. Héry[4], V. Tardy[4],
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ABSTRACT

Arsenic (As) is a toxic contaminant that locally accumulates in surface environments, thus potentially causing ecosystemic problems. Worldwide, high As concentrations in waters are essentially observed in aquifers subjected to inputs from igneous mountain ranges erosion, in geothermal fluids, or around mining sites, in particular those exploiting sulfide ore. In mining environments exposed to acid mine drainage (AMD), research is currently active for developing eco-compatible (*e.g.* using local resources) passive bioremediation technologies to immobilize As from As-rich waters. Key physico-chemical parameters have to be identified and controlled to promote highest As removal rates in complex bioprocesses. Such bioremediation issues require identifying the chemical reactions governing As chemistry at the molecular scale, for which redox- and ligand-sensitive synchrotron-based techniques are of particular interest.

In this presentation, I will first show how X-ray absorption spectroscopy at the As *K*-edge (XANES/EXAFS at the SAMBA BL) has been used to probe As speciation (redox and solid species) and helps identifying the geochemical processes at stake in both oxic and anoxic laboratory pilot systems, which were designed to decontaminate As-rich AMD waters in the framework of the INGECOST-DMA research project [1-4]. Taking as an example samples from anoxic bioprocesses dedicated to water decontamination [3-4], I will discuss the interest of spectral imaging through STXM at the As $L_{2,3}$-edges (performed at the HERMES BL) to reveal the spatial distribution of As species at the microscale in As-sulfide-encrusted biofilms. Then, I will discuss how high-resolution X-ray spectroscopies such as HERFD-XANES and RIXS (GALAXIES BL) at the As *K*-edge could help improving the determination of As speciation in complex biogeochemical systems where the chemical signature of different As species spectrally overlap in standard XAS measurements [5]. Finally, I plan to evoke preliminary work with XES-HEROS measurements (GALAXIES BL) performed at the As *K*-edge, which may open perspectives to depict As speciation in environmental samples.

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In-depth 3D Analysis of Iron Age Mineralised Textiles Using Synchrotron-based Techniques

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ABSTRACT

Archaeological textile remains from ancient times are rare because they are perishable in most environments. Their study provides valuable insights into the social and cultural life of ancient civilisations, such as burial practices, textile production and craftsmanship [1]. In temperate climates, the main preservation mechanism is "mineralisation", based on the nucleation and growth of mineral phases formed from metal cations from an adjacent archaeological artefact. Mineralisation can preserve morphological information as a cast or imprint of textile shapes [2-3]. In recent years, the use of semi-quantitative synchrotron X-ray micro-computed tomography (µCT) has greatly improved our understanding of the physico-chemical mechanisms leading to the preservation of archaeological textiles [4-5].

15 millimetre to centimetre-sized mineralised textile fragments from Iron Age sites (8th-5th century BC) in France and the Netherlands were analysed using µCT at the PSICHÉ beamline to reconstruct their internal morphology. The automated processing of the µCT data based on fibre orientation, which we developed, allowed detailed study even in their highly degraded state from the scale of the fibres, to yarns and weave types, which is a difficult endeavour for highly transformed textiles [6-8]. Individual mineralised fibres were analysed by µCT on the ANATOMIX beamline to better understand the chemistry leading to their mineralisation based on the distribution of copper corrosion phases. These data were coupled with X-ray fluorescence and X-ray diffraction data collected at the microscopic scale on the PUMA beamline, to better assess the nature of the mineral phases present and to provide deeper insights into the successive chemical steps involved in the mineralisation process that ultimately led to their preservation up to present day.

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Stability Field of FeO_2Hx in the Earth's Mantle from in situ X-ray Diffraction at Extreme Conditions

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ABSTRACT

Water plays a critical role on Earth's geodynamic and geochemical evolution as it modulates material properties and contributes to deep mantle magmas by reducing silicate melting temperatures. Understanding the storage and circulation of water within the Earth is crucial for grasping global dynamics. Water enters the Earth's interior through oceanic plate subduction, and its transport to the depths depends on the stability of water-bearing phases under mantle pressure (P) and temperature (T). Experimental studies have highlighted stable dense hydrous magnesium silicates (DHMS) in subducting slabs, facilitating water transport through the upper mantle (down to 670 km depth). In the lower mantle, aluminous and ferrous compositions play a vital role, with hydroxide phases such as δ-phase AlOOH[1] and ε-FeOOH[2], isostructural with DHMS phase-H[3], potentially forming a solid solution in the FeOOH-AlOOH-$MgSiO_2(OH)_2$ system[4]. Recent attention to the phase diagram of these solid solutions has unveiled high-pressure phases, including hexagonal (Fe,Al)OOH[5], hexagonal $(Fe,Al)(OH)_3$[6] and the unexpected oxygen-rich phases FeO_2 and FeO_2H_x (with $0<x<1$)[7,8]. They may form water reservoirs accumulating at the core-mantle boundary (CMB), influencing seismic features such as ultra-low velocity zones (ULVZ)[9].

The goal of the present study is to investigate the stability of FeO_2H_x within a mantle assemblage. We collected high-pressure and temperature X-ray diffraction (XRD) signals using the double-sided YAG laser heating diamond-anvil cell set up available on PSICHE beamline on FeOOH-AlOOH, FeOOH-AlOOH-$MgSiO_2(OH)_2$ and FeOOH-AlOOH-$CaSiO_3$ systems. We will discuss the phase diagram of FeO_2H_x as a function of pressure, temperature and composition and the possible interactions between FeO_2H_x and major mantle minerals bringing new light on the capacity of FeO_2H_x to transport water down to the CMB.

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Peptides Inspired by the Left-handed β-helix: Structural Characterization by Circular Dichroism and X-ray Diffraction

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ABSTRACT

In this presentation, we will describe how DISCO and PROXIMA-II beamlines provided us with insightful information that couldn't be obtained with equipments commonly available in labs. This information helped use better characterizing peptides that were rationally designed, taking inspiration from a fold that belongs to the β–solenoid family.

Effects of Environmental Factors on Co Speciation at the Surface of Magnetite

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ABSTRACT

Magnetite nanoparticles (MNs, Fe3O4) are abundant in the environment and are used for various applications due to their unique magnetic, adsorbing or redox properties. The stoichiometry of magnetite (Fe(II)/Fe(III)) is dependent on environmental factors (pH, presence of organic ligands, redox conditions,[1] which largely affects MNs physico-chemical properties, such as adsorption of contaminants.[2] However, the joint effects of environmental factors and MNs stoichiometry MNs-metal cations interaction are elusive. This study focusses on Co as an important contaminant in the environments, and because Co-doped MNs are of high interest for nanotechnology applications.[3]

Magnetite nanoparticles (~10nm) with different stoichiometries were synthesized by co-precipitation, and partially oxidized using H2O2 to obtain the desired stoichiometry. Batch studies were carried out with different [Co] ("adsorption isotherms"), using three different stoichiometries (0.1, 0.3 and 0.5), at different pH values and in the presence or the absence of natural organic matter (NOM) or atmospheric O2(g). The electronic and magnetic properties of Co bound to MNs was probed by X-ray absorption spectroscopy (XAS) and magnetic circular dichroism (XMCD) at the Co L2,3-edges.

Experimental and modeling results revealed three Co species according to Co concentration, which could be attributed to (i) surface complexed or incorporated Co2+ with a ferrimagnetic behavior at low loadings, (ii) magnetically-silent small Co polymers at intermediate loadings and (iii) precipitation of antiferromagnetic Co(OH)2(s)-like phase onto the MNs surface (i.e. core–shell Fe3O4@Co(OH)2 nanoparticles) for highest Co concentrations. Their proportions depended on the physico-chemical conditions: Co-polymers and precipitates were favored on high-stoichiometry MNs, at high pH and in the absence of NOM. Experiments with O2g) lead to the partial oxidation of Co(II) to Co(III).

This study provides detailed knowledge of the effects of environmental factors on the Co-MNs interaction mechanisms, and on the chemical and magnetic properties of these particles. This will help to predict the behavior and fate of Co in the environment and to understand the impact of environmental factors for an appropriate use of MNs for environmental applications.

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Structural Resolution of the Metabolic Activation Pathway of the Antiviral Drug Bemnifosbuvir: From Pro-drug to Target

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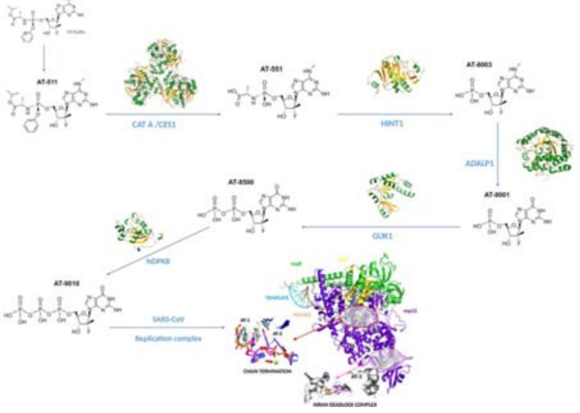
ABSTRACT

Bemnifosbuvir (AT-527) is a guanosine analog currently in clinical trial phase III against SARS-CoV-2, and phase II (with Ruzasvir) against HCV (1,2). This purine nucleotide analogue (NA) is modified at three positions relative to their natural nucleotide counterparts: the purine N6, the 2'-ribose, and the 5'-phosphate.

Here we show this NAs require a minimal set of 5 enzymes, namely CatA/CES1 esterase, HINT1, ADALP1, GUK1, and NDPK for activation to their common 5'-triphosphate active form AT-9010, with an obligate order of reactions prior hitting the main component of the Sars-CoV2 replication complex. AT-9010 inhibits essential viral activities enzymes, accounting for broad spectrum antiviral potency (3). Enzyme assays together with structural data at atomic resolution illuminate N6-purine deamination compatible with metabolic activation by the human ADALP1 enzyme. Crystal structures of human HINT1, ADALP1, GUK1, and NDPK at 2.09, 2.44, 1.76, and 1.9 Å resolution, respectively, with respective precursors of AT-9010 complete the five-steps activation pathway from the orally available drug Bemnifosbuvir to AT-9010, pointing to key drug-protein contacts along the activation pathway as well as chemical positions candidate for further modification on the purine nucleotide. Our work provides a structural and functional framework to integrate antiviral nucleotide analogue design from drug bioavailability and metabolic activation to antiviral potency.



