20th SOLEIL USERS' MEETING

JANUARY 14th - 16th, 2026

Synchrotron SOLEIL (Saint-Aubin)

SCIENTIFIC COMMITTEE

Paloma FERNANDEZ VARELA (CNRS - on availability)
Lorella PASCOLO (Institute for Maternal and Child Health - Burlo Garofolo Pediatric Institute - Trieste - Italy)
Charlotte CATROUILLET (Institut de Physique du Globe de Paris)
Simona RANERI (University of Florence - Department of Earth Sciences – Florence - Italy)
Pierre ASSELIN (De la Molécule aux Nano-objets : Réactivité, Interactions et Spectroscopies - Paris)
Helgi Rafn HRODMARSSON (Laboratoire inter-universitaire des systèmes atmosphèriques - Créteil)
Amélie BORDAGE (Institut de Chimie Moléculaire et des Matériaux d'Orsay - Orsay)
Eglantine BOULARD (Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie - Paris)
Sara GONZALEZ (Institut de Nanotechnologies de Lyon - Villeurbanne)
Fabien SILLY (CEA SPEC - Gif-Sur-Yvette)
Luis CARDENAS (Institut de recherches sur la catalyse et l'environnement - Villeurbanne)
Asma TOUGERTI (Unité de Catalyse et de Chimie du Solide - Université de Lille – Villeneuve d'Ascq)

SOLEIL SYNCHROTRON

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    - Physics & Advanced Materials (Structural, electronic and magnetic properties of matter / Physical surfaces and interfaces)

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Welcome

The 20th SOLEIL Users' Meeting takes place from Thursday January 15th to Friday 16th, 2026 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 beamlines.
It is also the occasion to share scientific, technical and practical issues about the Synchrotron radiation use.
The plenary talks cover recent research highlights of SOLEIL in the following areas:

- Soft Matter,
- Geoscience.

Scientific communications are presented during three parallel sessions, selected from the submitted abstracts.
In the afternoon of January 15th and 16th, a social time is held at SOLEIL with stands from Commercial exhibitors and the Conference dinner.

The novelty of this SUM2026 is the discussion times with two posters sessions: one dedicated to the synchrotron community (beamlines, scientific associations, …) and one dedicated to science.

The new session dedicated to the synchrotron community, on January 15th, offers time to discover all its sides and to discuss together as a community. For instance, the scientists of beamlines present an overview of their beamlines and their perspectives, while the scientific associations present their goal and some of their actions.

The science session on January 16th, is, as usual, dedicated to scientific results obtained (at least partially) thanks to SOLEIL, with a prize attributed to the best PhD student poster.

A multidisciplinary satellite workshop « Radiation Damage » is held on Wednesday 14th of January, 2026 at SOLEIL.

A satellite meeting is organized for the French community of X-ray absorption spectroscopists at SOLEIL on Friday afternoon the 16th of January, 2026.

Bienvenue

Le 20ème Colloque des Utilisateurs de SOLEIL se tient les jeudi 15 et vendredi 16 janvier 2026, 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.
Les conférences plénières couvrent les thèmes de recherche de la communauté des utilisateurs de SOLEIL suivants :

- Matière molle,
- Géosciences.

Les sessions parallèles sont composées d'exposés scientifiques originaux, sélectionnées à partir des résumés soumis.
Des temps de convivialités sont organisés à SOLEIL les jeudi 15 et vendredi 16 janvier 2026 avec les stands d'entreprises et le diner de la conférence.

La nouveauté de ce SUM2026 est dans les temps de discussions avec deux sessions posters : une dédiée à la communauté synchrotron (lignes, associations savantes, …) et une session scientifique.

La nouvelle session dédiée à la communauté synchrotron du 15/01, permet de découvrir tous ses aspects et de discuter ensemble en tant que communauté. Par exemple, les scientifiques de ligne présentent une vue d'ensemble et des perspectives pour leur ligne, et les associations savantes leur but et actions.

La session scientifique du 16/01, est dédiée, de manière plus traditionnelle, aux résultats scientifiques obtenus (au moins en partie) grâce à SOLEIL ; un prix est attribué au meilleur poster présenté par un doctorant.

Un atelier thématique multidisciplinaire « Radiation Damage » a lieu le mercredi 14 janvier 2026 à SOLEIL.

Une réunion-satellite de la communauté française des spectroscopistes d'absorption des rayons X est également organisée le vendredi 16 janvier 2026 après-midi à SOLEIL.

Radiation Damage Satellite Workshop

Chairpersons: Amélie Bordage, Laurent Tranchant, Simona Raneri,
Amelia Suzuki, Charlotte Catrouillet

Wednesday, January 14th, 2026

SOLEIL Auditorium - Main Building

09:00 - 09:30	Registration – Welcome – Coffee
09:30 - 09:40	Introduction to the workshop ***Amélie Bordage*** *- S2UO chair*
09:40 - 10:25	**Plenary Talk** Radiation damage in macromolecular crystallography: What is it and why do we care? ***Prof. Elspeth Garman*** *- Department of Biochemistry, University of Oxford, UK*
10:25 - 11:00	**Plenary Talk** Beam damage and safe analysis: A study of how perception, perspective, and vocabulary shape the construction of risk ***Dr. Mathieu Thoury*** *- IPANEMA, St Aubin, France*
11:00 - 12:30	A multidisciplinary viewpoint to radiation damage ***Stéphanie Belin, Christophe Sandt, Jean Susini*** *- Synchrotron SOLEIL, Saint-Aubin, France* ***Marine Fournier*** *- LCPMR Sorbonne Université, Paris, France*
12:30 - 13:45	*Lunch*
13:45 - 14:30	Introduction to round table ***Dr. Amelia Suzuki*** *- Institute of Heritage Science ISPC-CNR of Florence, Italy* ***Dr. Marine Cotte*** *- ESRF, Grenoble, France*
14:30 - 16:00	Interactive and multidisciplinary round table ***Dr. Amélie Bordage*** *- Institut de Chimie Moléculaire et des Matériaux d'Orsay, France* ***Dr. Laurent Tranchant*** *- Synchrotron SOLEIL, Saint-Aubin, France*
16:00 - 16:30	*Coffee break setting up in front of the SOLEIL amphitheater.*
16:30 - 17:20	**Tutorial** The RADDOSE-3D software program ***Prof. Elspeth Garman -*** *Department of Biochemistry, University of Oxford, UK*
17:20 - 17:30	**Conclusion** ***Myrtille Hunault*** *- Synchrotron SOLEIL, Saint-Aubin, France* ***Amélie Bordage*** *- S2UO chair*

Thursday, January 15th, 2026

SOLEIL Users' Meeting
January 14th - 16th, 2026
Synchrotron SOLEIL, Saint-Aubin - France

SOLEIL Auditorium - Main Building

09:00 - 10:00	Registration & coffee
10:00 - 10:10	Welcome / Introduction, S2UO Chair - ***Amélie Bordage***
10:10 - 10:50	Latest news from SOLEIL, General Director - ***Jean Susini***
10:50 - 11:35	**Plenary Talk** - Soft Matter Structure, properties and reactivity of oxide nanoparticles in solution: Synchrotron studies ***Olivier Diat & Matthieu Virot*** **-** *Institut de Chimie Séparative de Marcoule, Bagnols sur Cèze France*
11:35 - 12:05	Towards SOLEIL II: The Experiment Division Perspective - ***Eva Pereiro, Amina Taleb***
12:05 - 13:30	*Lunch*
13:30 - 15:40	**Parallel sessions** – 5 different rooms • Biology and Health • Chemistry & Soft Matter (Characterization of structure and properties of chemical materials, reactivity, catalysis, chemical surfaces and interfaces / Soft matter) • Diluted matter • Geosciences / Environment / Cultural Heritage • Physics & Advanced Materials (Structural, electronic and magnetic properties of matter / Physical surfaces and interfaces)
15:40 - 16:10	*Coffee break setting up in front of the SOLEIL amphitheater.*
16:10 - 18:20	**Parallel sessions** – 5 different rooms • Biology and Health • Chemistry & Soft Matter (Characterization of structure and properties of chemical materials, reactivity, catalysis, chemical surfaces and interfaces / Soft matter) • Diluted matter • Geosciences / Environment / Cultural Heritage • Physics & Advanced Materials (Structural, electronic and magnetic properties of matter / Physical surfaces and interfaces)
18:30 - 20:00	**The Synchrotron Community posters session** Commercial Exhibitors / Aperitif
20:00 - 21:30	*Dinner*
21:30	*Bus transfer*

Friday, January 16th, 2026

SOLEIL Auditorium - Main Building

9:00 - 09:45	**Plenary Talk -** Geosciences Structure Surface reactivity of tubular Al/Si nanoparticles: interactions with nucleic acids and implications for prebiotic scenarios ***Jérôme Rose*** *- CEREGE, Aix-en-Provence, France*
09:45 - 11:45	**Scientific Posters session -** *Coffee break setting up in front of the SOLEIL amphitheater.*
11:45 - 12:00	**Award of the best student poster** - **Roger Fourme Prize** Conclusion
12:00 - 13:30	*Lunch*
13:30 - 15:00	**Visit of 4 Beamlines** - *DESIRS / MARS / PROXIMA-1 / SIXS*

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13:30 - 16:30	**TEA-XAS Meeting** SOLEIL Auditorium - Main Building
13:30 - 13:35	Introduction
13:35 -14:50	Status and projects of the XAS beamlines and laboratory instruments ***Delphine Vantelon*** *(SOLEIL),* ***Olivier Proux*** *(FAME/FAME-UHD),* ***Marine Cotte*** *(ESRF),* ***Sophie Nowak*** *(ITODYS) &* ***Benoît Baptiste*** *(IMPMC)*
14:50 - 15:00	Status of the project to unite the French community of X-ray absorption spectroscopists ***Amélie Bordage*** *(S2UO)*
15:00 - 16:00	Interactive round table ***Amélie Bordage, Charlotte Catrouillet*** *(S2UO)*
16:00 - 16:30	Plenary discussion and conclusions

Parallel Session Schedule

Biology and Health

Chairpersons: Paloma Fernandez Varela & Lorella Pascolo

SOLEIL - Reception Building Auditorium

Thursday, January 15th, 2026

13:30 - 14:00 (25'+5')	From tissue to trace: an elemental investigation of bromine in healthy and diseased ovarian tissue ***Anna Flamigni*** *- IRCCS Ospedale Infantile Burlo Garofolo, Italy*
14:00 - 14:25 (20'+5')	Stuctural insights into tecovirimat antiviral activity and poxvirus resistance ***Riccardo Vernuccio*** *- Institut Pasteur, Paris, France*
14:25 - 14:50 (20'+5')	Small angle X-ray scattering structural characterization of quinones oxidoreductases ζcrystallins using SOLEIL SWING beamline ***Nicolas Mousnier*** *- Centre de Recherche Paul Pascal, Pessac, France*
14:50 - 15:15 (20+5')	Probing the colloidal behavior of polysaccharides-degrading enzyme in a highly constrained model system ***Hugo Voisin*** *- INRAE Nantes, France*
15:15 - 15:40 (20+5')	Tracing metal contaminants in environmental plastics pellets and mammalian tissues using XRF mapping at PUMA ***Alessandra Gianoncelli*** *- Elettra, Sincrotrone Trieste, Italy*
15:40 - 16:10	*Coffee break*
16:10 - 16:35 (20'+5')	Designing cryo-correlative workflows: Understanding radiation damage risks in HEK293-XpaQ ***Harisa Rista*** *- Synchrotron SOLEIL, Saint-Aubin, France*
16:35 - 17:00 (20+5')	Detection of titanium dioxide particles in human, animal and infant formula milk ***Anne Burtey*** *- Génétique Animale et Biologie Intégrative, Jouy-en-Josas, France*
17:00 - 17:30 (25'+5')	The role of the gut in dementia ***Alessia Cedola*** *- CNR-NANOTEC, Italie*
17:30 - 17:55 (20'+5')	Mechanical phenomena occurring in tissue during subcutaneous injections ***Aurélien Baquié*** *- Nemera, Lyon & INSERM Sainbiose, Saint-Étienne, France*
17:55 - 18:20 (20'+5')	Structural and functional characterization of human tissue nonspecific alkaline phosphatase ***Pierre-Damien Coureux*** *- I2BC, Gif-sur-Yvette, France : Présentation by* ***Iliass Imam*** *- Université Claude Bernard Lyon 1, France*

Parallel Session Schedule

Chemistry & Soft Matter
(Characterization of structure and properties of chemical materials, reactivity, catalysis, chemical surfaces and interfaces / Soft matter)

Chairpersons: Luis Cardenas, Asma Tougerti & Amélie Bordage

SOLEIL Auditorium - Main Building

Thursday, January 15th, 2026

13:30 - 14:00 (25'+5')	STXM as a tool for studying the morphology of organic semiconducting nanoparticles for energy applications ***Anne Hebraud*** *- Institut de Chimie et Procédés pour l'Energie, l'Environnement et la Santé, Strasbourg, France*
14:00 - 14:25 (20'+5')	Revealing the mechanisms of enhanced photo-electrocatalytic OER performance of Ni doped maghemite via operando XAFS ***Francesco Paparoni*** *- Synchrotron SOLEIL, Saint-Aubin, France*
14:25 - 14:50 (20'+5')	Comparison of STXM and SXP for the morphological study of organic semiconducting nanoparticles used for hydrogen production ***Sufal Swaraj*** *- Synchrotron SOLEIL, Saint-Aubin, France*
14:50 - 15:15 (20+5')	Tracking hydrogen-driven structural dynamics in supported Pd nanoparticles using full-field hyperspectral XAS imaging ***Marlon Muniz da Silva*** *- Brazilian Synchrotron Light Laboratory & Institute of Chemistry, Campinas, SP, Brazil*
15:15 - 15:40 (20+5')	Fate of self-assembled squalene nanoparticles in a biomimetic medium assessed by scattering techniques ***Hugo Roncin*** *- NIMBE/CEA Paris-Saclay, Gif-sur-Yvette, France*
15:40 - 16:10	*Coffee break*
16:10 - 16:40 (25'+5')	Realistic catalysts at work: APXPS insights into surface transformation for sustainable energy applications ***Spiros Zafeiratos*** *- Institut de Chimie et Procédés pour l'Energie, l'Environnement et la Santé, Strasbourg, France*
16:40 - 17:05 (20+5')	Probing protonation state dependent charge transfer-to-solvent in L-cysteine via sulfur Kβ Valence-to-core resonant inelastic X-ray Ssattering ***Sayantan Sarkar*** *- Laboratoire de Chimie Physique-Matière et Rayonnement, Paris, France*
17:05 - 17:30 (20'+5')	Strong coupling attraction in nanoconfined water between like-charged phospholipid layers ***Arnaud Hemmerle*** *- Synchrotron SOLEIL, Saint-Aubin, France*
17:30 - 17:55 (20'+5')	Cation ordering in synthetic stannoidite ($Cu_8Fe_3Sn_2S_{12}$) revealed by multiple-edge anomalous diffraction ***Carmelo Prestipino*** *- CRISMAT, Caen, France*
17:55 - 18:20 (20'+5')	Operando surface-sensitive X-ray scattering of Pd nanoparticles for selective NH_3 oxidation ***Alina Vlad*** *- Synchrotron SOLEIL, Saint-Aubin, France*

Parallel Session Schedule

Diluted matter

Chairpersons: Pierre Asselin & Helgi Rafn Hrodmarsson

ORION Room

Thursday, January 15th, 2026

13:30 - 14:00 (25'+5')	Are ketohydroperoxides from isoprene ozonolysis a missing major source of tropospheric OH? ***Jérémy Bourgalais*** *- Institut de Physique de Rennes, France*
14:00 - 14:25 (20'+5')	Tender X-ray induced fragmentation and charge release in halogenated radiosensitizers: A first electron–multi-ion coincidence study ***Oksana Travnikova*** *- LCPMR, Paris and Synchrotron SOLEIL, Saint-Aubin, France*
14:25 - 14:50 (20'+5')	Quantitative FTIR spectroscopy of corrosive and unstable atmospheric gases: Application to HNO_3, HONO and HOBr ***Alexandre Voute*** *- Synchrotron SOLEIL, Saint-Aubin, France*
14:50 - 15:15 (20+5')	Gas-phase interstellar ion-molecule reactivity driven by VUV Synchrotron light ***Corentin Rossi*** *- Institut des Sciences Moléculaires d'Orsay, France*
15:15 - 15:40 (20+5')	How do non-covalent interactions within small molecular cluster in the gas phase modify the ion molecule reactivity? ***Lucas Albouy*** *- MONARIS, Paris, France*
15:40 - 16:10	*Coffee break*
16:10 - 16:40 (25'+5')	Usage of the AILES beamline in support of molecular radio astronomy ***Sven Thorwith*** *- Physical Institute of Köln, Köln University, Germany*
16:40 - 17:05 (20+5')	The importance of Synchrotron spectroscopy in untangling the complex spectral patterns of deuterated methyl rotors ***Hayley A. Bunn*** *- Center for Astrochemical Studies, Garching, Germany*
17:05 - 17:30 (20'+5')	Direct experimental evidence of the roaming atom mechanism in a macromolecular noncovalent complex ***Jean-Christophe Poully*** *- CIMAP, Caen, France*
17:30 - 17:55 (20'+5')	Comparision of ethylene spectra at 10 µm recorded by Fourier transform and frequency comb spectrometers ***Hazem Ziadi*** *- Groupe de Spectrométrie Moléculaire et Atmosphérique, Reims, France*
17:55 - 18:20 (20'+5')	Rovibrational analysis of cyclopentadiene using ASAP and SOLEIL ***Luis Bonah*** *- I. Physikalisches Institut, Universität zu Köln, Germany*