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Synchrotron Radiation Techniques for the Characterization and Conservation of Painted Metal Objects of Industrial Heritage (The CoPaiM Project)

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ABSTRACT

Museum objects with a painted metal structure are often found within industrial, scientific and technical collections. The conservation of these objects presents a challenge because of their composite nature. The interactions between the components of the system can lead to different alteration phenomena than what would be expected for the paint or metal alone, resulting in the need for specific conservation strategies. The CoPaiM project (Conservation of Painted Metals) seeks to contribute to the development of new conservation strategies for historic painted metal objects. A first research aim of this project is to enhance the knowledge of the material system and its alteration phenomena through the study of historic objects. Samples of paint and corrosion products obtained from a corpus of 19th-early 20th century painted iron objects were prepared as cross-sections and studied using classic laboratory and synchrotron analytical techniques. The cross-sections were analysed on both the DiffAbs and PUMA beamlines using micro-XRF mapping to obtain a spatially resolved identification of the elemental composition. The elemental maps were often completed by micro-XANES point analysis to probe the chemical speciation of the components within the stratigraphy. This approach proved complementary to the results acquired by optical microscopy and micro-Raman spectroscopy, and led to the detailed characterization of the paint components and iron corrosion products present in the samples and to a qualitative micro-scale description of the alteration phenomena. Certain cross-sections were further investigated using deep-UV photoluminescence micro-imaging on the DISCO beamline, providing additional molecular information based on differences in optical emission. Indeed, the images demonstrate the highly heterogeneous nature of the samples which was not as evident from the elemental and visual observations and suggests the presence of many different molecular phases, possibly related to the formation of metal carboxylates. This study provides not only an improved understanding of the materials and techniques used for the preparation of the studied objects, but also a documentation of the possible states of alteration of the historic painted metal system, the discernment of which is crucial for the development of suitable conservation strategies.

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POSTERS SESSION

List of Posters

PO-AM-01-S	Permittivity and Schottky barrier height of $Ba_{0.45}Sr_{0.55}TiO_3$ (BST) varactors under bias ***S. Agudelo***
PO-AM-02	Recent developments in transition metal K-edge XMCD for molecular magnetism ***A. Bordage***
PO-AM-03	Ferroelectric controlled electronic band structure in doped β-Ga2O3 ***A. Boucly***
PO-AM-04-S	The spin-orbit induced insulator Ba_2IrO_4: Angle-resolved photoemission spectroscopy vs paramagnetic dynamical mean-field-theory ***F. Cassol***
PO-AM-05-S	Angular dependence of X-ray natural circular dichroism: X-ray optical activity beyond chirality ***A. De Frenza***
PO-AM-06	The charge-transfer in CoFe prussian blue analogs: New insights into the role of alkali cations using Synchrotron infrared spectroscopy ***M. Dronova***
PO-AM-07	3D imaging by ptychography X-ray computed tomography of single carbon and basalt fibers ***M. Ducousso***
PO-AM-08-S	Biopolymer-templated deposition of hierarchical 3D-structured graphene oxide/gold nanoparticle hybrids for surface-enhanced Raman scattering ***Y. Guo***
PO-AM-09	Operando characterization of Li ion batteries with XAS and Raman spectroscopy ***F. La Porta***
PO-AM-10-S	Modulation excitation XAS: How to go deeper, while remaining at the surface? ***S. Lips***
PO-AM-11-S	EC cell for operando XAS investigations on X-ray opaque supports ***E. Paparoni***
PO-AM-12	Structural Analyses and Properties of Complex Sulphides in the CrSnS System ***C. Prestipino***
PO-AM-13-S	Organic semi-conductor nanoparticles for photocatalytic hydrogen production: study of the internal morphology by soft X-ray spectromicroscopy techniques ***C. Rieb***

PO-AM-14	Investigating Ag growth on PET foil with dcMS and HiPIMS ***S.V. Roth***
PO-AM-15	Structural transformations in BiFe0.5Sc0.5O3 via in situ pressure SR diffraction dtudy at CRISTAL ***A.N. Salak***
PO-AM-16-S	Synchrotron-based electronic characterization of organic thin films for non-fullerene acceptor solar cells ***N. Vannucchi***
PO-DR-17	Operando XAS studies of copper porphyrin organic electrodes for lithium ion batteries ***Y. Hu***
PO-DR-18	Operando battery characterization via full-field quick-XAS imaging at ROCK beamline ***L. Pérez Ramírez***
PO-DR-19-S	Experimental study of polarization-dependent PCI effect in neon and water following K-shell photoionization ***A. Verma***
PO-HW-20	Analysis of the organic-inorganic interface in M. fruticosa: A multi-technique approach ***A-J. Álvarez-Valverde***
PO-HW-21	SAXS from cellulose solution: Interchain effects ***F. Boue***
PO-HW-22-S	Polyamino-isoprenic compound NV716 disrupts the outer membrane of Pseudomonas Aeruginosa and creates a new sensitivity to doxycycline ***M. Draveny***
PO-HW-23	The magic scroll of Ampus (Var, France) future “musée des écritures” ***J-P. Itié***
PO-HW-24	Functional and structural insights into the multi-step activation and catalytic mechanism of bacterial ExoY nucleotidyl cyclase toxins bound to actin-profilin ***L. Renault***
PO-HW-25-S	Characterizing red coloring matter samples from the Altamira cave using semi-quantitative chemical imaging and X-ray absorption at the PUMA beamline, SOLEIL ***J. Tapia Reguera***
PO-HW-26-S	Determination of the temperature dependence of the refractive index of ice in the Fir ***C. Taverna***
PO-HW-27	Ultrastructural insights into dentin using PXCT ***E. Vennat***
PO-DR-28	User-friendly tools implemented in Fastosh to visualize and interpret Wavelet Transform of the EXAFS ***G. Landrot***

Permittivity and Schottky Barrier Height of $Ba_{0.45}Sr_{0.55}TiO_3$ (BST) Varactors under Bias

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ABSTRACT

The perovskite solid solution BST is the most widely used ferroelectric in current varactors because maintains low dielectric losses at microwave frequencies and retains a high dielectric permittivity, which is very important in 5G and Near Field communication technologies. The top and bottom interface layer chemistry control the ε and SBH in varactors. We have used hard X-ray photoelectron spectroscopy to investigate the bias dependent permittivity and band line-up in a varactor stack. To do so, two samples were used 1. LSMO/BST/ICL/LSMO and 2. Pt/Cr/BST/ICL/LSMO.

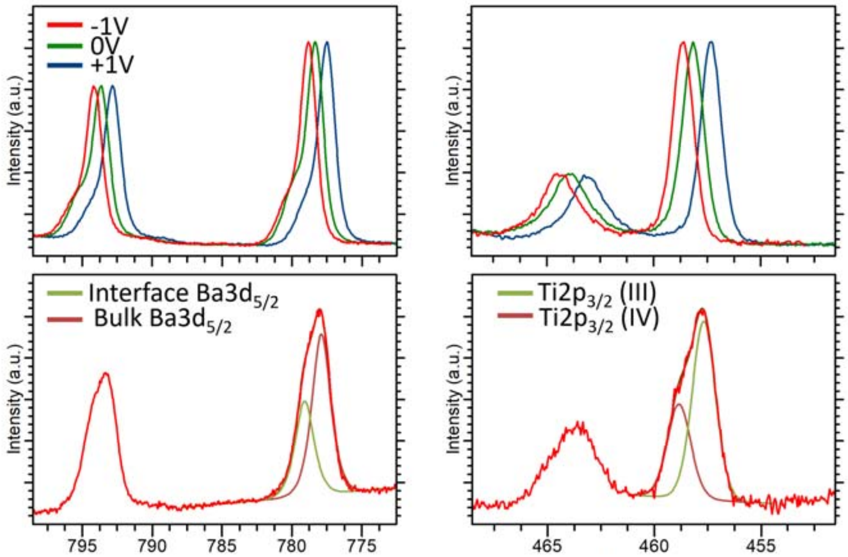

Figure 1. Ba3d and Ti2p core-level spectra at 6keV for different bias (top). Ba 3d and Ti 2p core-level spectra at 8keV and +1V bias (bottom).

The low field measurements (±0.2V) provided access to the bias dependent permittivity whereas the high field experiments (±1V) calibrated the ICL dependent Schottky barrier height.

Samples were prepared at GREMAN (Univ. Tours) by combinatorial pulsed laser deposition (CPLD). We have structured 400 x 400 µm² capacitors with four different ICL stoichiometries.

At the top interface (sample 1) we studied the band line up of $La_{0.7}Sr_{0.3}MnO_3$ (LSMO) top electrode and $Ba_{0.45}Sr_{0.55}TiO_3$ (BST) as a function of applied bias for two different energies (6 keV and 8keV). The top interface is revealed at 6keV whereas 8keV the full BST film is proved. The bias gives the core level shift. An internal field is formed and varies as a function of ICL stoichiometry and applied bias voltage. The Schottky Barrier Height is calculated using the Kraut method. The SBH varies as a function of the bias voltage and the hole carrier concentration of the ICL. The ICL stoichiometry defines the two possible regions: accumulation and depletion.

At the bottom interface (sample 2) we studied the chemistry of the BST/$La_{1-x}Sr_xMnO_3$ (LSMO1-x) ICL on a LSMO bottom electrode as a function of applied bias at 8keV.

From the Ba3d$_{5/2}$ spectra, two asymmetric species are identified: one from bulk BST at low BE, and one relative to the interface of BST/LSMO1-x at higher BE. The asymmetry is proportional to the applied bias voltage and the potential drop across the film. Ti 2p3/2 spectra is deconvoluted in Ti4+ and Ti3+. The presence of Ti reduced species at approximate 1.2eV from Ti4+ are probably due to charge transfer.