Parallel Session Schedule

Geosciences / Environment / Cultural Heritage

Chairpersons: Charlotte Catrouillet & Simona Raneri

LIBRA Room

Thursday, January 15th, 2026

13:30 - 14:00 (25'+5')	Invisible metals, visible impacts: Geochemical dynamics and the environment ***Alexandra Courtin*** *- GEOPS, Université Paris-Saclay, Orsay, France*
14:00 - 14:25 (20'+5')	Impact of redox conditions on the binding of redox-inert contaminants to magnetite ***Rémi Marsac*** *- Institut de physique du globe de Paris, France*
14:25 - 14:50 (20'+5')	Investigation of iron and copper speciation: Deciphering the green colourations of medieval stained-glass windows ***Cecile Bretonnet*** *- Ministère de la Culture, Paris, France*
14:50 - 15:15 (20+5')	Environmental degradation of plastics in soils: Example of polypropylene alteration investigated by Synchrotron-based GIXD and nano-CT ***Quentin Bollaert*** *- Synchrotron SOLEIL, Saint-Aubin, France*
15:15 - 15:40 (20+5')	Art gets the blues: Simple colorimetric tools for X-ray dose assessment ***Alice Gimat*** *- Muséum national d'Histoire naturelle, Paris, France*
15:40 - 16:10	*Coffee break*
16:10 - 16:40 (25'+5')	How Synchrotrons can help us understand the dangers of historical lead-based cosmetics ***Fiona E. McNeill*** *- McMaster University, Hamilton, Canada*
16:40 - 17:05 (20+5')	Quantifying the speciation of sulfur and associated metals in geological fluids using Synchrotron spectroscopy ***Gleb Pokrovski*** *- Géosciences Environnement Toulouse, France : Présentation by* ***Olivier Proux*** *- ESRF, Grenoble, France*
17:05 - 17:30 (20'+5')	Characterization of 19th and 20th century African glass beads using XRF band XAS spectroscopy ***Laurent Tranchant*** *- Synchrotron SOLEIL, Saint-Aubin, France*
17:30 - 17:55 (20'+5')	Impact of different micro-organisms (bacteria, archaea) on the platinum (Pt) speciation ***Justine Le Doaré*** *- Institut de physique du globe de Paris, France*
17:55 - 18:20 (20'+5')	Multi-scale Synchrotron study of critical-metal phases by XRF and XANES spectroscopies **Georgia Grypaiou Iskenteridou** - *Géosciences Paris-Saclay & Laboratoire de Physique du Solide, Orsay, France*

Parallel Session Schedule

Physics & Advanced Materials (Structural, electronic and magnetic properties of matter / Physical surfaces and interfaces)

Chairpersons: Eglantine Boulard, Sara Gonzalez & Fabien Silly

CEA BLOCH Auditorium

Thursday, January 15th, 2026

13:30 - 14:00	Deep strain field of surface reconstruction
(25'+5')	***Vincent Repain*** *- Université Paris Cité, Paris, France*
14:00 - 14:25	1s2p resonant inelastic X-ray scattering natural circular dichroism
(20'+5')	***Alessandro De Frenza*** *- Synchrotron SOLEIL, Saint-Aubin, France*
14:25 - 14:50	Deep learning approach for fixing limited angle artefacts in Synchrotron X-ray tomography
(20'+5')	***Shyam Pulickan*** *- Synchrotron SOLEIL, Saint-Aubin, France*
14:50 - 15:15	Imaging the indirect-to-direct band-gap crossover in PbI$_2$
(20+5')	***Marcin Rosmus*** *- Institut des Sciences Moléculaires d'Orsay, France*
15:15 - 15:40	Is there a liquid-liquid transition in realgar (As4S4) under extreme conditions? A comprehensive Synchrotron study
(20+5')	***Vincent Rajaji*** *- Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie, Paris, France*
15:40 - 16:10	*Coffee break*
16:10 - 16:40	Probing inversion symmetry breaking and related electronic properties in ultrathin tellurides
(25'+5')	***Fabien Cheynis*** *- CINaM Centre Interdisciplinaire de Nanoscience de Marseille*
16:40 - 17:05	Mechanical strain effects on the magnetic response of ferromagnetic thin films on polymer substrates
(20+5')	***Alejandro Toledano-Povedano*** *- Institut Pprime-CNRS, Poitiers, France*
17:05 - 17:30	Correlating RIXS and EELS and XEOL spectroscopies in Van der Waals materials
(20'+5')	***Alessandro Nicolaou*** *- Synchrotron SOLEIL, Saint-Aubin, France*
17:30 - 17:55	Structural and electrical characterization of Hf$_{0.5}$Zr$_{0.5}$O$_2$ and ZrO$_2$ thin films using grazing incidence Synchrotron X-ray diffraction
(20'+5')	***Grégoire Magagnin*** *- INSA Lyon, Villeurbanne, France*
17:55 - 18:20	*In situ* Synchrotron study of the 1T'/1H phase transition in colloidal WS$_2$ monolayers
(20'+5')	***Dario Mastrippolito*** *- Synchrotron SOLEIL, Saint-Aubin, France*

Radiation Damage Satellite Workshop

PLENARY TALKS

SOLEIL Auditorium - Main Building

Wednesday, January 14th, 2026

09:40 – 10:25	Radiation damage in macromolecular crystallography: What is it and why do we care? ***Prof. Elspeth Garman*** *- Department of Biochemistry, University of Oxford, UK*
10:25 - 11:00	Beam damage and safe analysis: A study of how perception, perspective, and vocabulary shape the construction of risk ***Dr. Mathieu Thoury*** *- IPANEMA, St Aubin, France*

Radiation Damage in Macromolecular Crystallography: What Is It and Why Do We Care?

Elspeth F. Garman

Department of Biochemistry, Dorothy Crowfoot Hodgkin Building, University of Oxford, South Parks Road, Oxford, OX1 3QU, U.K. Email: elspeth.garman@bioch.ox.ac.uk

ABSTRACT

Structural biology relies on X-ray crystallography to provide much of the three-dimensional information on proteins and other macromolecules that informs biological function [1], but radiation damage (RD) to the samples remains one of the major bottlenecks to accurate structure determined. The RD can manifest as `global' changes resulting in the fading of the diffraction pattern with increasing dose, or as `specific' structural and chemical changes in the protein structures obtained. It occurs during both room temperature (RT) and cryo-cooled (100 K) X-ray crystallographic diffraction experiments, and is a main-stream concern [2,3]. Our understanding of its characteristics and its effects have significantly increased over the last 60 years since the first study of the phenomenon at RT in 1962 [4]. It has become clear that it is vital for crystallographers to be aware of the artefacts that can result from overexposing crystals, and also important that they have some knowledge of how to minimise/avoid the deleterious effects of the unavoidable absorption of the incident X-rays by the sample.

The fundamental metric against which indicators of radiation damage are plotted is dose, the energy absorbed per unit mass of the sample (J/kg=Gy, gray). The dose can be estimated from knowledge of the beam characteristics (energy, flux, size, intensity profile) and the atomic contents of the sample (protein and solvent composition or small molecule constituents), which allows the amount of X-ray absorption to be calculated. The program RADDOSE-3D [5] permits the dose to be estimated, by full dose modelling of the macromolecular crystallography diffraction experiment. Over the last 10 years RADDOSE-3D [4] has been extended for use in a wide variety of diffraction and scattering experiments (MX, SMX, XFEL, SAXS, XPS, PXRD) and most recently, electron diffraction, RADDOSE-ED [6]. In addition, we have now released a new RADDOSE-3D GUI [6,7] which allows the estimation of dose for any of these modalities.

This contribution will present examples of the main symptoms of RD in MX and give pointers on how to monitor potential RD pathologies. By attention to the particular beam conditions and also inspection of the output from both the diffraction analysis software [8] and the modelling/refinement [9] stages of the experiment, the most deleterious effects of RD progression can be minimised.

REFERENCES

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2. E.F. Garman. *Acta Cryst D.* **D55,** 1641-1653 (1999).
3. E.F. Garman and M. Weik. *Current Opinion Struct. Biol.* **82**: 102662 (2023).
4. C.C.F. Blake and D.C. Phillips In 'Biological Effects of Ionising Radiation at the Molecular Level'. IAEA Symposium, Vienna, p183 (1962)
5. O.B. Zeldin, M. Gerstel and E.F. Garman *J. Appl. Cryst.* **46,** 1225-1230 (2013).
6. J.L. Dickerson, P.T.N. McCubbin, J.C. Brooks-Bartlett, and E.F. Garman. *Protein Science* **33**:e500 (2024)
7. https://github. com/GarmanGroup/RADDOSE-3D
8. K.S.Shelley and E.F. Garman *Acta Cryst.* **D80,** 314-327 (2024).
9. K.S.Shelley and E.F. Garman *Nature Communications* **13**,1314 (2022).

Beam Damage and Safe Analysis: A Study of How Perception, Perspective, and Vocabulary Shape the Construction of Risk

Mathieu Thoury

IPANEMA, St Aubin, France

SOLEIL Users’ Meeting

January 15th - 16th, 2026

PLENARY TALKS

SOLEIL Auditorium - Main Building

Thursday, January 15th, 2026

10:50 – 11:35	**Soft Matter** Structure, properties and reactivity of oxide nanoparticles in solution: Synchrotron studies ***Olivier Diat & Matthieu Virot -*** *Institut de Chimie Séparative de Marcoule, Bagnols sur Cèze France*

Friday, January 16th, 2026

9:00 - 09:45	**Geosciences** Structure Surface reactivity of tubular Al/Si nanoparticles: interactions with nucleic acids and implications for prebiotic scenarios ***Jérôme Rose –*** *CEREGE, Aix-en-Provence, France*

Structure, Properties and Reactivity of Oxide Nanoparticles in Solution: Synchrotron Studies

M. Virot et O. Diat

ICSM, Univ Montpellier, CEA, CNRS, ENSCM, Marcoule, France

ABSTRACT

For this presentation, we will explore two illustrative examples of the formation of ionic oxo- and oxo-hydroxo-metalate clusters dispersed in aqueous solutions. These species emerge through the hydrolysis of metal ions oxides, followed by recondensation and crystallization processes that yield intrinsic clusters or small colloids via olation and/or oxolation processes under mild acidic conditions. The formation pathways vary significantly depending on the surrounding electrolytes and the nature of the acid used.

In one case, the generation of specific iso- or hetero-polyoxometalates with low charge density give rises to the emergence of fascinating superchaotropic properties, opening new opportunities in soft-matter chemistry. In another context —radiochemistry— oxo-hydroxo clusters serve as key intermediates in the crystallization of actinide oxide nanoparticles, which are of major relevance for both environmental studies and nuclear industry applications.

Our presentation will showcase experimental insights gained through complementary synchrotron and neutron-based techniques, providing an integrated understanding of these complex species.

Structure and Surface Reactivity of Tubular Al/Si Nanoparticles: Interactions with Nucleic Acids and Implications for Prebiotic Scenarios

J. Rose

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ABSTRACT

The chemical reactivity of clay mineral surfaces plays a crucial role in many geochemical processes on Earth. Recent advancements have broadened research to include other fine, highly reactive particles, particularly nanoparticles. Among these, a unique class of naturally occurring nanoparticles—compositionally similar to clays but featuring a tubular structure—has been identified in volcanic soils. These aluminosilicate nanotubes, likely first synthesized as early as the 1970s[1], form through a process where tile-like structures curve into rings, followed by colloidal growth[2,3]. Their structure consists of an outer aluminum oxyhydroxide layer and an inner silicate layer.

The synthesis of these nanotubes has been extensively studied, and methods have been developed to produce both silicon-based and germanium-based imogolite nanotubes[3]. The surface of imogolite nanotubes can also be chemically modified to enhance their properties. For instance, the inner surface can be functionalized to make the nanotubes hydrophobic, which is advantageous for environmental applications such as the remediation of hydrophobic organic pollutants. Additionally, imogolite nanotubes can incorporate metals into their structure, making them effective for trapping metallic contaminants.[4]

Recent studies have further demonstrated their ability to adsorb nucleotides, which is significant for understanding their interactions with biological molecules. This research even explores the hypothesis that mineral surfaces may have played a role in the formation of oligomers before life emerged on Earth.

The adsorption of nucleotides onto imogolite nanotubes has been investigated using chemical techniques, separation methods, and spectroscopy. These studies have quantified the adsorption of monomers and determined the atomic structure of surface complexes through X-ray absorption spectroscopy at the phosphorus K-edge. The results emphasize the role of phosphate groups and reveal differences compared to their interactions with clays.

This raises the question: How does the surface of imogolite promote the formation of oligomers—precursors to DNA? This topic will be discussed

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PARALLEL SESSIONS

Parallel Session Schedule

Biology and Health

SOLEIL - Reception Building Auditorium

Chairpersons: Paloma Fernandez Varela & Lorella Pascolo

IT-01	From tissue to trace: an elemental investigation of bromine in healthy and diseased ovarian tissue ***Anna Flamigni***
OC-01	Stuctural insights into tecovirimat antiviral activity and poxvirus resistance ***Riccardo Vernuccio***
OC-02	Small angle X-ray scattering structural characterization of quinones oxidoreductases ζcrystallins using SOLEIL SWING beamline ***Nicolas Mousnier***
OC-03	Probing the colloidal behavior of polysaccharides-degrading enzyme in a highly constrained model system ***Hugo Voisin***
OC-04	Tracing metal contaminants in environmental plastics pellets and mammalian tissues using XRF mapping at PUMA ***Alessandra Gianoncelli***
OC-05	Designing cryo-correlative workflows: Understanding radiation damage risks in HEK293-XpaQ ***Harisa Rista***
OC-06	Detection of titanium dioxide particles in human, animal and infant formula milk ***Anne Burtey***
IT-02	The role of the gut in dementia ***Alessia Cedola***
OC-07	Mechanical phenomena occurring in tissue during subcutaneous injections ***Aurélien Baquié***
OC-08	Structural and functional characterization of human tissue nonspecific alkaline phosphatase ***Pierre-Damien Coureux*** *Présentation by* ***Iliass Imam***

From Tissue to Trace: An Elemental Investigation of Bromine in Healthy and Diseased Ovarian Tissue

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ABSTRACT

Halogens play essential yet often overlooked roles in human physiology and disease[1,2]. Among these elements, bromine has emerged as a pivotal component in tissue development, particularly as a cofactor for peroxidase enzymes involved in forming sulfilimine bonds within collagen IV—crucial for basement membrane integrity and function[3,4].

The objective of this study was to examine the elemental distribution of bromine in both healthy and pathological ovarian tissues using synchrotron-based X-ray fluorescence (XRF) spectroscopy[5]. The research was conducted at the Soleil Synchrotron (Puma beamline), and it employed high-resolution micro-XRF mapping on histological sections of cryo-preserved healthy bovine ovarian tissue and laparotomy-obtained ovarian cysts from human patients with endometriosis. Analyses were completed by nano-XRF means at ESRF (ID16B) in order to confirm distribution at the subcellular level.

Our analysis revealed distinct spatial patterns of bromine localization, notably within basement membranes, around blood vessels, and—importantly—surrounding ovarian follicles. The bromine signal exhibited variability in accordance with follicular development, thereby suggesting a potential dynamic physiological role. These findings lend support to the hypothesis that bromine plays a multifaceted role in collagen IV cross-linking and maintains a close association with the basal membrane.

The presence of bromine around ovarian follicles, in addition to vascular structures, lay the foundation for future studies that aim to elucidate the role of bromine in ovarian follicle development and its potential impact on female fertility. These studies offer novel perspectives in reproductive biology and clinical research.

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Stuctural Insights into Tecovirimat Antiviral Activity and Poxvirus Resistance

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ABSTRACT

Mpox, a zoonotic disease caused by the monkeypox virus (MPXV), is endemic to Central and West Africa. Since 2022, two major epidemics have emerged and spread beyond these regions, prompting the WHO to declare both outbreaks as Public Health Emergencies of International Concern (PHEIC). Neither outbreak has been resolved as of January 2025. Tecovirimat, the most widely used antiviral for mpox, targets the conserved viral phospholipase F13, blocking viral wrapping and egress. However, mutations in the F13 gene can confer resistance to Tecovirimat. The lack of molecular insight into Tecovirimat's mode of action hinders the development of improved drugs and the prediction of resistance mutations. To fill this gap, we aimed to elucidate Tecovirimat’s mode of action and investigate how resistant mutants escape its effect using a multidisciplinary approach that combined structural, biophysical, and virology approached.

Structural studies revealed that F13 might forms homodimers on membranes. Mapping resistant mutants from clinical MPXV isolates showed that these mutations cluster at the conserved dimer interface, identified as the Tecovirimat binding site through X-ray crystallography. Functional studies showed that tecovirimat act as a strong molecular glue, inducing F13 dimerization in solution and in cells. Resistant mutations alter the dimer interface, reducing the efficiency of Tecovirimat-induced dimerization.

In conclusion, these findings reveal that Tecovirimat induces F13 dimerization as a key mechanism of action, while resistance arises from mutations that weaken this dimerization. These insights and the assays developed here pave the way for the development of novel antivirals and the monitoring of resistance mutations during poxvirus outbreaks

Small Angle X-ray Scattering Structural Characterization of Quinones Oxidoreductases ζCrystallins using SOLEIL Swing Beamline

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ABSTRACT

Quinone Oxidoreductase (QOR) is a class of enzyme known for catalyzing the reduction of quinone alongside the concomitant oxidation of a nicotinamide cofactor NAD(P)H. Usually QOR catalyze a two electrons transfer from NAD(P)H to the quinone (e. g. DT-Diaphorase[1]). However, the existence of a subclass of QOR prone to catalyzes one electron transfer, releasing semiquinone radical products, has been enlighten since the 1980s. Because the first discovered protein showing such catalytic properties has been identified in guinea pig lenses, they were given the name of ζ-crystallins (ZCr)[2] . Semiquinone products tend to react actively with dissolved O_2, leading to the production of H_2O_2. Interestingly, ZCr's physiological role may be either of structural or catalytic nature, as the protein showed its importance in mammals lenses correct light refraction[3] or for oxidative stress response in plants[4,5], or yeasts[6,7] , respectively. As a result, study of the structural properties of ZCr is a requirement for the understanding and elucidation of the enzymatic mechanism behind the one electron transfer. Small Angle X-ray Scattering method gave the opportunity to assess structural properties of ZCr in a native state in different conditions. The comparative study of recombinant ZCr from various organisms: mammals, plants, yeast and bacteria is of interest as differences in protein oligomeric state (monomeric, dimeric or tetrameric) are observed according to the specie. SAXS data combined with other structural data such as analytical Size Exclusion Chromatography, Gel electrophoresis and resolved crystal structures certainly is an added value for ZCr structural analysis.

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Probing the Colloidal Behavior of Polysaccharides-degrading Enzyme in a Highly Constrained Model System

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ABSTRACT

Understanding the specific interaction of enzymes that degrade cell wall polysaccharides with their substrates is an important issue, both from a fundamental and practical point of view. Such interactions are difficult to clarify under real conditions (biomass) due to the structural complexity of the plant cell wall. In this study, we present complex, concentrated model systems of cholesteric cellulose nanocrystal (CNC) suspensions reaching dimensions aiming to approach those found in the cell wall of plants. Cellulose-xyloglucan (XG) assemblies were prepared, allowing us to probe the interactions and diffusion behavior of a glucanase both in diluted dynamic conditions and in an organized and concentrated cholesteric environment (110-140 g/L).

Experiments were designed specifically for the DISCO beamline in order to monitor in real-time the distribution of a glucanase enzyme using deep-UV fluorescence without labelling them, which could influence their activity. Experiments on droplets revealed a preferential accumulation of the enzyme in the on a synchrotron showed that XG adsorbed in an extended conformation (‘trains’) modified the interaction of glucanase with polysaccharides, changing from an attractive interaction to a repulsive interaction. They revealed the preferential accumulation of glucanase in less concentrated and organized areas exclusively in the presence of XG. Dynamic diffusion experiments revealed that it also translated into faster diffusion kinetics in medium containing XG-covered CNCs. This demonstrates that increased complexity in the environment (a mixture of soluble and insoluble polysaccharides) strongly influences the nature of the interaction between enzymes and solid components. This study enhances our understanding of how a protein's interaction with a substrate influences its transport in a constrained environment.