Recent Developments in Transition Metal K-edge XMCD for Molecular Magnetism

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ABSTRACT

For the last years, we have been involved in the study of Transition Metal (TM) K-edge X-ray Magnetic Circular Dichroism (XMCD) using Prussian Blue Analogs (PBAs ; $A_4[B(CN)_6]_{2.7}.nH_2O$; A,B=transition metal) in order to disentangle the physical effects originating these signals in molecular compounds [1-5]. A tool combining chemical selectivity and bulk sensitivity is indeed missing for the investigation of their magnetic properties. Our experiments first dedicated to the bimetallic $A_4[Fe(CN)_6]_{2.7}$ (A=Mn,Co,Ni,Cu) and $A_4[Cr(CN)_6]_{2.7}$ PBAs (A=Mn,Fe,Co,Ni) PBAs and more recently to the trimetallic $(Ni_xCo_{1-x})_4[Fe(CN)_6]_{2.7}$ series brought unprecedented information. By analyzing first the A K-edge of the bimetallic PBAs, we could establish that qualitative and quantitative parameters of the main 1s→4p contribution to the XMCD signal are related to the magnetic behavior of the absorbing atom: (i) the shape to the filling of the 3d orbitals, (ii) the sign to the orientation of the magnetic moment with respect to the applied magnetic field, (iii) the intensity of the signal to the total spin number (SA) and (iv) the area-under-peak to the Curie constant (CA) [3]. Additionally, the results at the Ni and Co K-edge of the trimetallic series showed that TM K-edge XMCD is, at the N side of the cyanide bridge, a probe of only the absorbing atom (Ni or Co) and not of the whole sublattice [4]. The analyses of the Fe and Cr K-edges [5] showed that, at the C side of the cyanide bridge, TM K-edge XMCD is a probe of the absorbing atom as well as its interactions with its first magnetic neighbors. We could establish explicit relationships between the intensity and the total spin of the species to which the photoelectron is sensitive; [4,5] the agreement between the intensity calculated using our expressions and the experimental one is illustrated Fig. 1. Valuable information (i) on the exchange interactions between all involved 3d and 4p orbitals and (ii) on the local orientation of the magnetic moment carried by the absorbing atom (Fig. 2) were thus proposed. A summary of our previous results on the bimetallic PBAs and the last ones on the trimetallic series will be presented, with the new possibilities it offers to molecular magnetism.

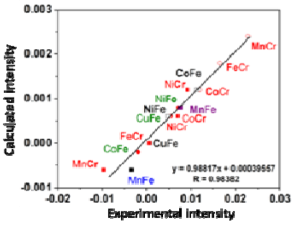

Fig. 1 Experimental intensity (I_{exp}) vs the one calculated using our expressions (I_{calc}) [3-4] for the bimetallic (dots) and trimetallic series

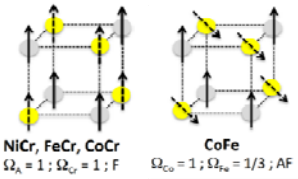

Fig. 2 Proposed orientations of the magnetic moments for an octant of the PBA structure

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Ferroelectric Controlled Electronic Band Structure in Doped β-Ga2O3

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ABSTRACT

Ga2O3 belongs to the family of ultra wide band gap semiconductors (EG ~ 4.8-4.9 eV) with large high quality single crystal substrates commercially available and potentially unrivalled performance in power electronics thanks to breakdown fields up to 8-12 MV/cm, are ideally suited for hostile or demanding environments[1,2]. There are three principle applications for Ga2O3 devices: UV light detectors, Schottky barrier diodes (two terminal device) and depletion mode MOSFETs (three terminal device). However, Ga2O3 also has drawbacks. Only n-type doping has been demonstrated, limiting applications (Ga2O3 FETs can only operate in depletion mode) and controlling the electronic structure requires logic compatible with power electronics. Thanks to their low thermal budget, excellent electrical properties and a maximum polarization obtained for films in the range of 8-12 nm, ferroelectric HfZrO4 (HZO) has received enormous interests[3,4] and could provide a solution. By integrating an ultra-thin ferroelectric HZO film to a Ga2O3 semiconductor, we plan to control the band alignment using the switchable polarization of the HZO to shift the electronic levels either downward or upward.

Here we present results of combined in-situ biasing and Hard X-ray photoemission spectroscopy (HAXPES) measurements carried out on a Ge:Ga2O3/HfZrO4 (HZO)/TiN capacitor-like structure. The goal of those measurements was to characterize in depth the response of our Ga2O3/HZO interface under different biasing conditions. Remarkably, we observed the presence of a hysteresis in the binding energy position of our hafnia peak during a biasing loop as well as a charge injection phenomenon.
This work was supported by the AFSOR grant FA9550-20-1-0164

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The Spin-orbit Induced Insulator Ba_2IrO_4: Angle-resolved Photoemission Spectroscopy vs Paramagnetic Dynamical Mean-field-theory

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ABSTRACT

Since its formulation during the 90's, dynamical mean-field theory (DMFT) has become a well-established numerical technique to describe strongly correlated materials. Thanks to its finite-temperature nature and its capability to treat the strong electron-electron interactions in these materials, it allows the realistic calculation of phase diagrams and observables measured in experiments, such as spectral functions.

In this talk, we will present a fully *ab initio* study of Ba_2IrO_4 comparing the momentum-resolved spectral function resulting from DMFT calculations with respect to available angle-resolved photoemission spectra (ARPES).

Ba_2IrO_4 is a simpler sister compound of the well known Sr_2IrO_4, which is considered a prototypical system for the so-called spin-orbit-induced Mott transition[1]. The physics of Sr_2IrO_4 has largely been described by a single band construction, involving the spin-orbital entangled band $j_{eff} = 1/2$ resulting from a mixture of Ir t_{2g} orbitals. In Ba_2IrO_4, however, structural distortions are absent which leads to several pseudospin states crossing the Fermi energy, thereby casting doubt on a single-band picture[2].

Here, we report an accurate multi-band DMFT study of Ba_2IrO_4 in the paramagnetic phase. First, we will briefly clarify the role of spin-orbit coupling in the Mott transition and then use an *ab initio* parametrization to focus on the electronic structure of Ba_2IrO_4. We will show that a modest amount of electronic interactions is sufficient to realize a paramagnetic Mott insulating state. Carefully analyzing the calculated **k**-resolved spectral function in comparison with available ARPES measurements[3,4], we will finally discuss the role of antiferromagnetic long-range order as well as of short-range antiferromagnetic fluctuations on the spectra.

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Angular Dependence of X-ray Natural Circular Dichroism: X-ray Optical Activity beyond Chirality

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ABSTRACT

Chirality is the absence of improper symmetry operations in a crystal and it is most often connected to optical activity. In some rather specific situations, it is known that optical activity can exist even in the absence of chirality. Our target is to understand X-ray Natural Circular Dichroism (XNCD) where a sample is shined with left and right circularly polarized light and a difference in X-ray absorption is observed.

In the present case, we shall consider the unusual situation where achiral crystals - i.e. crystals for which an improper symmetry operation is a symmetry of the space group of the crystal - present a large XNCD signal [1]. We shall restrict to the cases of crystals with D_{2d} (-42m) and S_4 (-4) symmetries, where XNCD has been observed (see companion Abstract by Elizabeth Hillard). Since S_4 is a sub-group of D_{2d}, the XNCD angular dependance for S_4 crystals is richer.

We shall compute the expressions for the XAS and XNCD cross-sections and detail the various geometric parameters that are present in the definition of the cross-sections. Great care will be brought to the symmetry properties at stake for XNCD where three different groups are to be considered : i) the crystal space group, ii) the point group of the space group and iii) the local point group of the absorbing atom. Through an analytical study of the angular dependances of XNCD, we shall show what type of information can be gained from the shape of the XNCD signal and how the XNCD signal for a D_{2d} crystal can unambiguously be distinguished from the one measured for a crystal with the lower S_4 symmetry. To conclude, we shall focus on the XNCD sum rules and outline the importance of the pseudo-deviator term and its connection with the anapole.

Connection shall be made with experimental results measured at Fe and Cu K-edges on ID12@ESRF and GALAXIES@SOLEIL [2].

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The Charge-transfer in CoFe Prussian Blue Analogs: New Insights into the Role of Alkali Cations using Synchrotron Infrared Spectroscopy

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ABSTRACT

Over the years, the (photo)magnetic properties of CoFe Prussian Blue Analogs (PBA) have been a subject of prominent research, as they offer appealing solutions for future data storage applications. For well-chosen stoichiometries, they indeed present a $\mathrm{Co_{III}Fe_{II}} \rightarrow \mathrm{Co_{II}Fe_{III}}$ charge transfer that can be induced by light, temperature or pressure. Our previous studies[1,2,3] demonstrated that these photo- and thermally-activated charge transfers can be modulated by varying the nature and amount of alkali metal ions inserted in the structure. Nevertheless, a full understanding of the phenomenon is still missing to be able to design photomagnetic PBA working at room temperature.

Here, we will present the latest results on our original investigation using synchrotron infrared spectroscopy of an alkali cation-containing CoFe PBA series having the A2Co4[Fe(CN)6]3.3□*n*H2O (A=Cs,Na, Rb) chemical composition. The series were synthesized and macroscopically characterized in the laboratory, and the IR investigation (both in the far and mid regions) was conducted on the AILES beamline. The effect of the alkali ion nature on the metal-to-ligand vibrations were examined in all electronic states involved in both thermally activated and photo-induced switching properties. Our findings revealed for the first time a characteristic signature of alkali cations interacting with the FeII-C≡N entities and their non-innocent role in the electron transfer between the CoIII(LS)-FeII and CoII(HS)-FeIII states. Our work therefore demonstrates the relevance of infrared spectroscopy in probing the fine structural changes accompanying these charge-transfers in CoFe PBAs, and so in gaining deeper understanding of their (photo)magnetic properties.

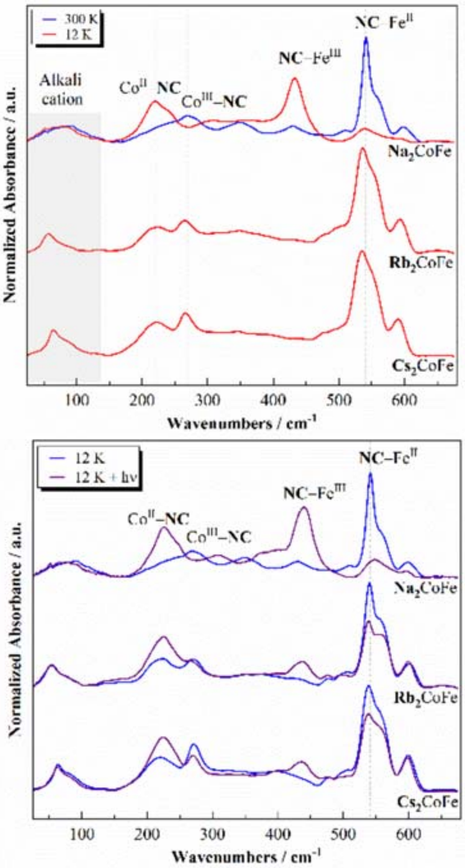

Figure 1. Far-Infrared spectra for the A2CoFe series (A=Na,Rb,Cs) showing the thermally-induced charge transfer for A=Na (top) and the photoinduced one for the whole series (bottom).

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3D Imaging by Ptychography X-ray Computed Tomography of Single Carbon and Basalt Fibers

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ABSTRACT

Carbon fibers are engineered fibers, formed of more than 95% of carbon, and often obtained from the graphitisation and oxidation of a polymer, the PolyAcryloNitrile (PAN) [1]. They are widely used for light structure design in aeronautics industry and are generally associated to polymers to form carbon fiber reinforced plastics (CFRP). Part of our research activity at Safran Group is to improve our basic knowledge in carbon fibers to optimize our composite structures.

A feature of interest concerns their surface chemistry. At the atomic scale, the carbon crystallite is arranged in layer planes, due to strong π-π interaction, but at the nanoscale, these crystallites are forming a less ordered structure [2]. This structure induces exposed edges of the crystallites in a partially oxidized state at the surface of the fiber, introducing polar chemical groups such as alcohol, ketone or aldehydes [3], which can improve the bonding state quality between the carbon fiber and polar resins. The presence of these heteroatoms results in local electronic density variations. Ptychography X-ray Computed Tomography (PXCT) is a unique method, which directly produces nanoscale 3D maps of the electron density in absolute units and therefore allows for direct comparison with theoretical values.

Another interesting characteristic is their surface morphology, which has a great influence on the carbon/polymer adhesion properties: high surface roughness leads to good interfacial adhesion with the resin through mechanical inking.

We will present here very first results obtained on SWING beamline of PXCT on single carbon and basalt fibers. Electron density and surface morphology are probed, with a spatial resolution around 100 nm. This work will contribute to improving the basic knowledge of carbon fibers and its adhesion with polymer.

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Biopolymer-templated Deposition of Hierarchical 3D-structured Graphene Oxide/Gold Nanoparticle Hybrids for Surface-enhanced Raman Scattering

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ABSTRACT

Cellulose, a well-known natural biopolymer, has emerged as a promising bio-based substrate capable of synergistically combining with conductive materials (e.g., metals or carbon-based materials) for diverse applications including sensors, smart windows, and bioelectronics. Typically, Surface Enhanced Raman Scattering (SERS), an advantageous analytical technique, allows for the rapid detection and structural analysis of biological and chemical compounds through their spectral patterns in nanotechnology [2]. Crucial for SERS is fabricating the substrates with strong and reproducible enhancements of the Raman signal over large areas and with a low fabrication cost. Herein, we present a straightforward approach utilizing the layer-by-layer spray coating method to fabricate (CNF) films loaded with gold nanoparticles (AuNPs) and graphene oxide (GO) to serve as SERS substrates. Compared to conventional SERS substrates, the hybrid three-dimensional (3D) structures comprising GO/AuNPs significantly enhance the SERS sensitivity due to their synergistic effect. In addition, the incorporation of 3D CNF substrates, which serve as templates for the morphology of GO/AuNPs, contributes to a more uniform distribution. To investigate the fundamental mechanisms of enhanced SERS performance, grazing incidence small-angle X-ray scattering combined with nano-Fourier-transform infrared-spectroscopy was employed to gain comprehensive insights into the nanostructure in ultra-small quantities and at ultrahigh spatial resolution. Therefore, our approach provides a reference for facile and scalable production of universally adaptable SERS substrates with exceptional sensitivity.

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Operando Characterization of Li Ion Batteries with XAS and Raman Spectroscopy

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ABSTRACT

The need for more performant energy storage devices drives the research on trying various electrode materials, and on understanding the electrochemical mechanisms[1]. *Operando* measurements performed on these systems typically yield more reliable results than *ex-situ* measurements for several reasons[2]. First, they allow to monitor the real-time evolution of key parameters under actual working conditions, such as pressure, temperature, and lithium concentration. Secondly, *operando* measurements prevent any alterations to the materials during cell disassembly and washing. Thus, the importance of reliable electrochemical cells cannot be overstated.

The primary objective of this work is to introduce an electrochemical cell capable of multimodal characterization in *operando* conditions. The latter is designed and developed at the ROCK beamline of SOLEIL. The cell design addresses 3 main constraints: first it must be electrochemical reliable, then it has to be geometrically suitable for photon in/photon out techniques e.g. X-ray Absorption Spectroscopy (XAS) and Raman Spectroscopy, and lastly it has to be easy to assemble in a glovebox. To demonstrate the reliability of this investigational cell, $LiNiO_2$ was employed as a benchmark material, given its well-documented behavior in XAS[3-4] and Raman spectroscopy[5].

The initial version of the cell allowed Raman and XAS measurements during the electrochemical cycle. The diamond windows equipped, however, introduced significant Raman background noise. To address this issue, the cell was updated replacing them with fused silica and beryllium windows. The new cell design presents also a larger solid angle capability to access the electrodes, and it allows multiple measurements at the same time. The updated device will be tested in the ROCK beamline on the first semester of 2024.

The activity described above is part of the European project BIG-MAP (Battery Interface Genome – Materials Acceleration Platform) that aims to develop the technological and scientific building blocks for accelerated battery discovery. The consortium is part of the long-term research initiative Battery 2030+.

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Modulation Excitation XAS: How to Go Deeper, while Remaining at the Surface?

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ABSTRACT

The development of MEXAS (Modulation Excitation X-ray Absorption Spectroscopy) opened up a wealth of possibilities to study the surface of catalysts at a high level of detail, while operating under reaction conditions.1 Since the modulation excitation technique is quite new, its experimental design is still subject of study.2 Maximizing the amount of information derived from this complex technique necessitates advanced data analysis. The application of PSD (Phase-Sensitive Detection) was already a big step forward in analysing MEXAS data, even giving access to kinetic information.2 To further enhance the spectral interpretation, simulation techniques are required. This is where DFT (Density Functional Theory) calculations come in.

When applying MCR-ALS (Multivariate Curve Resolution with Alternating Least Squares) data analysis on an experimental MEXAS dataset, one obtains the spectra of a number of 'pure' components.[3] To characterize these pure components based on their spectra, EXAFS modelling is used. This gives a lot of information about the bulk properties of the catalyst. However, catalysis researchers are also interested in the chemistry occurring at the surface. The presence of adsorbates will impact the XAS spectra of surface elements and as a result, details about these adsorbates can be found in the MEXAS data. To extract this information, a detour via DFT is needed. Based on the bulk properties of the pure components and chemical intuition, VASP (Vienna Ab-initio Software Package) can be used to construct an atom scale structure of the catalyst surface.[4] It should be stressed that this structure comprises both catalyst and adsorbates. Using the FDMNES (Finite Difference Method Near-Edge Spectrum) software, the XANES (X-ray Absorption Near Edge Structure) spectrum of this structure can be estimated.[5] If the predicted spectrum matches the spectrum of the pure component, the proposed VASP-structure is likely similar to the real structure. In this way, one has indirectly obtained information about the surface chemistry from the modulation experiments.

The proposed methodology, combining MEXAS with DFT, is in a conceptual phase and as such presents challenges. One is the fact that the errors from MCR-ALS, VASP and FDMNES all add up to the final product. Another lies in the question whether the FDMNES software is sensitive enough to predict the subtle differences, occurring during a MEXAS experiment. However, if this methodology proves functional, it provides a unique approach to simultaneously validate DFT calculation outcomes and analyse MEXAS results on a deeper level. All of this, while remaining at the surface ...

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EC Cell for Operando XAS Investigations on X-ray Opaque Supports

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ABSTRATCT

Investigating the electronic and structural dynamics of a catalyst in *operando* conditions has a crucial role in the development of more performant electrochemical devices. A special importance is to be assigned to the catalyst/electrolyte interface, whose understanding leads to improved electrochemical processes. Several approaches are available. The stringent experimental requirement imposed by imaging methods or vibrational spectroscopies often makes the investigation challenging, with respect to the more straightforward approach allowed by x-ray absorption spectroscopy (XAS). However, if hard x-rays have a long penetration depth, probing an absorption edge below 10 keV in the presence of a layer of electrolyte can be quite challenging. In most setups, this obstacle is overcome by depositing the sample on a conductive and x-ray transparent support like graphite or a thin silicon nitrate membrane [1,2], then probing the sample from the substrate side. However, this geometry not only limits the sensibility to the electrode/electrolyte interface but precludes the study on non-transparent supports. Different electrochemical cells have been designed to reduce the absorbance of the liquid layer by shrinking its thickness [3], but (to the best of our knowledge) no XAS measurement at energies below the Cu K edge are known. In this presentation, we will describe a novel electrochemical cell for *operando* XAS measurements in fluorescence mode. The thin layer of flowing electrolyte allows to probe energies as low as the Ti K-edge. We estimated a *photon-in photon-out* efficiency of the cell in the 45° configuration of 75% at the Fe K edge and 43% at the Ti K edge. In our poster, we will describe the cell and show operando XAS measurements at the Fe and Ni K-edges on thin Ni-doped maghemite films (111) epitaxially grown on Pt (001) single crystal substrates. As discussed in our recent work [4], we will describe the role of Ni doping in the catalytic performances of maghemite for the oxygen evolution reaction. The described electrochemical cell will be made available to the scientific community at SAMBA beam line. It will contribute to new research and results in the physical chemistry field.

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Structural Analyses and Properties of Complex Sulphides in the CrSnS System

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ABSTRACT

The design and optimization of thermoelectric (TE) materials rely on the intricate balance between thermopower (S), electrical resistivity (ρ) and thermal conductivity (κ). Perfecting such a balance is the key to reach high TE performances - determined by the dimensionless figure of merit ZT = S2T/ρκ - necessary to improve energy recovery systems and thermoelectric cooling devices.1 Among the most promising TE materials at medium temperature, complex copper-based sulphides are of double interests as they are usually made of eco-friendly and low cost elements2 and exhibit intrinsically low thermal conductivity.3 However, the use of copper-based sulphides in TE devices is limited by the lower TE performances of the n-type materials compared to those of the p-type.4 Hence, it appears necessary to develop more performant n-type sulphide materials.