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Tracing Metal Contaminants in Environmental Plastics Pellets and Mammalian Tissues using XRF Mapping at PUMA

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ABSTRACT

Synchrotron-based micro–X-ray fluorescence (µXRF) microscopy offers exceptional elemental sensitivity and spatial resolution, enabling trace-level mapping of metals in complex materials. Using the PUMA beamline at SOLEIL Synchrotron (France), we applied this technique to two complementary targets, environmental plastic debris and mammalian tissues, to explore links between environmental contamination and biological exposure.

Within the Italian Pellets Watch (ItPW) survey, the first national survey of plastic pollution along the Italian coastline, µXRF mapping of resin pellets collected along the Sardinian, Abruzzese, and Tuscan coasts revealed the presence of Pb, Fe, Cr, Ni, Sr, Mn, Br, and other elements. Their localization on both polymer surfaces and internal matrices indicates that plastics can act as carriers for toxic metals. Given their buoyancy and high pollutant adsorption capacity, up to hundreds of times higher than seawater, these pellets represent a critical pathway for contaminant transfer in marine systems.

Parallel analyses of a golden jackal kidney and human placental tissues uncovered comparable metal distributions, with Pb, Cr, Ni, Sr, Mn, Br, and Fe frequently co-localizing. The detection of these metals in jackal tissues supports the potential of this species as a sentinel for environmental metal contamination in northeastern Italy. Similarly, the presence of comparable metals in human placental tissues underscores potential fetal exposure to environmental pollutants and identifies possible biomarkers for assessing multi-elemental contamination at the maternal–fetal interface.

By integrating environmental, animal, and human data, this study underscores the value of synchrotron µXRF as a versatile tool for tracing pollutant pathways and evaluating the health implications of chronic exposure to contaminated ecosystems.

Designing Cryo-correlative Workflows: Understanding Radiation Damage Risks in HEK293-XpaQ

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ABSTRACT

Results from Correlative Microscopy Imaging (CMI) can only be correctly interpreted if the sample remains intact and as close as possible to its native state. Working under cryogenic conditions, with properly vitrified samples, is the first step toward preserving that integrity and allows, not without challenges, the same sample to be transferred across multiple imaging techniques.

The first challenge lies in achieving and maintaining proper vitrification while moving the sample from one microscope to another. The second is avoiding radiation damage from the imaging sources themselves. These effects are cumulative, and their impact must be considered carefully when interpreting images, especially when moving from whole-cell views to finer subcellular or molecular scales. What begins as biology can easily become artifact, and without acknowledging that, structural distortions can lead to false biological interpretations.

Using HEK293 cells expressing the fluorescent protein XpaQ as a model system, our work explores these challenges within a Cryo-Correlative Light and X-ray Microscopy (Cryo-CLXM) workflow, with the long-term goal of extending it to Cryo-Correlative Light, Electron, and X-ray Microscopy (Cryo-CLEXM). The focus is on understanding how vitrification quality, illumination dose, and ice thickness affect both fluorescence and structural fidelity, ensuring that the information we extract remains faithful to the real biological state.

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Detection of Titanium Dioxide Particles in Human, Animal and Infant Formula Milk

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ABSTRACT

Titanium (Ti) dioxide (TiO2) nanoparticles (NPs) are massively manufactured for countless industrial applications for their white pigment, UV filter and photocatalytic properties. They are classified as potential carcinogens to humans by inhalation and banned from food applications in France and Europe due to their suspected toxicity. Present in daily life products, medicine, agriculture, building paints and coatings, water and air remediation systems, they have been detected in water, air, and soils. Their presence in mammals remains however underexplored. Here, we investigated the existence of an actual contamination by TiO2-NPs of milk, a proxy for both maternal and offspring exposure. We analyzed human, animal, and infant formula milk samples using single particle inductively coupled plasma mass spectrometry (sp ICP-MS) and by synchrotron radiation-based X-ray fluorescence and absorption approaches at LUCIA beamline. We found that Ti microparticles and nanoparticles were present in all the samples tested, and characterized their size and concentration. Chemical speciation of Ti indicated predomination of rutile TiO2, followed by anatase TiO2, and to a lesser extent other Ti-bearing minerals (ilmenite FeTiO3, titanite CaTiSiO5, or pseudobrookite Fe2TiO5). We found variations in the levels of Ti in milk that depended on the genetic background in cows, and on unrecognized factors in humans. These results shed light on the existence of an exposure to Ti particles of humans at all ages who consume milk, including newborns from birth until weaning. They further raise concerns regarding the potential impact on health and development of mammals, particularly in the postnatal period which is critical for the development of mammalian physiological functions.

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The Role of the Gut in Dementia

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ABSTRACT

Alzheimer's disease (AD), a debilitating neurodegenerative disorder, remains one of the foremost public health challenges of our time. Despite decades of research, its etiology largely remains enigmatic. Recently, attention has turned to the gut-brain axis, a complex network of communication between the gastrointestinal tract and the brain, as a potential player in the pathogenesis of AD.

Here we exploited X-ray Phase Contrast Tomography to provide an in-depth analysis of the link between the gut condition and AD, exploring gut anatomy and structure in murine models.

We conducted a comprehensive analysis by comparing the outcomes in various mouse models of cognitive impairment, including AD, frail mice, and frontotemporal dementia (FTD) affected mice. We discovered an association between substantial changes in the gut structure and the presence of amyloid-beta (Aβ) in the brain. In particular, we investigated the gut morphology, the distribution of enteric micro-processes and neurons in the ileum.

Understanding the intricate interplay between gut condition and dementia may open new avenues for early AD diagnosis and treatment offering hope for a future where these diseases may be more effectively addressed.

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Mechanical Phenomena Occurring in Tissue During Subcutaneous Injections

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ABSTRACT

Introduction Although tolerable [1], subcutaneous (SC) injections of formulations presenting large volumes are currently not repeatable through self-administration [2]. To develop effective and safe delivery devices for these larger volumes, a thorough understanding of the mechanical phenomena occurring in the SC tissue during injections is thus necessary [1]. To identify the nature, the location, and the pressure at which these mechanical phenomena occur, we propose to visualize SC samples in 3D, before, during, and post-injection. Methods Ex-vivo swine samples containing epidermis, dermis and SC tissue were positioned in a partially confined chamber (part of their epidermis surface remained free). A catheter was introduced through the epidermis of each sample and was connected to a syringe through a tubing. To measure the hydrostatic pressure at the injection point during injections, an in-line pressure sensor was positioned between the syringe and the tubing. Injections of a contrast agent formulation (Iomeron® 150, Bracco Imaging, Italy) were then carried out using a push-syringe. Plateau pressures were successively and statically reached during injections. Samples were then free to inflate through their free epidermis surface. Samples were scanned before injection and at each plateau pressure at the ANATOMIX beamline by X-ray local phase contrast microtomography. Resulting scans corresponded to a cylinder centered on the injection point and at a reasonable distance from the sample constrained edges. Structures of interest (SC lobules, septa and contrast agent) were then segmented. The thicknesses of the contrast agent depots, the ratio of their volume to their surface, and the ratio of their volume to the volume pre-injection of the substructures in which contrast agent passed were extracted. Results Data post-processing is still on-going (48 scans from 9 samples). First results suggest that the organization of SC substructures is impacted by the catheter introduction in samples. Also, despite diffusion of contrast agent in samples, most of the contrast agent remained in septa. Their thicknesses increased significantly with the increase of pressure. Mechanical phenomena occurring in septa seemed irreversible and are likely related to hydraulic fracturing. Depending on samples, it occurred at pressures between 0 and 30 kPa.

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Structural and Functional Characterization of Human Tissue Nonspecific Alkaline Phosphatase

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ABSTRACT

Tissue-nonspecific alkaline phosphatase (TNAP) is an enzyme known for long for its necessary function in bone mineralization [1,2]. Indeed, the genetic deficiency in TNAP (also known as hypophosphatasia) leads in its most severe forms to the perinatal death of babies devoid of minerals in their skeleton. However, skeletal mineralization is not the only physiological function of TNAP, which is not specific of a particular substrate, but able to dephosphorylate very different compounds. For instance, TNAP dephosphorylates lipopolysaccharide (LPS) and ATP to exert anti-inflammatory functions, or pyridoxal phosphate to allow vitamin B6-dependent reactions. Moreover, TNAP was recently showed to participate in thermogenesis by dephosphorylating phosphocreatine [3]. Understanding how TNAP recognizes its different substrates and how TNAP activity can be inhibited is crucial, since an increasing number of patients with hypophosphatasia are treated with recombinant TNAP, and since on the opposite, TNAP inhibition is under clinical investigation in patients with pathological tissue calcification [2].

Human recombinant TNAP has been expressed in eukaryotic cells and purified, followed by enzymatic and structural characterization. Kinetic data showed TNAP activity toward ATP as well as ADP and AMP. Recombinant TNAP also displays activity on other known physiological substrates, including inorganic pyrophosphate, pyridoxal phosphate and phosphocreatine. An X-ray structure of a TNAP-phosphate complex reveals that substrate binding is mainly assured by the charge difference between the phosphate moiety and divalent cations in the catalytic site. Furthermore, TNAP inhibition studied by cryo-EM has revealed specific interactions with residues that are absent in other alkaline phosphatases [4]. Interactions with ATP have also been studied (with a resolution down to 1.5 Å), revealing two distinct binding conformations leading to substrate hydrolysis.

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Parallel Session Schedule

Chemistry & Soft Matter
(Characterization of structure and properties of chemical materials, reactivity, catalysis, chemical surfaces and interfaces / Soft matter)

SOLEIL Auditorium - Main Building

Chairpersons: Luis Cardenas, Asma Tougerti & Amélie Bordage

IT-03	STXM as a tool for studying the morphology of organic semiconducting nanoparticles for energy applications ***Anne Hebraud***
OC-09	Revealing the mechanisms of enhanced photo-electrocatalytic OER performance of Ni doped maghemite via operando XAFS ***Francesco Paparoni***
OC-10	Comparison of STXM and SXP for the morphological study of organic semiconducting nanoparticles used for hydrogen production ***Sufal Swaraj***
OC-11	Tracking hydrogen-driven structural dynamics in supported Pd nanoparticles using full-field hyperspectral XAS imaging ***Marlon Muniz da Silva***
OC-12	Fate of self-assembled squalene nanoparticles in a biomimetic medium assessed by scattering techniques ***Hugo Roncin***
IT-04	Realistic catalysts at work: APXPS insights into surface transformation for sustainable energy applications ***Spiros Zafeiratos***
OC-13	Probing protonation state dependent charge transfer-to-solvent in L-cysteine via sulfur Kβ Valence-to-core resonant inelastic X-ray Ssattering ***Sayantan Sarkar***
OC-14	Strong coupling attraction in nanoconfined water between like-charged phospholipid layers ***Arnaud Hemmerle***
OC-15	Cation ordering in synthetic stannoidite ($Cu_8Fe_3Sn_2S_{12}$) revealed by multiple-edge anomalous diffraction ***Carmelo Prestipino***
OC-16	Operando surface-sensitive X-ray scattering of Pd nanoparticles for selective NH_3 oxidation ***Alina Vlad***

STXM as a tool for studying the morphology of organic semiconducting nanoparticles for energy applications

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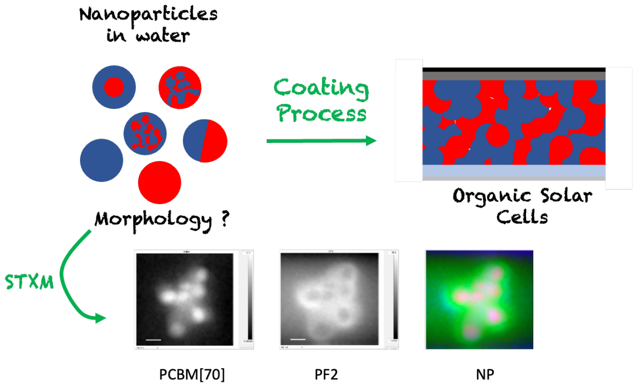
ABSTRACT

Organic semiconducting nanoparticles (NPs), made of electron donor (D) and electron acceptor (A) molecules, are increasingly used in advanced energy applications such as organic photovoltaics (OPV) or photocatalytic hydrogen production. In organic photovoltaics, aqueous suspensions of these NPs are used as an ecofriendly ink to print the active layer of OPV cells. Their internal morphology, fixed during their elaboration process plays a very important role in the device operation. However, this morphology is not so easy to determine by conventional characterization methods available in laboratories, such as TEM, because it does not offer sufficient contrast between the two types of materials, D and A. Soft X-ray Scanning Transmission X-ray Microscopy (STXM) was used to determine the NPs internal morphology. In this technique, a chemical contrast is obtained thanks to differences in the Near Edge X-ray Absorption Fine Structure (NEXAFS) spectra of the 2 materials, offering the possibility to map the chemical composition of the NPs thus showing the donor and acceptor domains as well as their purity. In this presentation, I will show how OSCs NP have been prepared, characterized by STXM and finally used for OPV devices.



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Revealing the Mechanisms of Enhanced Photo-electrocatalytic OER Performance of Ni Doped Maghemite via Operando XAFS

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ABSTRACT

Hydrogen is one of the most promising green energy carriers. H_2 can be produced without greenhouse gas emission via renewable energy-fueled electrolysis [1]. Solar energy stands out as the most abundant renewable energy source on Earth, and can be exploited to fuel electrolysis through a photovoltaic panel. However, a direct solar-to-chemical energy conversion is an attractive possibility, allowing device simplification and limiting intermediate losses [2]. This can be accomplished in photoelectrochemical (PEC) cells, where the e^-/h^+ pairs formed upon light absorption on the photoelectrode are injected into the electrolyte, promoting water redox reactions. Despite their currently low STH conversion efficiency, PEC cells represent a young technology with substantial room for development. Most of the efforts are currently focusing on the oxygen evolution reaction (OER) catalysis, which, due to its complex four-step electron transfer mechanism, is commonly regarded as the bottleneck of electrochemical technologies [3]. Maghemite (γ-Fe_2O_3), is a promising, cost-effective photoanode material in this matter, given its optimal band gap (2 - 2.2 eV). Despite being less known than its polymorph hematite, the cubic spinel phase offers a higher conductivity and a versatile structure that allows dual-site catalytic activity and a more facile and stable adjustment of composition by doping. However, PEC performance tuning via doping passes through the understanding of the photocatalytic mechanism under *operando* conditions. In this matter, a special importance must be assigned to the catalyst/electrolyte interface, where reactant intermediates form.

To this end, at the SAMBA beamline we developed an electrochemical cell to perform *operando* XAS compatible with samples on X-ray opaque supports, since the sample is probed from the electrolyte side [4]. Compared to other cells working with similar geometry, ours allows for the collection of high-quality XAS data in fluorescence mode even at a lower energy range (down to the Ti K-edge). Moreover, to unravel the tiny surface-bound electronic effects resulting from reactant intermediates formation, a setup was developed to perform Fixed Energy X-Ray absorption under chopped light illumination (FEXRAP). Combining *operando* XAS investigations with conventional electrochemical and electronic analysis, we will describe the photoanodic performances and relative catalytic mechanism of Ni-doped γ-Fe_2O_3 films (111) epitaxially grown on Pt (001) single crystal. We will show how Ni ions modify the material local structure and electronic configuration, and how such modulations impact the photoanodic performances for solar OER as a function of the Ni concentration.

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Comparison of STXM and SXP for the Morphological Study of Organic Semiconducting Nanoparticles used for Hydrogen Production

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ABSTRACT

Organic Semiconducting (OSC) Nanoparticles composed of carefully selected mixtures of electron donor and acceptor materials were synthesized using mini-emulsion and nanoprecipitation techniques. These nanoparticles were employed in H_2 production through photocatalysis. It was found that the PTQ10/ITIC-4F pair without surfactant, in a morphology intermixed with Pt as a co-catalyst, has a 10 times higher hydrogen production rate than the core-shell morphology, but a reduced production stability over 24h (Figure 1C) [1].

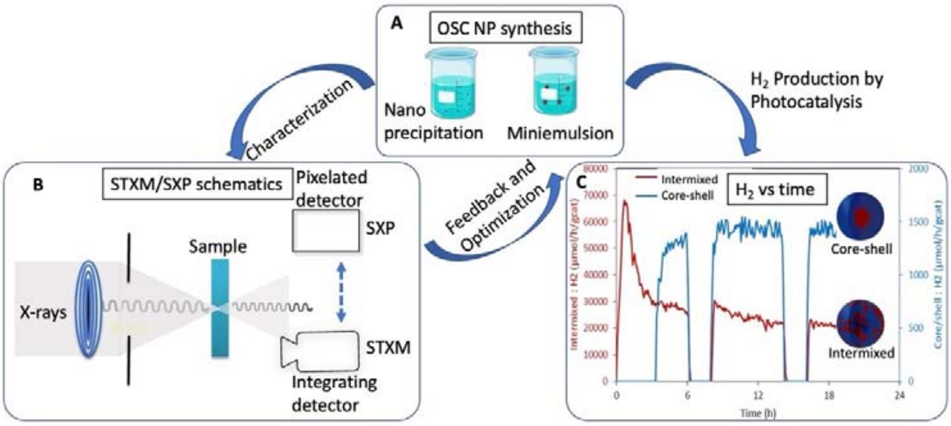

Figure 1: Overall schematics depicting (A) OSC synthesis (B) STXM/SXP schematics (C) H_2 production from photocatalysis vs time

In this presentation I will focus on the role STXM (Scanning Transmission X-ray Microscopy) and SXP (Soft X-ray Ptychography) has played in chemical and morphological characterization of these nanoparticles [2]. I will present practical aspects of these two techniques such as spatial resolution, radiation damage, and acquisition time along with some open questions.

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Tracking Hydrogen-driven Structural Dynamics in Supported Pd Nanoparticles Using Full-field Hyperspectral XAS Imaging

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ABSTRACT

The strong affinity of palladium nanoparticles (PdNP) for hydrogen makes them one of the most important model systems for understanding of metal–hydrogen interactions 1. Hydrogen absorption into the Pd catalyst structure leads to the formation of a palladium hydride (PdHx) phase, which has several industrially relevant catalytic applications 2,3. Developing a comprehensive understanding of the factors governing these transitions could help enhance catalytic performance. The composition of the support in heterogeneous catalysts containing Pd nanoparticles has been shown to strongly influence hydride formation. Specifically, strong metal–support interactions with highly active supports can inhibit the transition from the metallic state to PdHx, resulting in lower concentrations of the hydride phase 4.