In this context, we have synthesized and studied the structural and physical properties of two phases in the Cr-Sn-S ternary system: Cr2Sn3S7 and Cr2SnS4. The former is characterised by a semi-ordered crystal structure and a n-type semiconductor behaviour, and the latter is characterised by a complex crystal structure (Figure 1) and a p-type semiconductor behaviour. The intrinsic structural complexity of these materials leads to very low thermal conductivities, which are promising features to develop new performant thermoelectric materials.

In this presentation, I will (i) present results obtained from X-ray diffraction, scanning and transmission electron microscopies, magnetic measurements, spectroscopy techniques and transport measurements and (ii) discuss on the relationships between chemical compositions, crystal structures and properties (TE and magnetic) of Cr2Sn3S7 and Cr2SnS4. 5

Organic semi-conductor nanoparticles for photocatalytic hydrogen production: study of the internal morphology by soft X-ray spectromicroscopy techniques.

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ABSTRACT

Global warming is encouraging humanity to give up fossil resources, replacing them by renewable energies. However, most of them are intermittent. The production of hydrogen would be a good way to store and distribute energy. Here, we focus on the photocatalytic production of green hydrogen by water splitting by organic semi-conducting (OSC) nanoparticles (NPs). Contrary to classical inorganic semi-conductors (ISC) who absorb only UV light, OSC can absorb a larger part of the sun emission spectrum (44% for OSC and 6.6% for ISC of sun emission spectrum) [1]. However, due to the low dielectric permittivity of these materials, separation of the excitons into free charges requires the presence of a heterojunction between an electron donor (D) and an electron acceptor (A). The objective of this work is to prepare, by miniemulsion and nanoprecipitation, such NP's that are morphologically and chemically optimized for their application in photocatalytic production of hydrogen. The optimization of these materials will be done by constant feedback from various laboratory based as well as advanced characterization techniques.

PTQ10 and ITIC-4F were chosen as a well-known D:A pair model in order to produce NPs with different morphologies. These and similar systems will be prepared and their internal morphology will be observed by Transmission Electron Microscopy (TEM) and Scanning Transmission X-ray Microscopy (STXM). They will also be used to validate the application of recently developed ptychography assisted soft x-ray STXM [2] for the characterization of these materials. The use of Ptychography will allow us to reach a higher spatial resolution (<20 nm, beyond the present limits of conventional STXM, ~30 nm) for obtaining the compositional and morphological maps of these NPs. A feedback from these spectromicroscopy techniques eventually should allow us to understand the influence of the OSC NPs morphologies on the H_2 evolution for well-designed D:A pairs (energies levels, chemicals functions, …).

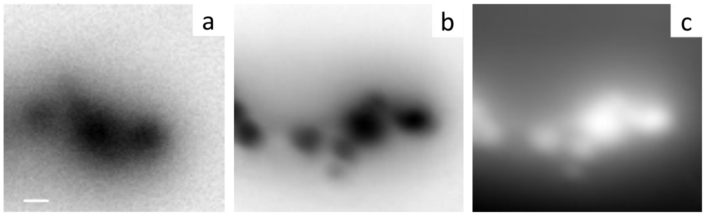

Figure 1: (a) STXM image of PTQ10/ITIC-4F NPs made by miniemulsion (scale bar = 200nm), (b) amplitude and (c) phase image obtained by ptychography of the same NPs.

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Investigating Ag Growth on PET Foil with dcMS and HiPIMS

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ABSTRACT

High Power impulse magnetron sputtering (HIPIMS) is a novel industrially-relevant deposition technique enabling increased adhesion between and density of thin deposited metal layers on polymers. No pre- and post-treatment is required to achieve these properties. In our recent study [1], we exploited this advantage for lithographic patterning. Yet, no report has discussed the nucleation and growth process during HiPIMS deposition. In this new study, polyethylenterephthalate (PET) foil is studied under various deposition conditions. In detail, we compare direct magnetron sputter deposition and HiPIMS. We present our results of a combined study from in situ growth by simultaneous in situ grazing-incidence small angle X-ray scattering (GISAXS), grazing incidence wide-angle X-ray scattering (GIWAXS) as well as ex-situ field emission scanning electron microscopy (FESEM) and SNOM measurements, which were performed at the SMIS beamline.

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Structural Transformations in $BiFe_{0.5}Sc_{0.5}O_3$ *via in situ* Pressure SR Diffraction Study at CRISTAL

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ABSTRACT

The phenomenon of annealing-stimulated irreversible transformations of the high-pressure stabilized phases (conversion polymorphism) [1] offers a promising approach to produce novel multiferroic materials. The polar *Ima*2 polymorph of the multiferroic $BiFe_{0.5}Sc_{0.5}O_3$ perovskite obtained *via* conversion polymorphism is a rare example of a polar weak ferromagnet with a non-collinear polar structure.

Pressure-induced transformations in $BiFe_{0.5}Sc_{0.5}O_3$ were studied *in situ* between ambient pressure and 20 GPa using synchrotron x-ray diffraction at the CRISTAL beamline in the SOLEIL synchrotron at room temperature. The structural phase sequence and the phase transition (coexistence) ranges were found to be essentially different upon compression and upon decompression. Two new polymorphs, namely polar *Imm*2 and non-polar *Pnma* in addition to the three previously discovered in $BiFe_{0.5}Sc_{0.5}O_3$ were found (Figure 1).

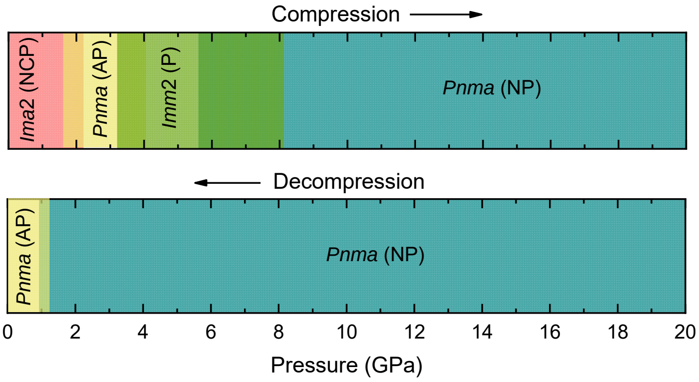

Figure 1. Schematic presentation of the pressure-induced structural phase transformations and the phase coexistence fields in the high-pressure synthesized perovskite $BiFe_{0.5}Sc_{0.5}O_3$ upon compression (top panel) and upon decompression (bottom panel). The phases indicated correspond to the noncollinear polar (NCP) orthorhombic *Ima*2; antipolar (AP) orthorhombic *Pnma*; the polar (P) orthorhombic *Imm*2, and the nonpolar (NP) orthorhombic *Pnma*, respectively.

The obtained data are important to design those phases as epitaxial films *via* thin-film strain engineering and consequently to optimize their multiferroic behavior.

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Synchrotron-based Electronic Characterization of Organic Thin Films for Non-fullerene Acceptor Solar Cells

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ABSTRACT

The transition from fullerene to non-fullerene acceptors (NFAs) has increased the power conversion efficiency (PCE) of organic photovoltaics (OPV) drastically, reaching PCEs above 19% [1]. As opposed to fullerene acceptors, NFAs have tuneable energy levels, stronger absorption across the solar spectrum, and better thermal stability. The PM6/Y7 polymer donor/NFA binary blend is one of the most promising systems [2] thanks to its broad absorption range, which favors high photocurrents in such based devices [3]. Frontier orbital band alignment is a key factor affecting the device's efficiency. This aspect remains unexplored in the PM6/Y7 blend system, especially with varying donor-acceptor ratios.

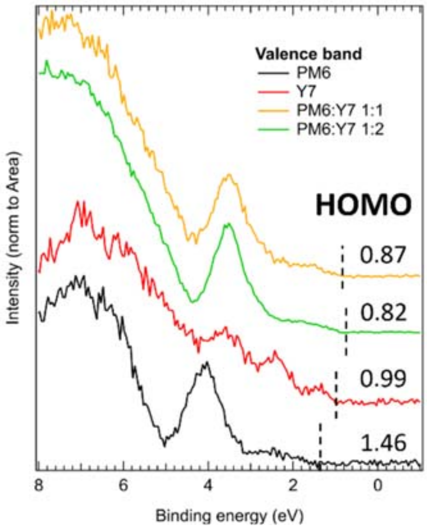

Figure 1. Valence band spectra of the neat PM6 and Y7 thin films and the blend PM6:Y7 with different ratios.

This work aims to investigate the electronic structure and the energy band alignment of spin-coated PM6/Y7 thin films, by studying the evolution of the core levels, the work function, and the frontier orbitals (valence and conduction bands) as a function of the different ratio between the donor and acceptor molecule in the blend (1:0, 0:1, 1:1, 2:1, 1:2). By recording X-ray and UV photoemission spectroscopy and X-ray absorption spectroscopy spectra during several synchrotron campaigns, we observed a decrease in the bandgap from the neat molecules to the 1:1 blend and a further decrease when transitioning to the 1:2 or 2:1 blend (Fig. 1).

In standard blend junction solar cell architectures, organic blends are linked to transition metal oxide electron transport layers (ETLs). Since the interplay at the interface between the oxide and the acceptor molecule also plays an important role in the device's performance, we examined the ETL ZnO nanoparticles spin-coated on ITO, particularly its interface with the Y7 acceptor. This has been possible thanks to the spray deposition technique that allowed a vacuum deposition of a Y7 thin film on the ZnO substrate directly connected to in-situ characterization. Starting from the confirmation

In standard blend junction solar cell architectures, organic blends are linked to transition metal oxide electron transport layers (ETLs). Since the interplay at the interface between the oxide and the acceptor molecule also plays an important role in the device's performance, we examined the ETL ZnO nanoparticles spin-coated on ITO, particularly its interface with the Y7 acceptor. This has been possible thanks to the spray deposition technique that allowed a vacuum deposition of a Y7 thin film on the ZnO substrate directly connected to in-situ characterization. Starting from the confirmation of our successful deposition, we noticed a strong modification of the Cl 2p core level shape as a function of the thickness of the sprayed film, which is highlighted by the appearance of a new feature.