Advances in synchrotron characterization have made it possible to extract information at the reactor scale in situ, enabling measurements under realistic environmental conditions. The application of full-field hyperspectral X-ray absorption spectroscopy (XAS) imaging at ROCK 5, using a pixelated array camera, combines micrometer-scale spatial resolution with Quick-EXAFS (quick extended X-ray absorption fine structure) measurements, achieving optimal time resolution in the order of seconds. This innovative technique allows the tracking of dynamic chemical changes across the catalytic bed and reveals spatial heterogeneities induced by temperature variations or phase transformations 6.

In this work, we applied in situ spatially resolved full-field hyperspectral XAS imaging to track dynamic modifications in PdNP catalysts supported on Al2O3 and TiO2 (inactive and active supports, respectively). The catalysts, with similar size and morphology, were examined under varying hydrogen concentrations. This approach allowed us to follow the transitions from oxidized Pd to metallic and then hydride Pd, as well as to identify spatial heterogeneities within the catalytic bed. In contrast to the pronounced differences observed during the initial PdO-to-Pd0 transition, marked by a wavefront in alumina- but not in titania-supported samples, this behavior reflects the known influence of the support, which also affects hydride formation 4. The hydride phase developed as a uniform spatial transformation across the entire catalytic bed, with varying PdHx concentrations depending on the hydrogen content in the atmosphere and the support composition. Full-field hyperspectral XAS imaging revealed spatial differences between the two samples and provided deeper insight into phase transitions in Pd catalysts at the reactor scale. This work lays the foundation for operando studies of reactions such as CO oxidation, linking spatially resolved structural dynamics with catalytic performance.

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Fate of Self-assembled Squalene Nanoparticles in a Biomimetic Medium Assessed by Scattering Techniques

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ABSTRACT

Over the last 20 years, pharmaceutical industries gained interest towards therapeutic nanoparticles (NPs) so-called nanomedicines. The NP formulations demonstrated enhanced properties compared to the drug alone such as improved targeting, reduced toxicity, and enhanced pharmacokinetics. However, there is still a lack of data and understanding of the physicochemical properties of such compounds in particular after their injection in biological media leading to numerous failures in clinical trials[1].

In this context, we proposed to study a particular case of “soft” NPs composed of a pro-drug which consists of a squalene (SQ) linked through an amide bond to Leucine-enkephaline (LENK). Feng et al. demonstrated that LENK-SQ NPs produced an analgesic effect comparable in duration to that of morphine, unlike LENK alone[2-4]. Moreover, contrary to the opioids currently used as painkillers, LENK allows to get rid of the development of an addiction over time by acting on peripherally localized receptors rather than central nervous system opioid receptors.

In this study, we characterized the assembly state of LENK-SQ bioconjugates in a biomimetic environment using physicochemical techniques focusing on small/wide angle X-ray scattering (SAXS/WAXS on SWING at SOLEIL) and small angle neutron scattering (SANS on D22 and SAM at ILL). Taking benefit of the BioSAXS sample changer, we were able to evidence and characterize the micellization of the bioconjugate in conditions that mimic physiological conditions of blood in terms of pH and ionic strength. The influence of different buffers was assessed across a range of concentrations, resulting in various pH and ionic strength conditions in the final suspension. These results were put into perspective with SANS analyses.

The study revealed an equilibrium between LENK-SQ bioconjugates, LENK-SQ NPs and micelles, which depended on buffer concentration[5]. Consequently, the relative proportion of each species appears to be primarily governed by the pH, highlighting its critical role in the relationship between drug efficacy and morphology of self-assembled bioconjugates. These findings provide key insights into how the physicochemical environment can influence NP formation and, ultimately, therapeutic performance.

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Realistic Catalysts at Work: APXPS Insights into Surface Transformations for Sustainable Energy Applications

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ABSTRACT

CO_2 methanation ($CO_2 + 4H_2 \rightarrow CH_4 + 2H_2O$) is of significant environmental interest as a sustainable pathway for energy production and storage [1]. Ni-based catalysts are widely used in this reaction due to their low cost and high CH_4 selectivity. These systems typically consist of nanoscale Ni particles dispersed on high-surface-area oxide supports such as Al_2O_3, SiO_2, or CeO_2. The support plays a crucial role in controlling Ni particle dispersion, morphology, and stability through metal–support interactions. However, stabilizing Ni nanoparticles under reaction conditions remains challenging, as they tend to agglomerate, leading to performance degradation. In this context, exsolution? a high-temperature process that drives metal species initially dissolved in the parent oxide to emerge as nanoparticles at the surface, has attracted significant attention as a route to generate strongly anchored particles with enhanced resistance to sintering [2].

In this presentation, we focus on Ni-doped CeO_2 and $LaNiO_3$ perovskite as precursors that, upon thermal activation, generate the active surface phase [3-5]. To elucidate the structural and chemical evolution of these materials, we combine a suite of advanced in situ and operando spectroscopies, spanning a wide pressure range (from mbar to bar) and probing depths (from nanometers to micrometers), across five European synchrotron facilities. We will show how the integration of ambient-pressure soft and hard X-ray photoelectron spectroscopies (static and time-resolved APXPS, HAXPES) with X-ray absorption spectroscopy (XAS) enables direct monitoring of key surface transformations during activation and under working conditions. Beyond capturing the chemical state of the catalyst, these techniques provide crucial insights into adsorbed species and their mechanistic role during CO_2 methanation. We further examine how controlled oxidative and reductive thermal treatments influence the formation, stabilization, and reactivity of the active phase. Overall, while the talk will focus on the unique capabilities of APXPS, it will also illustrate its inherent limitations and show how an integrated multitechnique operando approach, combining multiple probing depths and pressure regimes, is essential to fully unravel structure–function relationships and guide the rational design of next-generation Ni-based catalysts for efficient and durable CO_2 methanation.

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Probing Protonation State Dependent Charge Transfer-to-solvent in *L*-cysteine via Sulfur *Kβ* Valence-to-core Resonant Inelastic X-ray Scattering

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ABSTRACT

L-cysteine is a highly versatile amino acid capable of undertaking several diverse functional roles within proteins, owing largely to the ability of its thiol group to deprotonate and engage in bonding giving rise to unique structural feature like disulfide bonds and strong coordination with metal centres. [1] The electronic structure of aqua-solvated *L*-cysteine has been a subject of long-standing interest due to its fundamental biological relevance. [2] While previous studies have successfully established a foundational understanding of static properties like speciation and hydrogen-bonding networks surrounding the thiol moiety, the dynamic ultrafast electronic phenomena remain largely unexplored. [3-5]

L-cysteine in aqueous solution exists predominantly in its zwitterionic thiol form, whereas increasingly alkalinity shifts the equilibrium towards a deprotonated thiolate species, becoming dominant at higher pH values. This study examines the influence of these protonation states on charge delocalisation at the sulfur site following *X*-ray induced core-shell excitation. Sulfur *Kβ* valence-to-core Resonant Inelastic *X*-ray Scattering (RIXS) provides a valence sensitive probe to explore the nature of charge delocalisation processes occurring on the timescale of core-hole lifetimes but due to the relatively weak signal strength at the sulfur *Kβ* emission line, it has been difficult thus far to access it with sufficient photon flux to obtain meaningful electronic structure information.

The multi-crystal *X*-ray spectrometer – MOSARIX, developed recently by our group provides us unprecedented access, making it possible to perform highly photon efficient high-resolution measurements in this tender *X*-ray region. [6] With this capability, we resolve distinct spectral signatures corresponding to the thiol and thiolate forms of *L*-cysteine. While the thiol species remains largely inert to the solvent environment, the thiolate engages with the solvent and exhibits pronounced charge transfer-to-solvent features below the ionization threshold. Using Molecular Dynamics and Ab initio Quantum Chemistry calculations, we showcase the existence of diffused molecular orbitals in the thiolate form that extend into the solvent continuum in contrast to the thiol form where the orbitals are largely localized on the sulfur site.

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Strong Coupling Attraction in Nanoconfined Water between Like-charged Phospholipid Layers

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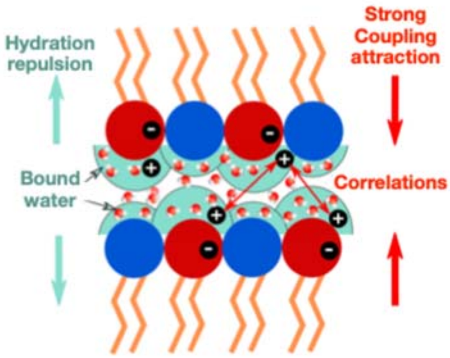
ABSTRACT

When a surface is immersed in water, it becomes spontaneously charged. Interactions between charged surfaces play a key role in many phenomena, such as the cohesion of cement, the behaviour of polymers, and the adhesion of living cells. Yet under certain conditions, a surprising effect occurs: two surfaces carrying the same charge can attract each other. To elucidate the mechanisms behind this counterintuitive attraction, we investigate stacks of charged lipid bilayers as a model system.

Traditionally, this so-called "strong coupling" electrostatic attraction [1] has been associated with multivalent counterions, yet recent experimental evidence suggests that nanoconfined water can also drive attraction even in the presence of monovalent counterions [2, 3]. We explore this phenomenon by examining the balance between hydration repulsion and strong coupling attraction in charged phospholipid layers.

Using X-ray reflectivity and fluorescence on the beamline SIRIUS, we studied multilayered structures composed of negatively charged DPPS and zwitterionic DPPC phospholipids under varying relative humidity and surface charge densities. These measurements allowed us to quantify water layer thickness, hydration forces, and dielectric properties in nanoconfined environments. Our findings reveal that hydration water near charged surfaces exhibits reduced rotational freedom, as observed previously in confined water [4], which enhances electrostatic interactions and leads to strong coupling attraction between like-charged layers. Our results provide new insight into electrostatic interactions in biological and colloidal systems, with implications for membrane stability and charged interfaces under confinement.



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Cation Ordering in Synthetic Stannoidite ($Cu_8Fe_3Sn_2S_{12}$) Revealed by Multiple-edge Anomalous Diffraction

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ABSTRACT

Understanding cation ordering in complex copper-based sulfides is crucial for optimizing their thermoelectric performance. We report a comprehensive study of the cationic distribution in synthetic stannoidite, $Cu_8Fe_3Sn_2S_{12}$, by combining X-ray powder diffraction, X-ray absorption spectroscopy (**EXAFS**), and Multiple-Edge Anomalous Diffraction[1] (**MEAD**) at the Cu and Fe K-edges, performed at the DIFFABS and SAMBA beamline of Synchrotron SOLEIL.

The close scattering factors of Cu^+ and Fe^{2+} make their discrimination by conventional diffraction difficult and traditional anomalous diffraction show show some difficulties as low energy diffraction scale, absorbtion correction, and fluorescence contribution coulde strongly correlate with structural refinement. MEAD overcomes this limitation by exploiting the energy dependence of selected Bragg reflections across absorption edges, enabling direct insight into site occupancies. Complementary EXAFS analysis confirms interatomic Fe–Fe/Cu interactions characteristic of Fe occupation at interstitial positions.

The combined dataset consistently supports a **single cationic configuration**, contrasting with earlier structural models.[2] This configuration provides improved agreement with both experimental Bragg intensity evolution and local structural parameters, as further validated by DFT modeling.

This work demonstrates the effectiveness of MEAD in resolving subtle cation-ordering phenomena in complex sulfides, underscoring its value for the rational design of next-generation thermoelectric materials.

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Operando Surface-sensitive X-ray Scattering of Pd Nanoparticles for Selective NH_3 Oxidation

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ABSTRACT

In the transition towards decarbonized energy solutions, ammonia (NH_3) is emerging as a promising carbon-free fuel and hydrogen carrier. It offers the advantage of large-scale production using well-established infrastructure and can be efficiently stored and transported. Beyond its traditional role in fertilizer production, NH_3 is being explored for direct combustion, fuel cells, and hydrogen storage/release applications. In this context, controlling its oxidation to maximize N_2 selectivity is crucial, as this minimizes NO_x emissions. To this end, we have investigated oxide-supported arrays of Pd NPs, prepared via plasma-assisted micelle nanolithography, as catalysts for NH_3 oxidation, focusing on the role of subsurface species in governing activity and selectivity.

Simultaneous operando grazing incidence X-ray diffraction (GIXRD) and grazing incidence small-angle X-ray scattering (GISAXS) were performed at the SixS beamline of Synchrotron SOLEIL (France). We demonstrate that plasma-assisted synthesis allows for tuning the reactivity of Pd NPs and their activity in oxidation reactions. Our experimental results highlight the crucial role of plasma-assisted synthesis in the architectural design of nanomaterials: by precisely altering the synthesis procedure, one can effectively tailor metal-support interactions, ultimately impacting the structure, morphology, and catalytic performance of the nanoparticles.

Parallel Session Schedule

Diluted matter

ORION Room

Chairpersons: Pierre Asselin & Helgi Rafn Hrodmarsson

IT-05	Are ketohydroperoxides from isoprene ozonolysis a missing major source of tropospheric OH? ***Jérémy Bourgalais***
OC-17	Tender X-ray induced fragmentation and charge release in halogenated radiosensitizers: A first electron–multi-ion coincidence study ***Oksana Travnikova***
OC-18	Quantitative FTIR spectroscopy of corrosive and unstable atmospheric gases: Application to HNO_3, HONO and HOBr ***Alexandre Voute***
OC-19	Gas-phase interstellar ion-molecule reactivity driven by VUV Synchrotron light ***Corentin Rossi***
OC-20	How do non-covalent interactions within small molecular cluster in the gas phase modify the ion molecule reactivity? ***Lucas Albouy***
IT-06	Usage of the AILES beamline in support of molecular radio astronomy ***Sven Thorwith***
OC-21	The importance of Synchrotron spectroscopy in untangling the complex spectral patterns of deuterated methyl rotors ***Hayley A. Bunn***
OC-22	Direct experimental evidence of the roaming atom mechanism in a macromolecular noncovalent complex ***Jean-Christophe Poully***
OC-23	Comparision of ethylene spectra at 10 µm recorded by Fourier transform and frequency comb spectrometers ***Hazem Ziadi***
OC-24	Rovibrational analysis of cyclopentadiene using ASAP and SOLEIL ***Luis Bonah***

Are Ketohydroperoxides from Isoprene Ozonolysis a Missing Major Source of Tropospheric OH?

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ABSTRACT

This is the Ozonolysis is a central oxidation pathway for biogenic unsaturated volatile organic compounds (VOCs), leading to highly oxygenated molecules (HOM) and secondary organic aerosol (SOA) formation, often exceeding yields from OH or NO3 chemistry. [1] Its role is further amplified in biomass burning plumes, where abundant unsaturated compounds and enhanced ozone production strongly affect air quality. [2] Ozonolysis proceeds through the formation of a primary ozonide (POZ), which predominantly decomposes to yield Criegee intermediates (CIs), well known for their central role in tropospheric oxidation and SOA formation. [3,4]

An alternative pathway, however, involves POZ isomerization leading to ketohydroperoxide (KHP) formation. This mechanism was first proposed theoretically [5] and later confirmed experimentally [6] for ethylene, and more recently in 1-hexene ozonolysis. [7] While KHPs are established in combustion, they are generally overlooked in the atmosphere due to insufficient energy to cleave the O-O bond. Yet, the exothermicity of ozonolysis may provide enough internal energy to drive rapid O–O scission, yielding OH, the key oxidant of the atmosphere.

To test this hypothesis, we investigated the ozonolysis of isoprene, the most abundant biogenic VOC and a key system for HOx recycling. Experiments were conducted at the SOLEIL synchrotron (France) and the Hefei synchrotron (China) using a laminar flow tube reactor and product characterization via photoelectron–photoion coincidence (PEPICO) spectroscopy, supported by high-level quantum chemical calculations. We will present preliminary results providing direct spectroscopic evidence of KHP formation and quantification during isoprene ozonolysis, pointing to a potentially missing OH source in the troposphere

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Tender X-ray Induced Fragmentation and Charge Release in Halogenated Radiosensitizers: A First Electron–multi-ion Coincidence Study

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ABSTRACT

Absorption of high-energy X-rays by molecules initiates a cascade of electronic relaxation processes that redistribute charge and energy on femtosecond timescales. These ultrafast steps determine how the system evolves from a localized excitation to widespread ionization of the molecular framework and, ultimately, to fragmentation through Coulomb explosion. Despite their central role in X-ray science and radiation chemistry, the pathways of charge buildup and energy flow at the molecular level remain incompletely understood. Molecules containing high-Z atoms such as bromine or iodine are of particular interest because their large inner-shell ionization cross sections make them dominant sites of X-ray absorption ("hotspots"), triggering rich electronic decay cascades that drive rapid and extensive molecular damage. Beyond their fundamental relevance to ultrafast radiation–matter interactions, these processes are also of practical importance in X-ray-mediated cancer therapy, where halogenated nucleoside analogs act as radiosensitizers in hypoxic tumor cells. Current biological models typically describe radiation damage in terms of low-energy secondary electrons and hydroxyl radicals generated from water radiolysis, while largely overlooking the direct contribution of the radiosensitizer molecules themselves.

Addressing this gap requires experiments capable of disentangling charge redistribution, fragmentation dynamics, and the role of embedded high-Z atoms within complex molecular systems. Our new high-resolution electron–multi-ion coincidence setup, MUSTACHE, is designed for this type of investigation and is optimized for tender and hard X-ray studies [1]. By correlating energy-resolved electrons with multiple ionic fragments, MUSTACHE provides a unique means to probe how molecular structure and halogen "hotspot" characteristics govern charge flow and fragmentation pathways. Our first measurements on halogen-containing radiosensitizers – the uridine derivatives 5-iodo-4-thio-2′-deoxyuridine and 5-bromo-4-thio-2′-deoxyuridine – performed at the GALAXIES beamline reveal that absorption of a single hard X-ray photon can induce a violent Coulomb explosion, producing predominantly small (atomic) and multiply charged fragments. These results demonstrate that such molecules release not only cascades of Auger electrons but also energetic ionic fragments capable of inflicting localized chemical and mechanical damage – species not accounted for in existing radiobiological models. Together, these insights can help advancing our understanding of the molecular-scale mechanisms underlying radiosensitizer action and their potential impact in X-ray-based therapies.

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Quantitative FTIR Spectroscopy of Corrosive and Unstable Atmospheric Gases: Application to HNO_3, HONO and HOBr

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ABSTRACT

Nitric acid (HNO_3), nitrous acid (HONO), or hypobromous acid (HOBr), are known to play an important role in the complex chemical reactions that occur in the Earth atmosphere. Remote IR sensing satellites such as IASI, its successor IASI-NG, and FORUM[$] can, possibly, provide quantitative identifications on these species. However, to take full advantage of the spectra recorded by these satellite measurements, it is necessary to have at one's disposal, good quality spectroscopic parameters for these molecules. These data are achieved during theoretical investigation of high-quality laboratory spectra. However, getting “absolute” line intensities is quite a challenge for chemically unstable or highly reactive molecules like those investigated here.