In summary, we have taken a significant step forward in understanding this efficient, unexplored system by observing notable electronic structure changes between the pure molecules and the blend and the emergence of a new feature at the interface between NFA and ETL.

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Operando XAS Studies of Copper Porphyrin Organic Electrodes for Lithium Ion Batteries

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ABSTRACT

Porphyrin materials have demonstrated promising electrochemical properties in different battery chemistries [1-4]. The advantage of these materials lies in fast kinetics allowing rapid charging, which is interlinked to a high-power density, and outstanding cycling stability. Especially, the copper porphyrin derivatives reveals beneficial qualities like higher energy densities. CuDEPP, shortly for 15-bis(ethynyl)-10,20-diphenylpor-phinato] copper (II), has proven that it can be efficiently used in Li, Na- and K- Ion batteries. [5-7]. However, the present understanding of the redox mechanism for CuDEPP electrode remains incomplete and the role of central metal atom was not clearly revealed. Previous XPS results suggested a reduction reaction of Cu(II) to Cu(I) during the first discharge, and recent studies [8] stated that this Cu reduction already occurred during the initial charging, and Cu atoms reversibly participated in the redox reaction. To further improve the properties of these organic electrode materials, a deeper investigation of the redox chemistry and the materials evolution is needed.

This work was dedicated to address the fundamental mechanism for CuDEPP electrodes in Li-ion batteries by means of synchrotron *operando* X-ray absorption spectroscopy. It aims to monitor the oxidation states and local environment of Cu during cycling and to confirm the role of the central atoms as well as how they contribute to the overall charge storage mechanism. We expect to exploit this knowledge to aid the purposeful design of novel porphyrin materials with improved performance for the development of full organic Li-ion batteries as well as post-Li storage systems.

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Operando Battery Characterization via Full-field Quick-XAS Imaging at ROCK Beamline

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ABSTRACT

Full-field XAS hyperspectral imaging has been recently developed at ROCK beamline [1, 2]; a technical advancement that exploits the beam size tunability and the quick-XAS setup, together with a bidimensional detector with high-rate micrometric pixel size. This technique is of special relevance for the characterization of functional materials under working conditions (*operando*), as it adds spatial information to the hitherto time-resolved experiments. Here, we show the first results in the context of operando battery characterization. The analysed sample was a half-cell Li-ion battery, with $LiNiO_2$ (LNO) used as positive electrode and LP57 as electrolyte. The in situ electrochemical cell [3] was cycled from OCV to 4.3 V at the C/4 c-rate, corresponding to the extraction of 1 Li^+ in 4 hours. The experimental setup allowed obtaining a complete set of spatially resolved XAS spectra (a hyperspectral cube) in only 11 seconds. Having access to single-pixel spectral information, we are able to detect differences in the local structure and oxidation state of LNO electrode upon cycling, which can be related to the homogeneity of the Li extraction mechanism.

Additionally, new tools for data analysis have been developed at ROCK. They allow a smooth analysis of these hyperspectral maps, and facilitate their correlation with the evolution of electrochemical parameters. The use of Jupyter notebooks has demonstrated to be a user-friendly option with an open-access interface that allows to easily perform all steps of image data treatment, including pixel binning, energy calibration, and normalization of each single pixel XAS spectrum.

This experiment was done in the framework of the BIG-MAP European project, which has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 957189. The project is part of BATTERY 2030+, the large-scale European research initiative for inventing the sustainable batteries of the future.

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Experimental Study of Polarization-dependent PCI Effect in Neon and Water following K-shell Photoionization

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ABSTRACT

***Keywords**: Photoelectron, post-collision interaction, polarization, recapture of photoelectron*

Photoionization of an atom near the ionization threshold of an inner shell induces the emission of a slow photoelectron, followed by the emission of a high kinetic energy Auger electron during the subsequent relaxation process, leading to the atom acquiring a doubly positive charge [1]. The three-body interaction between the emitted electrons and the ion involves energy and angular momentum exchange [2]. This phenomenon is termed post-collision interaction (PCI). Despite more than three decades of study [3], a comprehensive understanding of PCI remains elusive. In a pursuit to refine our understanding of PCI, our experimental investigation focuses on delineating various aspects of this interaction, particularly the exchange of energy and angular momentum. The study is specifically conducted on neon atoms and water molecules, two isoelectronic species in the gas phase, examining the O 1s edge for water and the 1s edge in neon. Slow photoelectron spectra, recorded using polarized light at energies above the ionization thresholds, were analyzed. The experimental setup utilized the PLEIADES beamline at SOLEIL, providing access to the relevant soft X-ray energy range with high energy resolution and variable polarization. A SCIENTA analyzer permitted the recording of spectra at high resolution. Our observations reveal a significant PCI shift for both neon and water, depending on the photon energy. Moreover, a more pronounced effect was observed with horizontally polarized X-rays compared to vertically polarized X-rays at identical photon energies. Notably, the considerable energy exchange in neon 1s ionization led to the recapture of photoelectrons in higher Rydberg states.

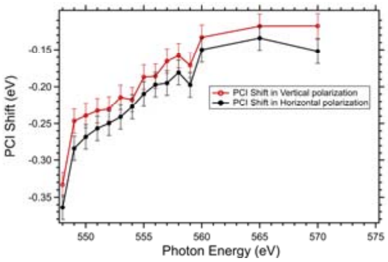

Figure 1: Energy shift observed for water vapor above the Oxygen 1s edge. The graphical representation is asfollows: The X-axis denotes the post-collision interaction (PCI) shifts, while the Y-axis shows the photon energy. The red curve, marked with circles, shows the PCI shift under vertical polarization, and the black curve, annotated with dots, shows the PCI shift under horizontal polarization.

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Analysis of the Organic-inorganic Interface in M. Fruticosa: A Multi-technique Approach

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ABSTRACT

Muricea fruticosa is a species of octocorals found near the Pacific coast of Costa Rica, in Cocos Island, National Park.[1] Like other octocorals, this species is characterized by a reddish coloration, originating from the presence of organic pigments. These pigments belong to the polyene family and are included within the inorganic matrix biomineralized by the organism.[2] This matrix is formed by sclerites, skeletal structures composed of magnesian calcite and 1% organic matter, predominantly formed by acidic proteins.[3]

In addition to these structures, within the branches, there is another structural unit composed of a protein called gorgonin. In this species, the axis has been poorly studied, and due to its characteristics, it is believed to be mineralized.[4] Thus, octocorals of the M. fruticosa species comprise a binary skeletal system. For this reason, it becomes an ideal system to study the organic-inorganic interface in this type of biominerals.

Through Raman imaging, it was determined that the distribution of pigment within the calcite is heterogeneous and associated with the presence of microprotuberances in the sclerites. Synchrotron radiation fluorescence microscopy allowed distinguishing signals associated with the autofluorescence of the pigment and its distribution within the sclerite, reflecting the radial growth of the structure. By coupling this technique with Second Harmonic Generation Microscopy, it was determined that this pigment has nanoscale ordering, where pigment molecules are aligned with each other.[5] Although the pigment exhibits a high degree of intermolecular ordering, it does not appear to be directly associated with calcite since x-Ray diffraction patterns show no change in the crystalline structure of pigmented calcite.

Additionally, through the combination of scanning electron microscopy (SEM) coupled with EDX and powder X-ray diffraction, it was determined that the coral axis is mineralized with hydroxyapatite nanocrystals. It was demonstrated through synchrotron X-ray microcomputed tomography that the composition of the axis is highly heterogeneous.[6] Thus, the axis is composed of regions with different degrees of mineralization according to the mechanical requirements of the coral branch. These results not only prove the presence of a new biomineral but also confirm the existence of one of the few organisms that mineralize both calcite exoskeleton and hydroxyapatite endoskeleton simultaneously.[4]

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SAXS from Cellulose Solution: Interchain Effects

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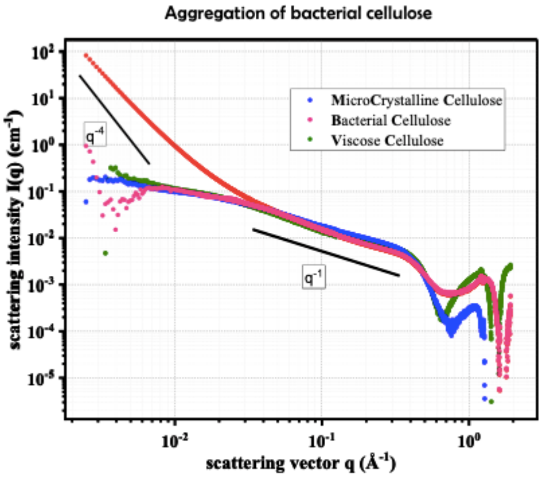
ABSTRACT.

Cellulose is a renewable bio-polymer that has the potential to replace non-biodegradable materials in various technological applications. In many processes, it is first dissolved, then processed (e.g. by spinning), and finally “regenerated” (recrystallization by adding water). However, dissolution from the very stable crystal structure requires harsh, pollutant solvents for individual chains to stay in solution. Ionic liquids (ILs) have emerged as a non-polluting solvent that can dissolve cellulose effectively since 2002. The mechanism by which ILs are successful solvents for cellulose has garnered much interest and some controversy.

We have undertaken studies of such solutions using SAXS, in particular at SWING, which is very useful since the contrast is low and the chain conformation close to the one of a thin rod (intensity lower than 1 cm^{-1}). Our **large concentration** range (0.0005 - 0.3 g/g), enables us to revisit former results, showing progressively interchain effects:

- in well dissolved cases, solution scattering implies a **structure factor**, which applies in two successive regimes of concentration and is interesting from a basic point of view, and in relation with solutions rheology.
- for very high concentration, **crystals** are observed at large q (WAXS). We have modelled that by studying solvent penetration **in** nanocellulose crystals of a fiber, through scanning of a gradient of concentration during swelling, using the unique possibilities offered by the narrow beam available on SWING.
- in presence of a small **percentage of water** (the good IL solvents are hygroscopic), a stronger scattering can be measured suggesting strong concentration fluctuations, or **biphasic structure**, which can be useful to understand the first stages of the “regeneration” step (recrystallization by adding water), necessary to obtain the final products, such as fibers.



- comparison **between plant and bacterial** cellulose scattering evidences nice super-position at large q with additional low q scattering from aggregates, which can be subtracted (see red points in Figure). This widens the way to neutron scattering experiments using deuteriated chains.

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Polyamino-isoprenic Compound NV716 Disrupts the Outer Membrane of *Pseudomonas Aeruginosa* and Creates a New Sensitivity to Doxycycline

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ABSTRACT

Increasing antibacterial resistance represents a major challenge in antibiotic discovery. Attractive targets in Gram-negative bacteria are (i) their unique asymmetric outer membrane, which acts as a permeability barrier that protects the cells from external stresses, such as antibiotics, and (ii) multidrug efflux pumps, which actively expel a wide range of antibiotic substrates. We previously identified novel polyamino-isoprenic compounds that act synergistically with doxycycline against *Pseudomonas aeruginosa* (1).

In this work, we describe the impact of compound NV716 on antibiotic accumulation and its mode of action on bacterial envelopes. Based on the intrinsic fluorescence properties of doxycycline, accumulation was quantified in bacteria by using spectrofluorimetry and fluorescent microscopy on DISCO beamline. First, we found that the presence of NV716 significantly increases accumulation of doxycycline in *Pseudomonas aeruginosa* in both the wild-type (PAO1) strain and in a derivative mutant deleted of the major efflux pumps (PA403, D*mex4*), suggesting NV716 does not targets efflux. We then measured the initial accumulation rates in the presence of various external concentration of doxycycline and concluded that NV716 increased permeation rate of doxycycline by a factor of 4.

We next investigated the mode of action of NV716 using biochemical assays and several microscopy techniques. Results indicate that NV716 induces outer membrane perturbation probably by interacting with the lipopolysaccharide.

Altogether, our results open a new avenue for the use of compounds to renew sensitivity for non-permeable antibiotic by disrupting the primary barrier to accumulation.

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The Magic Scroll of Ampus (Var, France) Future “Musée des Ecritures”

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UMR9022 Héritage/s: culture/s, patrimoine/s, création/s, Conseil scientifique du Musée des Ecritures
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ABSTRACT

The magic scroll belongs to the collection of the future “Musée des Ecritures” in Ampus (Var, France). Some engraved characters can be observed on the outside of the roll, indicating that something was written on the surface (figure 1). Unfortunately, due to the corrosion of the metal, it is impossible to unroll it physically without deterioration, destroying the object.

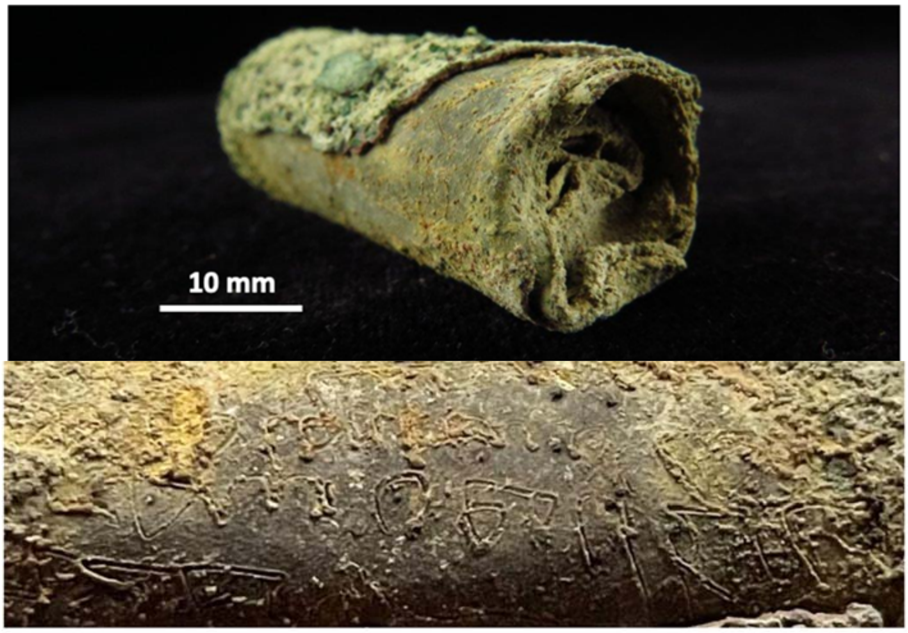

Figure 1: image of the magic scroll; close up of characters engraved on the outside surface.

To determine the origin of the characters scratched onto the roll and to read them, a tomographic study has been performed on the PSICHÉ beamline of SOLEIL. Due to the unexpectedly strong absorption of the metal, we were forced to increase the photon energy to the maximum available 120 keV in pink beam mode. The attenuation is due to the alloy containing a large proportion of lead, subsequently confirmed by fluorescence measurements performed at the PUMA beamline of SOLEIL.

A tomograph of the full axial length of the scroll (~45mm) was acquired using a helicoidal scanning acquisition. Using the reconstructed volume, the scroll has been virtually unrolled using Python routines, and visualized using Avizo software. The reconstruction shows that both faces of the metal foil are engraved with text. This was possible because of the thickness of the metallic sheet (250 µm).

A film, recorded during the experiment, will be shown in the first part of this presentation, and the reconstructed data will be presented.

Functional and Structural Insights into the Multi-step Activation and Catalytic Mechanism of Bacterial ExoY Nucleotidyl Cyclase Toxins Bound to Actin-profilin

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ABSTRACT

Nucleotidyl cyclase (NC) enzymes are important ubiquitous enzymes that catalyze the production of cyclic nucleotides, crucial second messengers involved in numerous signaling pathways. Bacterial virulence factors known as ExoY-like toxins are produced by diverse Gram-negative γ- and β-proteobacteria. These toxins are part of a broader family of bacterial NC toxins, sharing a structurally-related catalytic NC domain [1, 2]. When delivered into eukaryotic cells, they rely on eukaryote-specific proteins as cofactors to become potent NC enzymes. They subsequently disrupt host cell signalling by overproducing both cyclic purine (cAMP, cGMP) and pyrimidine (cCMP, cUMP) nucleotides. The molecular and mechanistic intricacies governing the activation and catalytic specificities of NC toxins remain partly elusive, yet are vital for unraveling their virulence mechanisms in host cells. We have shown that ExoY toxins employ an atypical eukaryotic cofactor, namely actin [3]. Adding to the complexity, homologous ExoY-like NC toxins that exhibit significant sequence variations use either polymerized/filamentous actin (F-actin) or monomeric/globular actin (G-actin) as a cofactor [4]. In this study, we investigate the Vibrio nigripulchritudo Multifunctional-Autoprocessing Repeats-in-ToXin (MARTX) ExoY effector domain (Vn-ExoY) as a model for ExoY-type members that interact with G-actin but not F-actin.

Our in vitro investigations first revealed the physiological cofactor at work within host eukaryotic cells. These ExoYs activate by capturing and sequestering the cytoskeletal G-actin-profilin complex, disrupting its regulatory functions in the dynamic assembly of actin [5].

Using X-ray crystallography, we have intercepted several structural snapshots along the ExoY activation pathway by G-actin or G-actin-profilin. These structural data reveal unprecedented mechanistic details of how the active site of all NC toxins undergoes progressive remodeling upon cofactor and substrate binding. They reveal how NC toxins can accommodate nucleotides of different sizes as substrates and clarify crucial aspects for their catalytic reaction of purinyl and pyrimidinyl cyclases. These structural insights into the multi-step activation of NC toxins may open new avenues to inhibit specifically this class of toxic bacterial NCs [5].

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Characterizing Red Coloring Matter Samples from the Altamira Cave using Semi-quantitative Chemical Imaging and X-ray Absorption at the PUMA Beamline, SOLEIL

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ABSTRACT

Paleolithic cave art stands as one of the earliest forms of art of modern humans, and as such it is important and necessary to analyze it and aim for a better comprehension of it. The coloring matters that can frequently be found are black, red or yellow. The study of black Paleolithic coloring matter has been well developed, and analytical procedures have been established [1],[2]. However, the study of reds is more complicated, as the coloring matter and the cave wall support present a similar chemical composition [3]. The aims pursued in our ongoing research are to improve the red Paleolithic pigments' characterization with respect to the *in situ* analyses that can be undertaken with a portable instrument in a cave, and to find differentiation criteria between the composition of the walls and that of the coloring matter, which would help to improve the performances of these *in situ* measurements [4].

In this study we present the results of the micro-X-ray fluorescence (µXRF) and X-ray absorption (XANES) analyses at PUMA, SOLEIL, of red coloring matter samples coming from different figures from one of the most important and renown examples of polychrome cave art, the Techo de los Polícromos from the cave of Altamira in Northern Spain. Applying such sensitive non-destructive techniques allowed us to study trace elements, chemical markers, and phases and identify the coloring matter in a way that is not possible *in situ* as of today (namely with portable XRF and X-ray diffraction). Here we present results of the characterization of these red samples, along with a comparative analysis of different representations between them. These may yield new insights on the creation steps of these prehistoric figures. Finally, we further improved the identification of elements to be searched for during *in situ* analyses with a pXRF equipment such as Ti, Cr, Mn, Zn, Rb, Sr or Br in tis cave or in others.

Figure 1. Techo de Los Polícromos, Altamira, with one of the analyzed locations marked with a white cross. © J. Tapia /CNRS-C2RMF

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Determination of the Temperature Dependence of the Refractive Index of Ice in the Fir

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ABSTRACT

Ice clouds play a major role in the atmospheric radiation budget. Therefore, being able to accurately simulate the radiative impact of ice clouds and its evolution under climate change is a key issue in climate science. For these simulations, models rely on datasets of ice cloud optical properties themselves computed from the complex refractive index (CRI) of ice. However, until now, experimental data of ice CRI in the far infrared were limited to temperatures under 195 K, with higher temperatures data (relevant to the Earth atmosphere) being linearly extrapolated from these low temperature values and may therefore be questionable for temperatures measured in cirrus clouds. In this context, we performed FIR transmission measurements on water ice films in a wide range including the temperature range useful for atmospheric simulations (50 - 300 K). To optimize the signal to noise ratio, the measurements were performed using synchrotron radiation at the beamline AILES of the Synchrotron SOLEIL facility. From transmission experiments we are able to obtain absorptivity, which is directly related to the imaginary part of the CRI, and use a Kramers-Kroenig based algorithm to compute the real part.