In recent years, the far-infrared (FIR) and THz spectroscopy AILES beamline at synchrotron SOLEIL has developed equipment dedicated to the study of such unstable molecules. The beamline couples the high-brilliance IR beam from the synchrotron to a high-resolution Bruker IFS125HR FTIR spectrometer whose ultimate spectral resolution is $0.001\ cm^{-1}$. The sample gas environment installed on the spectrometer consists in a White optical system embedded in a three-walled coolable glass cell. [1] Its non-glass parts in contact with the gas are carefully protected in order to prevent reactions at their surface. As a result, corrosive gas samples can be held as long as needed for averaging long high-resolution FTIR measurements. On the other hand, a special dual-channel detector [2] capable of recording two simultaneous spectra in the FIR and mid-infrared (MIR) regions has been designed for dealing with (polar) molecules in a mixture like HONO and HOBr. Provided the dipole moment of the target molecule is known, the pure rotational spectrum in the FIR region gives access to its partial pressure in the mixture. Hence, the relationship between the latter and the intensities of bands recorded simultaneously in the MIR region can be determined.

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Gas-phase Interstellar Ion-molecule Reactivity Driven by VUV Synchrotron Light

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ABSTRACT

The polycyclic aromatic hydrocarbons (PAHs) are universally acknowledged as key molecular species in space, potentially accounting for up to 25% of the carbon budget in the interstellar medium (ISM).1 They are also thought to be responsible for the aromatic infrared bands. However, their formation pathways under interstellar conditions remain poorly understood. In the bottom-up formation scenario, i.e. building up large molecular species from small hydrocarbons, ion–molecule reactions are of central importance, as they are typically exothermic and barrierless. However, astrochemical models crucially lack laboratory reactivity data such as reaction rates and product formation branching ratios to understand and accurately modelled the complex chemical network of the ISM. The work that will be presented investigates hydrocarbon ion-molecule chemical growth routes. Using the CERISES instrument on the DESIRS beamline, we measured absolute reaction cross section (RCS) for reaction between a cation generated by vacuum-ultraviolet (VUV) photoionization and a neutral partner. RCS are recorded as a function of the photon energy used to ionize the precursor, providing insights on the isomeric nature of the reactant as more energy is deposited in the system above their appearance energy. 2 These measurements can be converted into reaction rate coefficients, thereby supplying essential input parameters for astrochemical models.

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How Do Non-covalent Interactions within Small Molecular Cluster in the Gas Phase Modify the Ion Molecule Reactivity?

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ABSTRACT

Intermolecular interactions can strongly affect the local electron density, and therefore the reactivity of species. A better phenomenological description of these changes in reactivity seems essential for an accurate description of atmospheric and astrochemical processes.

To this end, we have studied the reactivity of aggregates as a function of their size. Photoionization by VUV radiation from SOLEIL has been used as a source suitable for generating aggregates, providing the ability to fine tune the energy content of the reactive ion. We have recently developed a coupling between the CERISES set-up and a molecular beam for generating aggregates, providing with particularly sensitive analyser and detector to identify and correlate reaction products that are present in small quantities. Measurements were carried out with the CERISES set-up on the DESIRS beamline at the SOLEIL synchrotron.

As a proof of concept, we were able to probe the reactivity of protonated aggregates of acetic acid (up to the pentamer) and with methylamine. The reactivity of the formic acid protonated aggregates was also investigated for the sake of comparison.

Quantum chemistry calculations were performed to interpret the results observed experimentally, aiming at finding an explanation for systematic behaviours observed as a function of the aggregate size and collision energy. The geometries were obtained with the software CREST (Conformer-Rotamer Ensemble Sampling Tool). The structures with the lowest energy were chosen. The complexation and reaction energies were calculated using Density Functional Theory (DFT) calculations (Gaussian 16). The functional LC ω-PBE with the basis set 6-311 ++ G(d,p) and the empirical dispersion GD3BBJ were used. Then, the enthalpy of the reaction between the methylamine and the protonated aggregates of acetic acid was calculated. We were able to highlight the possible geometries of protonated aggregates resulting from photoionization. The enthalpy of the reaction between the methylamine and the protonated aggregates were calculated.

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Usage of the AILES Beamline in Support of Molecular Radio Astronomy

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ABSTRACT

Star-forming regions, specifically hot molecular cores, are known to drive a very rich chemistry leading to the formation of many (complex organic) molecules. Radio astronomical observations reveal that - because of elevated temperatures in these regions - gas-phase molecules are not only present in their ground vibrational but also in vibrationally excited states. In fact, in the millimeter- and submillimeter regime so-called 'vibrational satellites', i.e., pure rotational transitions of molecules in vibrationally excited states, may contribute substantially to the overall molecular line emission. Vibrational satellites of some species may be comparably strong in astronomical spectra but weaker lines will also contribute to a dense floor of lines sometimes referred to as 'astronomical weeds'.[1] With this contribution, we would like to highlight the role of the AILES beamline at the SOLEIL synchrotron in tackling the astronomical 'weed problem'. Although vibrational satellites can be observed directly in millimeter-wave pure rotational spectroscopy, we will show that a detour through the far-infrared can be very much worthwhile, particularly when the spectroscopic analysis is significantly accelerated by using modern software such as that based on the Automated Spectral Assignment Procedure, ASAP.[2,3]

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The Importance of Synchrotron Spectroscopy in Untangling the Complex Spectral Patterns of Deuterated Methyl Rotors

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ABSTRACT

The internal rotation of a methyl group in a molecule such as methanol is well known to result in the splitting of energy levels into two states referred to as A and E. The introduction of a deuterium atom into the methyl group removes the 3-fold symmetry of this rotor resulting in three substates corresponding to structures differing by an almost 120 degree internal rotation of the asymmetrical methyl group. The torsion for a deuterated asymmetrical methyl rotor is more complicated than a symmetric methyl rotor because of the dependence of the inertia tensor on the angle of internal rotation in addition to the coupling of the internal and overall rotation. The global analysis approach1-4 designed to account for this dependence requires an accurate torsional potential derived from the analysis of experimentally determined torsional subbands located at far infrared frequencies. The high flux of synchrotron radiation and high resolution facilities like those at SOLEIL are required to measure these torsional subbands and therefore correctly model the rotational spectrum of deuterated species such as methyl mercaptan and methanol. The accurate rotational frequencies provided from such an analysis is essential for the identification of these isotopologues in the interstellar medium, where deuterium fractionation is an important tool to understand their formation pathways and inheritance through the stages of star and planetary formation. I will present an update on our efforts to correctly model the rotational spectra of the deuterated isotopologues of methanol and methyl mercaptan, highlighting the role the synchrotron spectra played in such analysis along with our efforts to identify these species towards the solar-like protostar IRAS 16293-2422.

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Direct Experimental Evidence of the Roaming Atom Mechanism in a Macromolecular Noncovalent Complex

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ABSTRACT

In the last twenty years, the “roaming atom” chemical mechanism emerged and gained enormous interest thanks to its success in explaining experimental results that are not accounted for by the widely accepted statistical transition state theory.[1] In the roaming atom mechanism, on the pathway from reactants to products of a given chemical reaction, there is no tight transition state, defined as a saddle point on the potential-energy surface (PES) of the system. Instead, the roaming atom (or group of atoms) explores large and relatively flat regions of the PES, bypassing saddle points. Along its trajectory, “frustrated bonds” between the roaming species and other atoms of the system are successively formed and cleaved.[2]

Despite intense efforts for describing this new mechanism, crucial questions remain: is it statistical or nonstatistical? Does it play a role in molecular systems larger than 20 atoms, in particular those relevant to life sciences and pharmacology? Here, we present data on HCl transfer within a noncovalent complex built upon vancomycin, an antibiotic containing more than 170 atoms, and a tripeptide, following UV-VUV photoabsorption in the gas phase. In this molecular system, the released HCl is not internally hot, at least in some cases. Furthermore, the underlying process appears to be nonstatistical and requires a remarkably low total activation energy that is incompatible with the values obtained by quantum-chemical calculations, assuming a straightforward transition state mechanism. Instead, our results are consistent with a nonstatistical “roaming atom” mechanism. These pioneering results call for further investigation, in order to shed light on the precise mechanism at play as well as the energetics of the reaction. We thus propose to study noncovalent complexes between chemical derivatives of vancomycin and the tripeptide, using the SRMS2 set-up at the DESIRS beamline.

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Comparision of Ethylene Spectra at 10 µm Recorded by Fourier Transform and Frequency Comb Spectrometers

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ABSTRACT

High-resolution Fourier transform infrared (FTIR) spectra of methyl fluoride (CH_3F) were recorded in the mid- and far-infrared regions using the Bruker IFS 125HR spectrometers at GSMA (Reims, France) and at the SOLEIL synchrotron facility (Saint-Aubin, France). The measurements cover both the pure rotational transitions of the ground state (20 – 100 cm^{-1}) and the vibrational triad region (1950 – 2450 cm^{-1}), which includes the $2_{v3,\ v3}$ + $_{v6}$, and 2_{v6} bands. Spectra were recorded under various pressure conditions to optimize line visibility, with a high resolution. Line assignments were performed using predictions from the tensorial effective Hamiltonian implemented in the MIRS package, together with a newly developed automated assignment tool, SpectraMatcher, which facilitates line matching and discrimination of CH_3F transitions from overlapping CO_2 features. More than 5000 transitions (up to $J = 52$ in the ground state and up to $J = 45$ in the triad and $K = 19$) were assigned and included in a global fit. The sixth-order tensorial effective Hamiltonian model yielded excellent agreement with experiment, with rootmean-square (RMS) deviations better than 7×10^{-4} cm^{-1} across all regions. This paper presents the first continuous rovibrational study of CH_3F over both the triad and far-infrared ground state regions. The improved accuracy from previous studies stems from the improved set of effective Hamiltonian parameters which will also form a good basis from future applications in atmospheric modelling and spectroscopic databases.

Rovibrational Analysis of Cyclopentadiene using ASAP and SOLEIL

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ABSTRACT

The spectroscopic fingerprints of vibrationally excited states of astronomical molecules are interesting for multiple reasons. They are excellent temperature probes of the corresponding astronomical regions and are thought to be the origin of many unknown lines in astronomical survey spectra. Rovibrational spectra provide accurate vibrational energies and can guide subsequent pure rotational studies. The *Automated Spectral Assignment Procedure* (ASAP) greatly simplifies the rovibrational analysis when the rotational spectrum of either the upper or lower vibrational state is known with a high degree of accuracy (e.g., from a rotational analysis)[1].

Here, we present a new implementation of ASAP for the analysis of cyclopentadiene, a cyclic pure hydrocarbon that has already been detected astronomically toward the cold core of the Taurus Molecular Cloud[2]. Using the synchrotron radiation extracted by the AILES beamline of the SOLEIL facility, we recorded mid- and far-infrared high-resolution spectra of cyclopentadiene. We analyzed the rovibrational spectrum of the v_{21} fundamental with ASAP and used ASAP^2 to determine the vibrational energies of the eight vibrational modes below 860 cm^{-1}. ASAP^2 is an extension of ASAP for rovibrational bands where the rotational structures of the lower and upper states are known with high accuracy, leaving only the vibrational band center to be determined.

The presented rovibrational fingerprints agree with the results from pure rotational spectroscopy[3], demonstrating the efficiency and reliability of our new ASAP implementation.

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Parallel Session Schedule

Geosciences / Environment / Cultural Heritage

LIBRA Room

Chairpersons: Charlotte Catrouillet & Simona Raneri

IT-07	Invisible metals, visible impacts: Geochemical dynamics and the environment ***Alexandra Courtin***
OC-25	Impact of redox conditions on the binding of redox-inert contaminants to magnetite ***Rémi Marsac***
OC-26	Investigation of iron and copper speciation: Deciphering the green colourations of medieval stained-glass windows ***Cecile Bretonnet***
OC-27	Environmental degradation of plastics in soils: Example of polypropylene alteration investigated by Synchrotron-based GIXD and nano-CT ***Quentin Bollaert***
OC-28	Art gets the blues: Simple colorimetric tools for X-ray dose assessment ***Alice Gimat***
IT-08	How Synchrotrons can help us understand the dangers of historical lead-based cosmetics ***Fiona E. McNeill***
OC-29	Quantifying the speciation of sulfur and associated metals in geological fluids using Synchrotron spectroscopy ***Gleb Pokrovski,*** *Presentation by* ***Olivier Proux***
OC-30	Characterization of 19th and 20th century African glass beads using XRF band XAS spectroscopy ***Laurent Tranchant***
OC-31	Impact of different micro-organisms (bacteria, archaea) on the platinum (Pt) speciation ***Justine Le Doaré***
OC-32	Multi-scale Synchrotron study of critical-metal phases by XRF and XANES spectroscopies ***Georgia Grypaiou Iskenteridou***

Invisible Metals, Visible Impacts: Geochemical Dynamics and the Environment

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L. Darricau[d] , A. Mangeret[d] , J. Gorny[d] , S. Schoeder[e] , L. Tranchant[e] ,
D. Vantelon[e] , C. Rivard[e] , Q. Bollaert[e] , E. Léger[a] , J. Nouet[a] ,
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ABSTRACT

Since the beginning of the industrial and technosphere eras, there has been increased demand for various industrial minerals worldwide, leading nations to strive for self-sufficiency. From this perspective, pressure to reopen old mines is growing, meanwhile mining waste is also considered as a new opportunity for mineral extraction. However, mining activities are still considered as a potential source of metallic pollution, leading to profound modifications of environmental compartments in the subsurface, called the critical zone. Regarding these two perspectives, As, Bi, and W were studied in various materials for their speciation and crystal chemistry. The aim was to understand their new distribution in the subsurface environment and acknowledge their potential as resources. While there is a substantial body of data on As geochemistry and mineralogy, there is a severe lack of information on Bi and W. This hinders the ability to accurately predict their behavior, abundance, and mobility. Given tungsten's widespread use in alloys and carbides[1], it is essential to understand its dynamics to ensure sustainable management, particularly in the event of resumed mining activities. Bismuth is also an interesting element due to its increasing utilization (e.g., in hunting ammunition and fishing weights as an alternative to Pb[2]; in cosmetic products[3]). Furthermore, its geochemical cycle[4] and its substitution for As or Fe in some minerals must be assessed to predict its mobility in post-mining waste environments. XRF mapping and XANES analyses of waste materials, soils, and sediments provide essential knowledge about the local environments of these metals and metalloids. Microfocused data from X-ray fluorescence (XRF) mapping and X-ray absorption near-edge structure (XANES) analysis allows us to determine the importance of element redistribution, providing insight into their dynamics (e.g., remobilization or new retention), as well as the significant role played by organic matter and secondary phases of sulfate and phosphate in As and Bi sequestration. This highlights the metastability of the primary phases and demonstrates a certain resilience of some of the environmental compartments.

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Impact of Redox Conditions on the Binding of Redox-inert Contaminants to Magnetite

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ABSTRACT

Magnetite nanoparticles (MNs, $Fe^{II}Fe^{III}{}_2O_4$) play an important role on the behavior and fate of many contaminants and are widely used in environmental applications due to their small size, high surface area, redox and magnetic properties. Structural Fe(II) in stoichiometric MNs (R = [Fe(II)]/[Fe(III)] = 0.5) is extremely sensitive to oxidation, proton and ligand-promoted dissolution, leading to the formation of non-stoichiometric magnetite ($0 < R < 0.5$) or maghemite (R = 0; $Fe^{III}{}_2O_3$).[1] MNs stoichiometry can then be restored with Fe(II) or chemical reductants, which makes their structure highly dynamic in fluctuating redox environments.

The effect of redox conditions (or magnetite stoichiometry) on the reduction processes of various contaminants (e.g. U(VI), Cr(VI), organics) have been studied carefully.[2] However, most of the sorption experiments with redox-inert elements were carried out in O_2 atmosphere, using NO_3^- as background electrolyte or at acidic pH. Therefore, the impact of R on the binding of redox-inert contaminants to magnetite has been overlooked, although its ability to bind ions and molecules may heavily rely on R, as evidence for silicate, humic acid and quinolone antibiotics.[3]

Here we summarize our results on the interaction of Co(II),[4] Ni(II),[5] and Cr(III)[6] (considered redox-inert in reduced environments) with magnetite for various stoichiometries ($0.1 \leq R \leq 0.5$). Surface speciation of metal ions (M) was probed by X-ray absorption spectroscopy (XAS) and/or X-ray magnetic circular dichroism (XMCD) at Co/Ni $L_{2,3}$-edges on DEIMOS, XAS at Cr K-edge on LUCIA, and HERFD-XAS at Ni K-edge on FAME-UHD. Stoichiometric magnetite (R0.5) incorporates metal ions in its structure at low [M] (as MFe_2O_4-like phases), whereas surface complexes form on quasi-maghemite (R0.1). At high [M], R0.5 surface was a better template for M-hydroxide surface precipitation than R0.1. These results highlight the necessity to carefully preserve, control or monitor magnetite stoichiometry and will help to predict the effect of magnetite on metal fate and ecotoxicity in the environment.

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Investigation of Iron and Copper Speciation: Deciphering the Green Colourations of Medieval Stained-glass Windows

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ABSTRACT

Colour is one of the most striking properties of glass. This property is of interest in stained-glass windows, where the colour of the glass pieces is obtained thanks to the vdoping of the glass matrices with transition metals. The physicochemical origin of the colour is deeply linked to their speciation. For instance, copper is a widely used dopant, which can produce blue (absorption of diluted Cu^{2+} in distorted octahedra) to red (surface plasmon resonant absorption of Cu^0 nanoparticles) colours in glass [1]. But copper is also involved in green colourations. In the literature, the copper green colourations are linked to the presence of possible Cu^{2+}-Cu^{+} clusters [2], or to the influence of iron, mainly as Fe^{3+} in the glass [3], as iron is always found in medieval glass compositions due to raw materials impurities.

This study reports on X-ray Absorption Spectroscopy (XAS) measurements carried out at the PUMA beamline of SOLEIL synchrotron to determine the iron and copper speciation of a selection of medieval green glass pieces from the Reims cathedral, dated from the 13th century. Quantitative redox and sites of Fe and Cu in our samples were determined. In order to retrieve the elaboration condition of these historical samples, the results were compared to model glass pieces synthetized varying the Cu/Fe ratio and equilibrating temperatures (from 1500°C – reducing conditions – to 1200°C – more oxidizing conditions –).

Finally, we propose a new physicochemical description of the origin of the colour and elaboration conditions of medieval green glass pieces.

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Environmental Degradation of Plastics in Soils: Example of Polypropylene Alteration Investigated by Synchrotron-based GIXD and Nano-CT

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ABSTRACT

Plastic waste has become a major environmental concern due to uncontrolled littering across ecosystems, including soils. Compost amendments contaminated with plastics are a significant source to land. Once in the soil, plastics can fragment into microplastics (MP, 1 µm–5 mm) and nanoplastics (< 1 µm), which can be transported through the soil profile (1). Mobility of nanoplastics is particularly concerning because these particles can transport adsorbed metal(loid)s such as lead and rare earth elements (2,3). While thermal, photo- and mechanical degradation pathways are documented (4,5), the structural changes that accompany environmental alteration, and their role in generating nanoplastics, remain poorly constrained.

Here, we examine macroplastic fragments sampled from plastic-contaminated agricultural soils at Meung-sur-Loire (Loiret, France), which aged ~ 30 years in situ. Polypropylene (PP) fragments were analyzed using synchrotron-based grazing-incident X-ray diffraction (GIXD) and nano-computed tomography (CT). At 0° incidence, GIXD resolves only two of PP's four characteristic reflections, whereas increasing the incidence to 20° recovers the full diffraction pattern. The constant intensity of the (110) reflection, contrasted with the loss of others at low incidence angles, indicates the anisotropic alteration of plastic. Nano-CT imaging reveals sub-micron pores and micron-scale cracks forming in porous zones. Cracks network is characterized by fractures parallel to each other, with an almost vertical dip starting from the plastic surface and extending to depths of ~150 µm, demonstrating that degradation penetrated well below the surface. We observed porosity up to ~300 µm in diameter just below the surface, which seems to capture the fragmentation of the polymer into smaller fragments. These alteration features will be compared with those observed in other polymers from the same soil profile to identify which types of polymers are most susceptible to degradation, and to link with the nature, size and shape of the nanoplastics present in the soil.

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Art Gets the Blues: Simple Colorimetric Tools for X-ray Dose Assessment

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ABSTRACT

A variety of X-ray–based techniques can be employed to analyze Cultural Heritage (CH) artefacts[1,2]. However, the chemical reactions triggered by ionizing radiation and the potential subsequent damage remain poorly understood. This damage is mostly related to the X-ray dose absorbed during the analysis[3,4]. Measuring the dose is however challenging and, even with known instrumental and radiation parameters, rough estimations are at best based on assumptions (unknown absorption of the irradiated target).

We developed a simple radiochromic system to evaluate X-ray doses in CH artefacts. The indicator device consists of diacetylene molecules in a paper substrate. Upon X-ray exposure, the system undergoes a distinct and gradual colour change—from white to blue—, the kinetics of which depend on the diacetylene molecule used and its concentration. The quantitative evaluation of the absorbed dose correlates with the total colour difference (ΔE_{ab}). The dose–response was investigated across a wide dose range, relevant to CH studies, using both a large-area micro-X-ray fluorescence (MA-XRF) scanner and synchrotron radiation (PUMA beamline, SOLEIL). Two indicators, based on two different diacetylene molecules, were developed, for a dose interval coverage from 21 Gy to 37 kGy. The dependency of the response to X-ray energy, dose rate, beam accumulation, light and ambient air (temperature and humidity) was studied to determine the use conditions and give shelf-life recommendations. Associated with the calibrated colour scale, the indicators can be used as an early warning system during CH artefacts analysis and examination.

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How Synchrotrons Can Help Us Understand the Dangers of Historical Lead-based Cosmetics

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ABSTRACT

Lead compounds were used in cosmetics and hair dyes for millennia and there are well documented cases of poisonings. For example, the cosmetic Laird's Bloom of Youth killed one young woman and poisoned others in America in the 1870s[1,2] a hair dye caused encephalopathy in men in Ireland in the 1890s[3] and the traditional Hindu cosmetic sindoor poisoned women and children in India and the U.S.A.[4]

The exact mechanisms of the poisonings are not well understood. Inorganic lead compounds have generally been considered to be minimally absorbed through skin, but my laboratory has been studying whether transdermal absorption of lead from cosmetics could be possible.

In this presentation, I plan to show you our µXRF maps of lead in skin, measured using the PUMA beam line at Soleil which demonstrate how lead acetate in hair dyes permeated the skin around the hair follicle and how lead tetroxide in sindoor entered the skin. Further, I will show you how XAS measurements have shown us that lead compounds are changing form in cosmetics and this alters how they enter the skin. I will also show you that lead creates different compounds in deeper skin layers.

In addition, I will share data from the BioXAS beam line at the Canadian Light Source which explain how Laird's Bloom of Youth could penetrate the skin, and which demonstrate that if Queen Elizabeth the 1st was using a white lead and vinegar mixture as a cosmetic, she was likely poisoning herself through skin absorption of lead.

While our cosmetics research has been interesting, it is also providing health and safety data for today. I will share µXRF maps of lead acetate in skin (from both Soleil and CLS) which have revealed a measurement artifact that arises from using the gold standard testing method for penetration of compounds through skin. Our data suggest that transdermal absorption of inorganic lead may be a hundred times greater than believed. I will also share some remarkable µXRF maps which have revealed that that lead binds to specific cells in skin, is taken up in sweat glands, and is transported through connective tissue, suggesting alternative transport routes of lead through the body.

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Quantifying the Speciation of Sulfur and Associated Metals in Geological Fluids using Synchrotron Spectroscopy

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ABSTRACT

Sulfur is the key ingredient of the hydrothermal fluids that form metal economic resources on Earth. Knowledge of sulfur redox and chemical speciation in the fluid phase is thus necessary for assessing sulfur transfers, along with associated, metals to ore deposits. However, the extraordinary aqueous chemistry of sulfur, with a plethora of intermediate-valence species, including radical ions, polysulfides, sulfur dioxide and sulfites, coexisting with the two major redox end-members, sulfide S(-II) and sulfate S(+VI), makes quantitative assessment challenging[1]. This is because most of those sulfur forms and their complexes with metals are unquenchable, undergoing rapid transformations upon fluid cooling thereby making impossible their preservation in ex-situ studies. Quantifying such fugitive species requires in-situ spectroscopic approaches applicable to the fluid phase under elevated temperatures (T) and pressures (P). However, traditional lab spectroscopic techniques have multiple limitations intrinsic to measurements on high T-P fluids.

In this contribution, we highlight some promising venues that exploit synchrotron radiation for sulfur and its metal complexes. Our studies used perforated diamond anvil cells[2] developed at ID12 beamline, hydrothermal autoclaves[3] at FAME, FAME-UHD, and ID20 beamlines of the ESRF, and silicate minerals as traps for sulfur. These setups allow sulfur to be probed by K-edge XANES and $L_{2,3}$-edge NRIXS spectroscopy, whereas sulfur complexes with metals (Au, Pt, Pd, Mo) are quantifiable using both traditional and high resolution (HERFD) XAS. Combination of the spectroscopic data with solubility measurements and molecular modeling allows the quantification of both identity and stability of metal complexes with the major sulfur ligands - hydrogen sulfide and trisulfur radical ion[4-8], enabling more accurate geochemical models of sulfur and metal transfers across the lithosphere[8,9].

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Characterization of 19th and 20th Century African Glass Beads using XRF Band XAS Spectroscopy

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ABSTRACT

The cultural anthropology collections of the Musée de l'Homme (MH), part of the Muséum National d'Histoire Naturelle (MNHN), intend to document the history of societies and the evolution of their material know-how. This study focuses on African beads, which appeared very early on the continent and used as currency for several centuries. At the end of the XIXth century, the massive import of European glass beads, mainly from Venice and Murano, led to the development of a local craft industry, today emblematic of countries such as Ghana, Nigeria or South Africa [1].

The corpus studied includes African glass beads preserved at the MH, dated approximately from the end of the XIXth and XXth centuries. Some are important trade beads manufactured in Europe, sometimes recognizable by their patterns like *millefiori*, while others have been locally made from recycled glass. The mixture of stylistic and technical influences makes the provenance of the majority of them difficult to establish by a simple visual examination [2].

For this reason, these beads were characterized using non-invasive and non-destructive techniques in search of chemical markers to distinguish them. X-ray fluorescence (XRF) and X-ray absorption (XAS) spectroscopy measurements were carried out in April 2025 at the PUMA beamline. This allowed us to conduct a first qualitative study of the composition of the glasses. The results enable us to discuss the provenance of several beads of the studied corpus and also to precise the date or the manufacturing technique thanks to the trace elements detected in the glass matrix, to coloring agents and to glass heterogeneities.

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Impact of Different Micro-organisms (Bacteria, Archaea) on the Platinum (Pt) Speciation

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ABSTRACT

The anthropogenic use of platinum (Pt) has significantly altered its biogeochemical cycle over recent decades[1], leading to its increased dispersion in the environment. Microorganisms, ubiquitous in ecosystems, strongly influence metal speciation. While some metals are essential for microbial metabolism, their transformations can also generate toxic forms that microorganisms detoxify through chelation or redox processes[2] . However, the impact of microorganisms on Pt speciation remains poorly understood, despite Pt's high affinity for sulfur-bearing ligands[3] .This study investigates the influence of the common bacterium Escherichia coli and of the hyperthermophilic archaeon *Thermococcus kodakarensis,* on Pt and S speciation. These species compass a diversity of metabolic pathways: E. coli is a ubiquitous mesophilic bacterium common to human and animals, and the hyperthermophilic *T. kodakarensis,* relies on S-assisted fermentative metabolism.

X-ray absorption spectroscopy (XAS) at the Pt L_3-edge revealed that both microorganisms, when exposed to 100 µM of Pt(IV) in nutritive media, can reduce Pt(IV) to Pt(II) within 1 hour and to Pt(0) after 24 hours, involving S-bearing ligands in E. coli. In contrast, *T. kodakarensis* reduced Pt(IV) directly to Pt(0) within 1 hour, indicating faster reduction kinetics. These independent analyses also showed a more reduced intracellular sulfur pool in *T. kodakarensis* than in E. coli Similarly, XAS analyses at the S K-edge, performed under the same Pt(IV) exposure conditions (100 µM), revealed an increase in reduced S(-II) and a decrease in oxidized S(+V) species in E. coli, whereas *T. kodakarensis* exhibited the opposite trend, highlighting the key role of sulfur in microbial Pt detoxification. This work provides new insight into the microbial S metabolism driving distinct Pt transformation pathways and emphasizes the key role of microbial diversity on Pt environmental mobility by comparing two phylogenetically and metabolically different microorganisms.

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Multi-scale Synchrotron Study of Critical-metal Phases by XRF and XANES Spectroscopies

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ABSTRACT

Mining operations are essential for extracting valuable resources although they produce large volumes of waste with different mineralogical compositions, as well as various physical and chemical properties. Mining waste can be considered in two ways: as valuable secondary resources or as a potential source of pollution. The remediation of mining residues is always challenging due to the aforementioned issues, the age of the mine heaps — in France, dating back to antiquity and extending to the end of the 20th century — and the widespread distribution of the waste.

Here, we investigate how a non-remediated site (W district - French Massif Central) evolved over time, especially regarding the formation of new minerals after weathering processes of mining waste and their role in natural attenuation strategies.

To address this issue, the hardpans (indurated iron layers) are of high interest as they are considered to be an efficient sink for metal(loid)s. Hardpans are formed from indurated mining waste thanks to the weathering of sulfide-rich phases (mainly As-rich pyrite). In addition to W, other trace elements present in the waste were studied, notably As because of its well-known toxicity, and Bi given the lack of knowledge about its geochemical behavior and toxicity. Moreover, these three elements are classified as critical raw materials.

This work aims to understand the on-site hardpans formation, their role in retaining critical and/or potentially toxic trace elements (long-term efficiency), especially at the sub-micron scale. We therefore used a multiscale strategy that integrates synchrotron XRF and XANES, with As, Bi, and W edges acquired at PUMA, complemented by Fe and S edge analyses at LUCIA.

The mineralogical composition of the various wastes present on site was determined, with a focus on hardpans, as well as the fractionation of metal(loid) elements within the mining waste. Crystal chemistry, substitutions, and competitive effects between ions were studied within metal bearing phases, particularly sulfates and iron oxides, using natural and synthetic samples. The results provide an initial overview of the trace elements mobility and gives insights into the weathering of mineral phases, and the elemental redistribution toward various environmental compartments in the surrounding area.

Parallel Session Schedule

Physics & Advanced Materials
(Structural, electronic and magnetic properties of matter / Physical surfaces and interfaces)

CEA BLOCH Auditorium

Chairpersons: Eglantine Boulard, Sara Gonzalez & Fabien Silly

IT-09	Deep strain field of surface reconstruction ***Vincent Repain***
OC-33	1s2p resonant inelastic X-ray scattering natural circular dichroism ***Alessandro De Frenza***
OC-34	Deep learning approach for fixing limited angle artefacts in Synchrotron X-ray tomography ***Shyam Pulickan***
OC-35	Imaging the indirect-to-direct band-gap crossover in PbI$_2$ ***Marcin Rosmus***
OC-36	Is there a liquid-liquid transition in realgar (As4S4) under extreme conditions? A comprehensive Synchrotron study ***Vincent Rajaji***
IT-10	Probing inversion symmetry breaking and related electronic properties in ultrathin tellurides ***Fabien Cheynis***
OC-37	Mechanical strain effects on the magnetic response of ferromagnetic thin films on polymer substrates ***Alejandro Toledano-Povedano***
OC-38	Correlating RIXS and EELS and XEOL spectroscopies in Van der Waals materials ***Alessandro Nicolaou***
OC-39	Structural and electrical characterization of Hf$_{0.5}$Zr$_{0.5}$O$_2$ and ZrO$_2$ thin films using grazing incidence Synchrotron X-ray diffraction ***Grégoire Magagnin***
OC-40	*In situ* Synchrotron study of the 1T'/1H phase transition in colloidal WS$_2$ monolayers ***Dario Mastrippolito***

Deep Strain Field of Surface Reconstruction

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ABSTRACT

The knowledge of the atomic structure at the surface of a material is fundamental to understand its properties and control the interaction of the material with the environment. It is in particular essential to master the growth of new nanostructured materials. Most of the surfaces show a structure of the last atomic layer which is different from the bulk, which is called surface reconstruction. In common models, only atomic displacements in the surface layer and interplanar relaxations of the first subsurface layers are taken into account. On metals, a famous example is the 22x√3 reconstruction of Au(111), also called discommensuration lines. Very surprisingly, although it is a very popular surface for many applications, its investigation by x-ray diffraction is very scarce[1].

By a comprehensive grazing x-ray diffraction study of a reconstructed vicinal surface of Au(111) and comparison with atomistic models, we were able to demonstrate some novel features[2]. First, the structure of the surface layer displays a surface dislocation which is resolved with an unprecedented resolution for the first time. Second, we measure a strong signal of deep atomic displacements, which penetrates more than tens of layers into the bulk. We can decompose this strain field into several components generated by different surface patterns. On one hand, the surface dislocation induces a strong strain field which stabilizes a highly regular surface pattern. On the other hand, the discommensuration lines induce a dipolar like strain field, with a vortex of displacements located in the fifth subsurface layer, and penetrating at least in the first fifteen layers. Those deep strain fields have to be taken into account in the calculation of the energetics of the surface, with significant errors when not considered. Our results shed a new light on the complexity of subsurface displacements induced by surface reconstruction.

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1s2p Resonant Inelastic X-ray Scattering Natural Circular Dichroism

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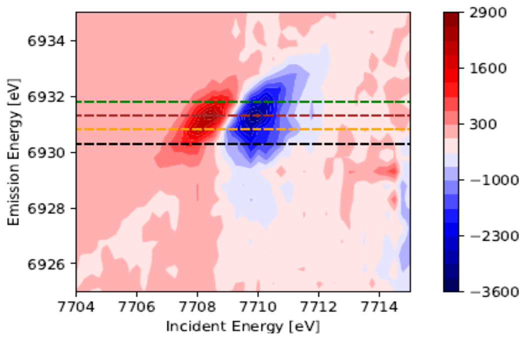
ABSTRACT

X-ray natural circular dichroism (XNCD), that is the differential absorption with circularly polarized X-rays having opposite helicity by an optically active material, is a powerful characterization technique for probing local chiral and magneto-electric properties of a material. Resonant inelastic X-ray scattering (RIXS) is an element-selective and high-energy resolved spectroscopic technique implied to investigate electronic structure of molecules, similar to X-ray absorption (XAS). In this work, we employ 1s2p RIXS, which probes the Kα emission following the excitation of a 1s electron to empty 3d–4p orbitals in a transition metal. The compounds investigated are single crystals of metal-organic complexes of $[Co(en)_3](No_3)_2$ that crystallize in the $P6_322$ space group. We previously measured a strong X-ray natural circular dichroic signal in these crystals [2] from measurements conducted at the GALAXIES RIXS end-station at SOLEIL [1]. High-Energy-Resolved Fluorescence-Detected X-ray Absorption (HERFD-XAS) spectra recorded with right- and left-circularly polarized light reveal a pronounced RIXS-NCD signal of about 23% relative to the pre-edge maximum. This represents a significant enhancement compared with previous XNCD measurements on the same compound, where the signal was approximately 9% [2]. RIXS-NCD also offers the possibility to measure full dichroic spectra for the emission. These spectra were recorded for the Δ- $[Co(en)_3](No_3)_2$ with the incident x-ray energy tuned close to the maximum of the RIXS-NCD signal at 7710 eV. The emission energy was scanned across the Co $K\alpha_1$ and $K\alpha_2$ lines for both helicities and for both axial and orthoaxial geometries. The observed dichroic signals follow the predicted angular dependence for XNCD in the $P6_322$ symmetry [3]. As last result, a two-dimensional RIXS map combining both the 1s absorption and the 1s2p emission shows a clear dichroism over a wide energy range in the Co 1s pre-edge region.



RIXS-NCD map at Co K-edge in
Δ- $[Co(en)_3](NO_3)_2$

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Deep Learning Approach for Fixing Limited Angle Artefacts in Synchrotron X-Ray Tomography

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ABSTRACT

Recovering missing information for angular data has been a topic of interest for decades predominantly in the field of research with the rise of technologies like electron microscopy, computer aided tomography, optical astronomy and so on. Various analytical solutions have been developed to fix these problems mainly using interpolation algorithms and iterative algorithms [1]. Recently with the development of Artificial Intelligence (AI) different Deep Learning (DL) algorithms have been developed to fix the missing angle artefacts.

A recent DL algorithm called DeepDeWedge (DDW), developed for cryo-transmission electron microscopy (cryo-TEM) tomography, has proven effective in correcting missing angle artefacts and image noise [2]. DDW uses cubic Representative Element Volumes (RVEs) from two tomograms reconstructed from the even and odd projections of a scan for training, relying on a 3D U-Net architecture to identify and correct these artefacts.