From the preliminary analysis of absorbance spectra, we obtained interesting results regarding the temperature behavior of the refractive index of ice in the FIR. The main reference values used to compute ice cloud optical properties in atmospheric models in the FIR region are those compiled by Warren and Brandt (2008) (WB08) at 266 K, who linearly extrapolated the spectrum from the data of Curtis et al. (2005). We first compared the temperature dependence of the position of the main peak of the connectivity band (around 220 cm-1) and found significant discrepancies.

This presentation will also describe the set up used to date and detail its limitations as well as the new optimizing set up in order to reduce the experimental uncertainties.

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Ultrastructural Insights into Dentin using PXCT

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INTRODUCTION

Dentin is the most important component of the tooth, located beneath the enamel, surrounding the pulp tissue. This highly mineralized tissue is composed of numerous microscale tubules. We can distinguish peritubular dentin (PTD) and intertubular dentin (ITD). ITD mostly contains type 1 collagen matrix mineralized with hydroxyapatite crystals. At the nanoscale, ITD is structured as a complex interweaving of collagen fibrils (100nm in diameter) and 5nm thick mineral platelets (1). PTD encircle tubules and are characterized by a dense mineral matrix. We present here an X-ray ptychotomography study of the dentinal tissue with a resolution of 31nm, allowing us to visualize this tissue hierarchical organization.

MATERIALS AND METHODS

One decidual tooth was examined. The tooth underwent cutting and polishing using classical techniques. Cylindrical samples measuring 20µm in both height and diameter were extracted, with a first step of coarse micromachining followed by the extraction and fixation of the sample on the pin, using FIB-SEM techniques. PXCT experiments were conducted at Synchrotron Soleil on the SWING beamline (2). A coherent X-ray beam with an energy of 8 keV was focused ahead of the sample position, resulting in a probe size of 4µm. For each tomographic projection, approximately 500 diffraction patterns were recorded, with an exposure time of 0.1s each by scanning the sample with a step size of 1µm. This procedure was repeated for about 600 evenly spaced angular positions as the sample rotated over 180°.

RESULTS AND CONCLUSION

Our observations have corroborated the existence of hypermineralized tissue encircling the tubules, with similar hypermineralized formations adjacent to the lateral branches emanating from these tubules. We also note the presence of two phases with different electron densities in the ITD, potentially corresponding to collagen fibrils intertwined with a denser phase, corresponding to the hydroxyapatite crystals. In the PTD, we observe two distinct phases: a peripheral interphase containing fibrils wrapping the inner PTD. This peripheral PTD is less mineralized. However peripheral PTD fibrils seem to be more mineralized than their counterparts in the ITD. In the ITD, we can distinguish and analyze the fibrils organization that seems to form a bird's nest structure around the tubules. These observations, not yet documented in the existing literature, were made possible through the extremely high resolution of PXCT data. They are expected to contribute to a deeper understanding of the physiology and pathology of dentin.

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User-friendly tools implemented in Fastosh to visualize and interpret Wavelet Transform of the EXAFS

Gautier Landrot & Emiliano Fonda

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ABSTRACT

Wavelet transform of the EXAFS may reveal some information that can be less obvious to notice from a simple observation of the Fourier Transform/Reverse Fourier Transform spectra. For instance, it can reveal the presence of two overlapping atomic shells occurring at similar distances and featuring neighboring atoms whose weights are significantly different from each other. Despite the development of Cauchy or Morlet Wavelets adapted to EXAFS is not recent (1,2), available algorithms to perform such operation are still scarce. The newest version of Fastosh features several functions that enable to visualize and interpret the Cauchy or Morlet Wavelet transform of an EXAFS spectrum. Similarly to Fourier Transform, Wavelet Transform can be simply performed directly from Fastosh's Main GUI where raw XAFS data is loaded and the results are plotted in a secondary window. Four approaches are available to display the results: 1) the Wavelet Transform map can be displayed by itself as a surface & contours, surface, or contours 2) The Wavelet spectrum can be interactively displayed: one can then visualize where the chi spectrum is locally processed by the Wavelet to obtain each pixel of the Wavelet Transform map, and understand what are the effects of the Wavelet parameters (e.g. Morlet Wavelet's η and sigma, or Cauchy's Wavelet's n) on the shape of the Wavelet spectrum employed. 3) The Reverse Wavelet Transform can be displayed 4) Additional Wavelet maps, corresponding to theoritical single-scattering chi spectra generated with FEFF8L using a user-friendly interface, can be stacked on top of the Wavelet map of the sample. This can be useful as a simple, pre- shell-by-shell fitting procedure to elucidate the local neighboring atomic environment of an absorber present in a sample, as demonstrated in this communication using examples of EXAFS spectra corresponding to known structures. The newest version of Fastosh (v1.0.7), which includes these new functionnalities and FEFF8L (no additionnal installation required), for Windows, Mac, or Linux, is available for free download on SAMBA beamline's website.

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TUTORIALS

TUTORIALS

Friday, January 19th

TU-01 *SOLEIL Reception Building Auditorium - Ground Floor*

15:00 - 17:00 Data Treatment and Analysis on SIXS

Surface X ray Diffraction (SXRD) data reduction and analysis

In this tutorial the reduction and analysis of surface diffraction and scattering data will be shown for users.
After a brief reminder on the technique basis and data collection strategy, the participants will be guided in the use of BINoculars-NG, a program developed at ESRF and refurbished at SOLEIL that allows to reduce the data, starting from images collected by a 2D hybrid detector. Data can be projected in a datacube in different spaces, depending on the experimental needs. Available spaces are *q*-space, *hkl*-space, angular-space, mixed (time, angle, q,…) – spaces. Once the dataset reduced in the desired space, data integration along desired space directions can be achieved. The tutorial will show how to manage the data collected on a sample surface and how to obtain the surface structure starting from the diffusion rods integrated by BINoculars. ROD program developed by E. Vleg will allow to solve the structure.

All the users who want to discover surface x-ray diffraction data treatments available at the SixS beamline are welcome.

The participant needs a PC with no special requirements but a wifi connection. The program and the data will be available on a dedicated space on the DARTS platform.

(1) http://dx.doi.org/10.1107/S1600576715009607
(2) https://doi.org/10.1107/S0021889899013655

Location: SOLEIL, Pavillon d’accueil

Organizers: SixS beamline (A. Coati, Y. Garreau, A. Resta, M. Sauvage-Simkin, A. Vlad) and GRADES group (F. Picca, E Farhi)

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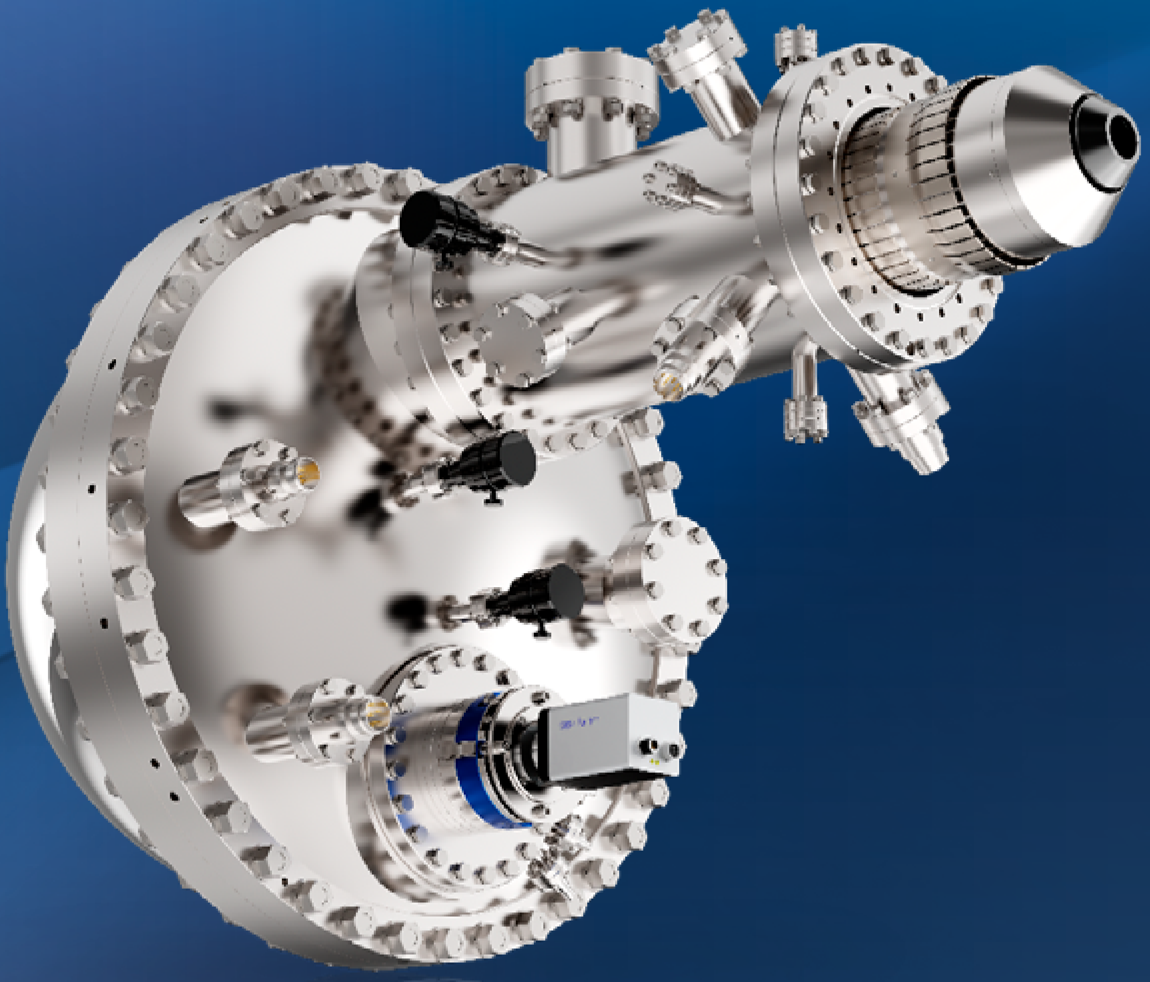

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