In synchrotron X-ray tomography, missing angles can appear due to the experimental configuration; for example, the columns of a high-pressure cell like the UToPEC (Ultra-Fast Tomography Paris-Edinburgh Cell) obstructing the beam [3]. The UToPEC used at the SOLEIL Synchrotron creates a ‘blind spot’ of 18.55°.

Missing angle artefacts are mainly visible in the XY plane (where Z denotes the tomographic rotation axis), which means that very few pixels are needed on the Z axis of a RVE when training the DL model. Therefore, the DDW algorithm is modified to adapt to synchrotron data. The modified version can use a single tomogram and handle RVEs with unequal side lengths (non-cubic).

This allows the DL to process more pixels in the XY plane, which are more relevant than those in the Z direction. Therefore, these can better contain the missing angle artefacts within a single RVE compared to its predecessor. This approach also reduces the load and time required for GPU calculations, and consequently the hardware requirements.

The adapted algorithm was tested on X-ray microtomography data from a 1 mm diameter aluminium cylinder with internal porosity and steel inclusions [4] and is found to be a good tool for fixing missing angle artefacts as well to a certain extend noises in the image.

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Imaging the Indirect-to-direct Band-gap Crossover in PbI_2

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ABSTRACT

We present direct experimental evidence for a thickness-driven crossover from an indirect to a direct band-gap in PbI_2 thin films. Using angle-resolved photoemission spectroscopy (ARPES) performed on films grown by molecular beam epitaxy on graphene/SiC, we observe a shift of the valence band maximum (VBM) from a position between $\bar{\Gamma}$ and $\bar{M}$ in monolayers to the $\bar{\Gamma}$ point in multilayers. This transition is accompanied by a dimensional crossover from a two-dimensional electronic structure in monolayers to three-dimensional dispersion in thicker films.

Our measurements are in excellent agreement with density functional theory calculations. The results identify the interlayer hybridization of iodine p_x and p_z orbitals as the driving mechanism for the band-gap transition. We further confirm that the VBM in multilayer PbI_2 resides at the A point of the bulk Brillouin zone, consistent with the emergence of a direct band-gap in the 2H polytype.

These findings provide a direct spectroscopic signature of band-gap tunability in a layered semiconductor, with implications for optoelectronic device applications.

Is there a Liquid-liquid Transition in Realgar (As_4S_4) under Extreme Conditions? A Comprehensive Synchrotron Study

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ABSTRACT

The possibility of having two or more liquid phases of the same substance, separated by a first-order liquid-liquid transition (LLT) where density discontinuously changes, has been discussed as early as the 1970's [1] and has been strongly debated in the case of supercooled water in the last 4 decades [2]. Experimental studies have clearly established the existence of first-order transitions in a few liquid systems, such as phosphorus [3,4] and sulfur [5]. However, our understanding of the LLT remains relatively primitive, and experimental realizations remain scarce and, in most cases, heavily disputed. In this context, the AsS system appears as a promising candidate for LLT according to recent literature [6-8]. Indeed, experiments [6] have revealed sharp and strong changes in the structural and dynamics properties of the AsS melt as pressure is increased. This led to the proposition that the AsS liquid undergoes two major transformations: first, from a molecular to a polymeric liquid around 2 GPa, and second, to a metallic liquid around 5 GPa. Moreover, according to two recent computer simulations using ab-initio molecular dynamics (AIMD) [7,8], a discontinuous volume jump occurs at the molecular-to-polymeric liquid transition.

Motivated by these findings, we have systematically investigated liquid As_4S_4 using synchrotron (PSICHE, SOLEIL) based in situ X-ray absorption, X-ray diffraction (XRD), X-ray radiography and tomography in the Paris–Edinburgh press. This set of various techniques enabled us to obtain the first measurements of the density of liquid AsS along various isotherms up to 6 GPa, as well as to explore the liquid structure and viscosity of AsS as a function of pressure and temperature. Furthermore, we measured the melting curve of AsS, and estimated the density changes along the melting line. The results will be shown in this presentation and discussed in relation with the proposed liquid-liquid transition.

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Probing Inversion Symmetry Breaking and Related Electronic Properties in Ultrathin Tellurides

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ABSTRACT

Crystalline tellurides characterized by an atomic arrangement with an inversion symmetry breaking such as α-SnTe, α-GeTe or Td-WTe$_2$ show multi-functional properties including ferroelectricity, a Rashba spin-split band structure, topological electronic states, … [1–4]. This is of significant importance in the perspective of all-electrically controlled and low-power spin-orbitronic applications [5–7]. In this context, device downscaling raises fundamental questions about the persistence of the targeted properties in ultrathin films. For instance, X. Yang *et al.* evidenced a reduction of the Rashba effect in α-GeTe(111) films below 5nm and extrapolated a critical thickness of 2nm, below which the Rashba spin splitting of the electronic band structure vanishes [8].

By appropriately analyzing and optimizing the growth conditions, we will show that Rashba spin-splitting and related electronic properties can be preserved in the ultrathin regime in α-GeTe and Td-WTe$_2$ films [9,10]. Our results based on photoemission spectroscopy techniques (ARPES, SR-ARPES, …), microscopies (TEM, STM) and a strong theoretical support from DFT calculations suggest to further investigate the limit of physical properties in the ultrathin film regime.

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Mechanical Strain Effects on the Magnetic Response of Ferromagnetic Thin Films on Polymer Substrates

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ABSTRACT

Ferromagnetic thin films are widely used in flexible electronics, being a key component in devices used as sensors, data storage and signal processing. To ensure the reliability of these systems, it is crucial to study the impact of mechanical deformations on their magnetic response. Such deformations can alter the magnetic behaviour of a material, creating both homogeneous elastic stresses and heterogeneous stresses arising from cracks [1] – associated with magnetoelastic coupling. After fragmentation, magnetostatic coupling can appear though dipolar interactions and shape anisotropy [2].

This study focuses on the impact of applied mechanical stress (from the elastic regime up to controlled crack propagation) on the magnetization curves of a ferromagnetic thin film (20 nm thick) of $Ni_{60}Fe_{40}$ deposited on a polymeric substrate. A new approach was implemented using a unique device developed at the SOLEIL synchrotron (DiffAbs beamline), combining four techniques to study in situ the crystalline and magnetic properties of the sample subjected to controlled biaxial tensile tests: X-ray diffraction to measure the deformation of the crystal lattice and deduce the stresses, digital image correlation to measure the applied macroscopic deformation, electrical resistivity to detect crack initiation, and the Longitudinal Magneto-Optical Kerr Effect (L-MOKE) to track the evolution of magnetic reversal.

In situ SOLEIL synchrotron diffraction allows demonstrating the direct correlation between the evolution of the thin film mechanical stress and the magnetization reversal cycles, where magnetoelastic effects dominate over magnetostatic effects (i.e. geometrical effects due to fragmentation) in both elasto-plastic and cracking regimes [3].

ACKNOWLEDGEMENTS

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Correlating RIXS and EELS and XEOL Spectroscopies in Van der Waals Materials

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ABSTRACT

In recent years, the inelastic branch of the SEXTANTS beamline has been developing a collaborative research initiative aimed at correlating different state-of-the-art spectroscopies. We perform resonant inelastic X-ray scattering (RIXS) in the soft X-ray regime (50 eV – 1000 eV), and on the same experimental setup, we can perform X-ray excited optical luminescence (XEOL). Both spectroscopies can be conducted down to 18 K and under electric and magnetic fields, thanks to the MAGELEC sample environment. Moreover, we closely collaborate to correlate RIXS and XEOL spectroscopies with electron energy loss spectroscopy (EELS) and cathodoluminescence on various van der Waals materials and correlated systems. In my talk, I will present our recent results. Specifically, I will discuss how, on the magnetic compound CrSBr, we have used crystal field calculations to model the linear dichroism measured in RIXS to determine the chromium crystal field scheme [1]. Additionally, to correlate magnetic properties with photoluminescence (PL) behavior, we measured both RIXS and PL under an applied magnetic field to track the antiferromagnetic-ferromagnetic transition at approximately 0.3 T. I will also present our correlative RIXS-XEOL and EELS study of hexagonal boron nitride (hBN), where the direct exciton responsible for strong luminescence at 6.4 eV was carefully characterized using these three spectroscopies [2]. Finally, I will emphasize the usefulness of combining complementary spectroscopies like RIXS and EELS, as well as excitation and recombination techniques.

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Structural and Electrical Characterization of $Hf_{0.5}Zr_{0.5}O_2$ and ZrO_2 Thin Films using Grazing Incidence Synchrotron X-ray Diffraction

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ABSTRACT

Ferroelectric hafnia-based oxides are promising for ultra-low-power, CMOS-compatible devices due to robust ferro/antiferroelectric responses at nanometric thickness. Among them, $Hf_{0.5}Zr_{0.5}O_2$ (HZO) can stabilize a polar orthorhombic phase enabling ferroelectricity, whereas ZrO_2 can exhibit antiferroelectric behavior through field-induced transitions. Understanding how deposition route and composition control phase assemblages is essential to optimize device performance.

We investigate 10-nm-thick HZO and ZrO_2 capacitors (TiN/HfZrO/TiN or TiN/ZrO_2/TiN on Si) prepared by atomic layer deposition (ALD) and RF sputtering. Grazing-incidence synchrotron X-ray diffraction (GIXRD) with θ–2θ scans and reciprocal-space mapping enables phase-sensitive analysis despite ultrathin films, resolving monoclinic, tetragonal, and orthorhombic fluorite-derived structures. The grazing geometry and high reciprocal-space resolution further reveal microstructural signatures: texture/preferential orientation and grain-size trends, systematically dependent on growth method and chemistry.

Electrical measurements performed on the same test structures (Dynamic Hysteresis Measurements) establish quantitative links between structure and properties. In HZO, ALD tends to favor higher fractions of the polar orthorhombic phase with correspondingly stronger ferroelectric switching; sputtered HZO shows comparatively reduced polar content and weaker remanence. In ZrO_2, both routes stabilize predominantly tetragonal, centrosymmetric character at rest, consistent with antiferroelectric-like double-loop behavior. The combined structural–electrical picture clarifies how processing parameters tune phase fractions, offering a practical pathway to engineer device-level metrics (coercive field, remanent polarization, and energy-storage figures) by targeted control of deposition conditions.

These results provide a comparative, probe-consistent map of phase stabilization across HZO and ZrO_2 stacks, delivering guidance for integrating hafnia-based ferroelectrics and antiferroelectrics into next-generation memory and energy-efficient electronics.

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In situ Synchrotron Study of the 1T′/1H Phase Transition in Colloidal WS_2 Monolayers

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ABSTRACT

Controlling the crystalline phase of transition metal dichalcogenides (TMDs) is crucial for tailoring their electronic and optical properties. Among the polymorphs of WS_2, the metastable 1T′ phase exhibits a semimetallic or narrow-bandgap character distinct from the semiconducting 1H phase, making their interconversion a key challenge in phase engineering.[1,2] Here, we employ a multi-technique synchrotron approach, combining in situ GIXD, XPS, and XAS measurements at the SOLEIL (TEMPO, SAMBA, ANTARES, SMIS) and DIAMOND (I07) facilities, to directly track both the structural and electronic evolution during the temperature-induced 1T′→1H phase transition in colloidally synthesized WS_2 monolayers stabilized with organic ligands.[3] The reducing ligands used during synthesis stabilize the 1T′ phase through strong electron doping, ensuring phase stability up to ~300 °C. Upon annealing above this threshold, ligand decomposition triggers a reconstructive transformation toward the 1H phase. The results reveal a progressive disappearance of the 1T′ superstructure and the emergence of the prismatic 1H lattice, accompanied by distinct changes in the local W coordination. We find that the kinetics of this transformation are strongly influenced by the nanosheet's lateral size and surface chemistry, highlighting the interplay between doping, ligand decomposition, and lattice reorganization. These insights open new perspectives for controlled phase stabilization and scalable synthesis of polymorphic TMDs nanostructures.

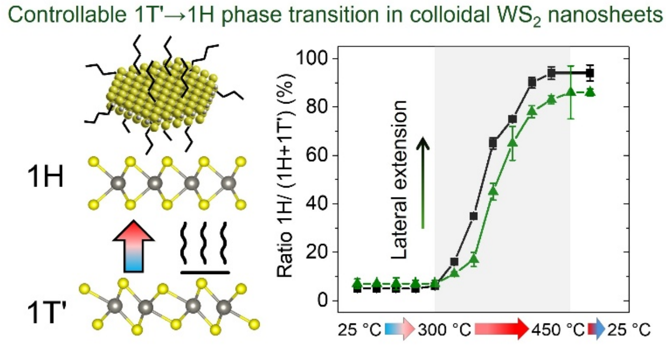
Controllable 1T'→1H phase transition in colloidal WS_2 nanosheets

Figure 1. Evolution scheme of the relative weight of the 1H phase with respect to the 1T′.

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The Synchrotron Community Posters Session

Thursday, January 15th, 2026

The Synchrotron Community

Amélie Bordage, in name of the S2UO committee
and of all the authors of the session

ABSTRACT

The Users'Meeting of a synchrotron is an ideal place to gather all the people involved in the life of a synchrotron. This new poster session of the SUM2026 is dedicated to all of them : beamline and support laboratory scientists, scientific associations, networks, BAGs, etc.

The scientists will present an overview and technical description of their beamlines and laboratories, as well as the science area in which they are involved and some examples of scientific results. This will be completed by their perspectives for future development and challenges. SOLEIL beamlines will be present as well as the French CRG beamlines of ESRF, for which beam access is granted through SOLEIL proposal review committees.

The scientific associations, the national network, the BAGs,… will present their status, their goal and some of their actions. Their role in making synchrotron a living and dynamic community is precious but sometimes not enough known and/or highlighted.

Such a session will offer time to discover all these sides of the synchrotron community and to discuss together as a community.

The titles of the poster is listed below.

The Synchrotron Community posters session

Thursday, January 15th, 2026

SOLEIL Beamlines and Support Laboratories

PO-01	X-ray Nano-Tomography at ANATOMIX
PO-02	CASSIOPEE - ARPES and spin-ARPES
PO-03	CRISTAL@SOLEIL
PO-04	DEIMOS Beamline
PO-05	GALAXIES Beamline
PO-06	LUCIA Beamline
PO-07	MARS, the beamline dedicated to radioactive studies at SOLEIL
PO-08	METROLOGY Beamline
PO-09	Multilength-scale and multimodale scanning hard X-ray imaging at NANOSCOPIUM at the dawn of the source upgrade
PO-10	PLEIADES Beamline
PO-11	The PUMA beamline
PO-12	ROCK: The quick-EXAFS beamline at SOLEIL
PO-13	SAMBA - XAFS for all
PO-14	Surfaces and interfaces x-ray Scattering (SixS) beamline at SOLEIL: From UHV to operando studies
PO-15	SMIS Beamline : Multiscale Infrared Spectromicroscopy
PO-16	SWING: A SAXS versatile beamline
PO-17	Operando nanoARPES probing of electronic structure
PO-18	Diffabs beamline
PO-19	Dichroism, Imaging, Spectroscopy for Chemistry and biology from molecule to tissue
PO-20	PSICHE beamline
PO-21	Presentation of support laboratories

CRG Beamlines

PO-22	The FAME-PIX and FAME-UHD CRG beamlines: Recent developments and perspectives
PO-23	BM02 - D2AM a french CRG beamline at the ESRF dedicated to Anomalous Diffraction and Scattering in Material Science
PO-24	Materials science and nanosciences on the French CRG IF beamline (BM32) at ESRF

PO-25	BM07: A versatile beamline for automated cryogenic (AMX) and functional room temperature crystallography (FMX)
PO-26	The in crystallo optical spectroscopy (icOS) Lab at the ESRF

Networks & Scientific Associations

PO-27	GDR CohereX - Science with coherent X-rays at 3rd and 4th generation Synchrotron sources
PO-28	RECIPROCS, le ЯÉseau des Chercheurs et ITA PROfessionnels de la Cristallographie Structurale
PO-29	SUO2: SOLEIL Synchrotron Users Organization
PO-30	AFURS

BAG Proposals

PO-31	The ‘Flat Fossils’ BAG At The PUMA Beamline: Rationale and First Results
PO-32	Virtual Histology in Biomedicine (ANATOMIX)
PO-33	The EXAFS BAG EXAFS for geosciences, environment and materials
PO-34	The Block Allocation Group Marseille
PO-35	BAG SWING - Synthesis and assembly of inorganic nanoparticles

Scientific Activities

PO-36	Research and network activities of the SOLEIL scientific section “Cultural and Natural Heritage Science”
PO-37	Scientific Section - Fundamental Processes in Isolated Systems
PO-38	CH logiciel - Irradiation Passport for Art
PO-39	Studies of macromolecules
PO-40	Chemical characterization of cells/tissues
PO-41	Structure characterization of cells/tissues

Scientific Posters Session

Friday, January 16th, 2026

Scientific Posters session

Friday, January 16th, 2026

PO-BIO-01	Exploring the interactions of elastin peptides with model membranes by molecular dynamics and circular dichorism *Jean-Marc Crowet*
PO-BIO-02	Lung-liver connective tissue interactions in rats assessed by the Synchrotron deep UV fluorescence microscopy *Petra Somogyi*
PO-BIO-03	AI-based design of RNA methyltransferase for RNA-based therapeutics *Priscila Sutto Ortiz*
PO-CHE-04	In situ evolution of SrMoO3 thin films probed by NAP-XPS *Rosinel Alfonzo*
PO-CHE-05	A new versatile operando photocatalytic cell for quick-EXAFS: The example of CO2 photoreduction *Anthony Beauvois*
PO-CHE-06	SAXS from rigid cellulose chains solutions in ionic liquids: Structure factor *François Boué*
PO-CHE-07-S	Formulation of lipid nanocapsules with microfluidic chips and characterisation *Etienne Chèvremont*
PO-CHE-08	The self-assembly of colloidal titania ribbons *Doru Constantin*
PO-CHE-09-S	Correlating supramolecular organization with chromatic transitions in ultra-thin functionalized polydiacetylene films *Maria Kandyli*
PO-CHE-10	LevSAXS: Exploring phase transitions under acoustic levitation combined with SAXS *Erwan Paineau*
PO-CHE-11-S	Formic acid production via CO$_2$ electroreduction using CeO$_2$–Bi catalysts supported on functionalized carbon nanotubes *Enrico Piasentier*
PO-CHE-12-S	Evaluating surface properties on high-density positive electrodes for li-batteries *Danish Quamar*
PO-CHE-13-S	Formation of a dense liquid precursor in mineral crystallization: Spinodal decomposition evidenced by sub-millisecond microfluidics coupled to time-resolved in situ SAXS *Jade Raimbault*

PO-CHE-14-S	Fate of self-assembled squalene nanoparticles in a biomimetic medium assessed by scattering techniques	*Hugo Roncin*
PO-CHE-15	Radiation damage with soft X-rays in organic and hybrid semiconducting materials	*Sufal Swaraj*
PO-CHE-16	Quantum crystallographic studies of phase transition in minerals under pressure	*Krzysztof Woźniak*
PO-CHE-17-S	Structure of assemblies of nanospheres confined in smectic liquid crystal defects	*Muyan Zhou*
PO-GEO-18	Contribution of infrared spectrometry to the understanding of calcareous biominerals	*Yannick Dauphin*
PO-GEO-19	Characterization & first performance evaluation of LEAPS-INNOV HPGe detector for spectroscopy applications	*Francisco-José Iguaz Gutierrez*
PO-GEO-20	Irradiation Passport for Art (IPA)	*Ineke Joosten*
PO-GEO-21	Redox speciation of cerium in the presence of natural organic matter	*Terjini Kiththangodage*
PO-GEO-22-S	Lacquer coatings on carriages: The possibilities of Synchrotron-based µFTIR spectroscopy for the study of multilayered historical samples	*Mathilde Occelli*
PO-GEO-23	Fragmentation of plastics induces Cr(VI) release : Implications upon environmental degradation	*Guillaume Pécheul*
PO-GEO-24	Localisation spatiale 2D et 3D de microsphères de polyéthylène chez la moule par techniques Synchrotron	*Camille Rivard*
PO-GEO-25	Structures of ices by quantum crystallography and PDF	*Krzysztof Woźniak*
PO-PHY-26	Structural phase transition in epitaxial lead-free $Bi_{0.5}Na_{0.5}TiO_3$-$BaTiO_3$ ferroelectric relaxor thin films	*Thomas W. Cornelius*
PO-PHY-27	Micro-fabrication using Synchrotron radiation	*Paulo Da Silva*
PO-PHY-28-S	Structural investigations of HfO_2-based transistor stacks during annealing and electric field cycling by in-situ XRD	*Tom Iung*

PO-PHY-29	Study of the phase composition in $Hf_xZr_{1-x}O_2$ depending on field-cycling via X-ray diffraction *Eunjin Koh*
PO-PHY-30	A unique experimental end-station enabling correlative RIXS and XEOL spectroscopies under electric and magnetic fields *Alessandro Nicolaou*
PO-PHY-31	1s2p rsonant ielastic X-ray sattering natural circular dichroism *Daniel Sier*
PO-PHY-32	Epitaxial growth of ultra-thin film on chiral substrates *Vanshika Singhania*
PO-PHY-33	Synchrotron-assisted HPHT annealing of quantum nanodiamonds: In situ control of phase stability *Boris Yavkin*

Exploring the Interactions of Elastin Peptides with Model Membranes by Molecular Dynamics and Circular Dichorism

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ABSTRACT

In vertebrates, elastin is a crucial extracellular matrix protein. It can be found in the elastic fibers that give many tissues their elasticity and resilience [1]. Elastin deteriorates with time, which can cause pathological disorders as well as function loss [2]. Hydrophobic peptides are produced when elastin takes damaged. The XGXXPG or XGXPGXGXG motif elastinderived peptides (EDPs) have biological activities due to their ability to bind to specific cell surface receptors [1]. By their very nature, it is possible that EDPs can interact directly with cell membranes. To test this possibility, molecular dynamics simulations were carried out. Analyses were carried out on the structure of the simulated peptides during the trajectory, as well as on the percentage of time spent at the membrane, to determine if and how they interact with it. The most promising peptides are analyzed by circular dichroim methods.

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Lung-liver Connective Tissue Interactions in Rats Assessed by the Synchrotron Deep UV Fluorescence Microscopy

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ABSTRACT

Introduction: The lungs and the liver are closely interconnected, influencing each other through physiological and pathophysiological processes. Both organs are rich in connective tissue, that has a major role in various disorders, such as type 1 diabetes mellitus (T1DM) and lung fibrosis (LF). Our aim is to characterize changes in the extracellular matrix and collagen remodeling in the lungs and liver in models of T1DM and LF, and to reveal potential lung-liver interactions. Methods: T1DM was induced by streptozotocin injection, while LF was induced by bleomycin instillation in young male and female Sprague-Dawley rats. Control animals received the solvents via the same routes. After the incubation periods, lung and liver samples were collected and sliced by cryostat. Images (1x1 mm, 40x magnification) were taken in the deep UV range using the DISCO beamline at SOLEIL Synchrotron on excitation wavelengths of 285, 290, 340 nm and emission wavelengths of 352-388, 380-420, 412-438, 510-560 nm. Signal intensities were quantified and compared. Results: Animals with T1DM showed increased signal intensity in the detection channels corresponding to extracellular matrix proteins such as collagen and elastin in the lungs. In contrast, no significant difference was found in the liver in any of used excitation and emission filters. The same was apparent for the LF animals. Significant differences were mostly detected in male rats. Conclusions: Both type 1 diabetes and lung fibrosis accumulate collagen and elastin fibers in the pulmonary tissues without affecting the liver. These findings suggest that lung fibrosis and diabetes exhibit organ-specific fibrotic remodeling, and additionally, male animals are more sensitive to these conditions.

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AI-based Design of RNA Methyltransferase for RNA-based Therapeutics

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ABSTRACT

In the cell, mRNAs are essentially unstable and their phenotypic outcome is modulated by >100 known post-transcriptional modifications, such as RNA methylations[1,2]. The past four years have brought mRNA therapeutics and vaccine potential in the spotlight, calling for controlled synthetic mRNA stability and selective functionalization to promote optimal residency and effectiveness in target cells[3]. Site-specific RNA methylation has the potential to achieve both increased stability and optimal balance between the cell innate immunity response coupled to its ability to express non-self proteins.

Facile synthesis and transfection of mRNAs has opened a wide field of investigation regarding their potential clinical use, and one next challenge is to dissect regio-specific functionalization provided by common mRNA methylations. This will unleash a vast area of applications in the health sciences field.

To do so, we need site-specific RNA methyltransferases (RMTases) able to counteract chemical and nuclease-mediated cleavages but also confer desired properties to future mRNA-based therapeutics or vaccinal RNAs.

Recent breakthroughs in artificial intelligence (AI)-generated enzyme backbones allow designing synthetic RMTase folds with mN6-adenine (m6A), mN1-adenine (m1A), mC5-cytidine (m5C), 2'-Oribose (Nm) specific MTase activities, further screened and selected using high-throughput methods.

The project's goal is to design and implement new strategies for a well-defined and challenging RNA target: the SARS-CoV-2 Spike mRNA, which has been used to immunize millions of people over the past three years. We will identify fragile and/or innate immunity-inducing sequences in the RNA and specifically methylate them using custom RMTases. The resulting novel mRNA with desired properties will be evaluated and refined in relevant cellular and animal models, aiming to develop next-generation vaccines, therapeutic RNAs, and tools for health and biological sciences.

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In Situ Evolution of SrMoO3 Thin Films Probed by NAP-XPS

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ABSTRACT

Perovskite-type oxides have attracted considerable interest due to their exceptional electronic and structural properties. In particular, their high electrical conductivity combined with optical transparency in the visible spectral range makes them promising candidates as transparent conducting oxides (TCOs) for optoelectronic applications.[1,2]

In this context, among many perovskites reported to date, $SrMoO_3$ (SMO) is considered a reference material, as it exhibits one of the highest electrical conductivities, surpassing even some conventional materials such as Au and Pt. DFT calculations seem to evidence that such metallic behaviour is related to the presence of Mo 4d electrons crossing the fermi level[3] in thin film containing Mo^{4+}. However, this high conductivity is accompanied by a strong surface reactivity, raising questions about its chemical stability and subsequent conductivity. Indeed, Mo^{6+} associated to oxidized surface states has no 4d electrons.

In this work, the surface chemical evolution of $SrMoO_3$ thin films deposited by pulsed laser deposition (PLD) on $SrTiO_3$ substrates is investigated under reactive atmosphere using near-ambient pressure X-ray photoelectron spectroscopy (NAP-XPS) with synchrotron radiation. The measurements were performed *in situ* under oxygen and hydrogen up to 3 mbar, combined with controlled temperature variations. Monitoring Mo 3d core level highlighted the oxidation and reduction processes occurring at the material surface ($Mo^{6+} \leftrightarrow Mo^{4+}$). The use of synchrotron radiation at different excitation energies allowed to distinguish the perovskite and the uppermost modified surface. In addition, the comparison of spectra acquired at different positions on the sample allows to disentangle the effect of the beam and the studied reactive atmosphere.

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A New Versatile Operando Photocatalytic Cell for Quick-EXAFS: The Example of CO_2 Photoreduction

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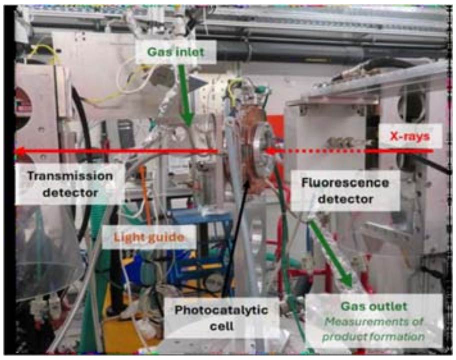
ABSTRACT

Over the past decade, photocatalysis has emerged as promising process for numerous applications including pollutant removal, water splitting or CO_2 conversion, through the harnessing of solar energy. However, achieving sufficient efficiency for industrial applications requires addressing several challenges. Most of these challenges relate to the design of the photocatalyst itself including light penetration and absorption, charges recombination, selectivity of the product formation, nature of active sites and photocatalyst deactivation[1]. Operando quick-EXAFS measurements is a powerful technique to unravel the structure-activity of the photocatalyst and to address these challenges by monitoring the electronic structure and local environment of a photocatalyst under working conditions.

In this work[2], we describe a versatile operando cell suitable for monitoring gas-phase photocatalytic reaction by quick-EXAFS in transmission or fluorescence in the energy range covered by the ROCK beamline[3], along with an in-line analysis of product formation by analytical methods such as mass spectrometry or gas chromatography. This development was carried out in the framework of the French 'PEPR LUMA'[4].



The capabilities of the operando cell will be demonstrated by studying Mo oxysulfides supported on TiO_2 used for the CO_2 photoreduction. After validating the cell by comparing the performances obtained at ROCK with that of a well-tested lab-cell, the behavior of these catalysts will be monitored by XAS at the Mo K-edge, using a Xe lamp (250-650 nm) as UV-visible source. To overcome the volume sensitivity of XAS for studying photocatalytic reactions (occurring at the sample surface where light interacts with the adsorbed species), a modulation-excitation[5] XAS was implemented. This technique has proven relevant and powerful to highlight the contribution of active species compared to silent spectator species during the photocatalytic process.

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SAXS from Rigid Cellulose Chains Solutions in Ionic Liquids: Structure Factor

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ABSTRACT

Ionic liquids (ILs) emerged as a non-polluting solvent that can dissolve cellulose effectively. The solvation mechanism is slightly controversial. In studies of such solutions using SAXS, in spite of low contrast and thin chain conformation giving very low intensity,

- we extracted a **form factor of core-shell semiflexible chain**.
- increasing concentration on a wide range (0.0005 - 0.3 g/g), we unveiled interchain effects:
    - in well dissolved cases, a **structure factor** can be proposed for independent softly aligned cellulose chains
    - at higher concentration, or in presence of a small percentage of water, a stronger scattering is observed suggesting **biphasic structures**, which can be useful to understand the first stages of the “regeneration”
- analysis of bacterial cellulose scattering evidences identical chain whereas aggregates additional low q scattering can be subtracted. This widens the way to neutron scattering experiments using deuteriated bacterial chains.

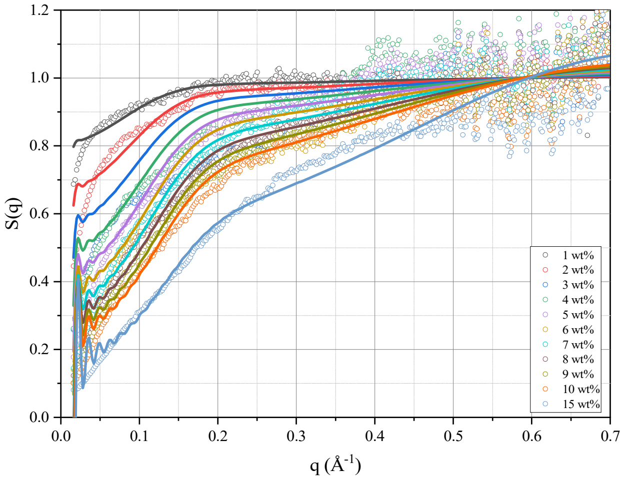

Figure 1 : Structure factor.

Formulation of Lipid Nanocapsules with Microfluidic Chips and Characterisation

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ABSTRACT

Nowadays, nanoscale drug delivery systems (DDS) are used for various medical purposes (e.g. vaccines, cancer treatments, …) and can be simply formulated from synthetic lipids: liposomes, cubosomes, or lipid nanoemulsions[1] so-called LNCs in our case. Lipidbased nanomedicines are obtained from the encapsulation of lipophilic drugs within a nanoparticle structure. Among possible LNCs formulation pathways, such as the phase inversion temperature (PIT) or the phase inversion in concentration (PIC)[2,3] we implemented a microfluidic lab-on-chip[4] process which offers many advantages such as high repeatability, continuous formation and the study of lyotropic phase evolution via in-situ and operando Xray scattering through the flow cell.

By comparing the rest phase diagrams of our formulations (non-ionic surfactant excipients, medium chain triglycerides and ultrapure water) with the flow phases that appears upon dilution in the microfluidic mixing channel, we shade some light on the pharmaceutical process of continuous production.

At SWING beamline (SOLEIL synchrotron), we used 3D stereolitography printed microfluidic chips including passive micromixers[5]; hydrodynamic flow focusing[6] between two solution phases (water and oil with surfactants) to study the operando Small Angle X-ray Scattering process, which allows one to study the nanoemulsification that determines the core-shell nanoparticles structure, composition size, shape and polydispersity. Several other techniques are used in parallel such as including Dynamic Light Scattering (hydrodynamical size of LNCs or micelles) and Asymmetric Flow Field-Flow Fractionation[7] to study the solutions homogeneity and seek of possible residual water soluble surfactants micelles.

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The Self-Assembly of Colloidal Titania Ribbons

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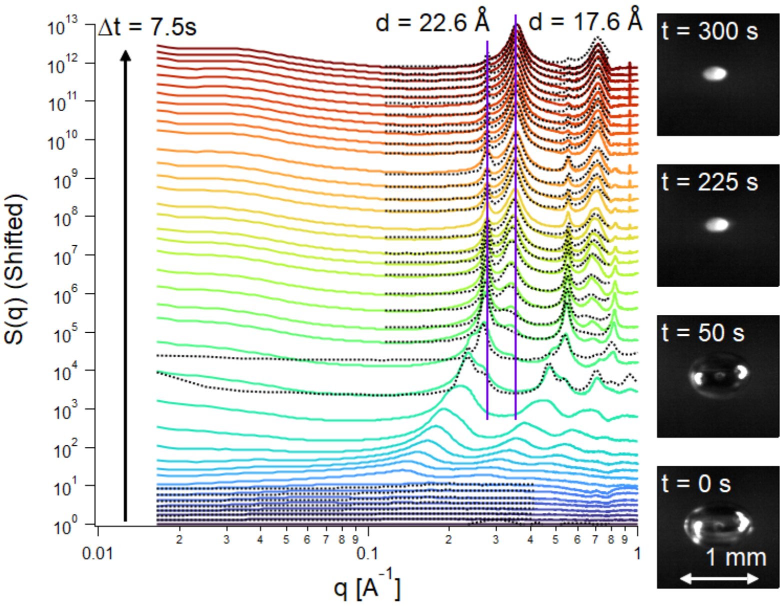
ABSTRACT

Titanium dioxide, TiO_2, is one of the most studied photocatalysts. Among TiO_2 nanostructures, recently-obtained 1D titanate lepidocrocite nanofilaments (NFs) are remarkable due to their very convenient (inexpensive, high-yield and environmentally friendly) synthesis strategy, but also exhibit fascinating structural and functional properties.[1]

We have recently shown that, in colloidal dispersion, the NFs loosely associate into ribbons, one lepidocrocite sheet thick (about 4 Å), 30 to 40 Å wide (5 to 8 NFs) and more than 300 Å long. After drying, their final state is that of extended sheets, stacked three to about twenty high, whose crystallinity increases with stack height.[2]

Our next goal is to follow in detail the evolution of the system as a function of concentration (in the colloidal state), allowing us to explore the phase diagram of this new family of colloidal objects. As the suspension dries, the kinetics of the stacking process becomes available.



First experiments, performed on levitated droplets (see the Figure) allowed us to quantify the interaction between ribbons and the resulting positional order within the dispersion, as well as their evolution during the drying process towards a final 3D crystalline state[3].

We will continue by studying in detail the morphology and internal degree of order within the ribbons and stacks. We will explore the role of the initial concentration, of the synthesis method, and of the nature of the solvent, which has been shown to influence profoundly the texture of the final material.[4]

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Correlating Supramolecular Organization with Chromatic Transitions in Ultra-thin Functionalized Polydiacetylene Films

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ABSTRACT

Polydiacetylenes (PDAs) are promising candidates for smart optical sensors due to their stimuli-responsive blue-to-red colorimetric transitions. However, quantitatively linking these optical properties to specific molecular packing remains a challenge, particularly in ultrathin systems.[1] This study investigates the structure-property relationships of functionalized, fluorescent PDA-based monolayers (approx. 5 nm) assembled at the air–water interface using the Langmuir technique.[2] To elucidate the structural origin of the polymerization efficiency and optical response, we employed synchrotron Grazing Incidence X-ray Diffraction (GIXD) and X-ray Reflectivity (XRR). GIXD analysis allowed for the precise determination of in-plane lattice parameters and coherence lengths, revealing that the supramolecular organization is the governing factor in the topochemical polymerization process. Complementary XRR data provided high-resolution electron density profiles, confirming the film thickness and interfacial roughness. By correlating these structural metrics with UV–Visible absorption spectroscopy and Atomic Force Microscopy (AFM), we demonstrate that specific molecular packing motifs maximize chromatic intensity and stability. These results underscore the necessity of high-brilliance X-ray scattering in rationalizing the design of highly sensitive, ultra-thin PDA sensors.

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LevSAXS: Exploring Phase Transitions under Acoustic Levitation Combined with SAXS

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ABSTRACT

Self-assembly of liquid crystals is of key relevance for the design of materials with enhanced electrical, electrochemical or optical properties [1]. Evaporation induced self-assembly on various solid substrate has already received a lot of attention providing an easy way to produce nano-assemblies [2]. However, the method suffers from the influence of solid-liquid interface which provide a non-uniform dispersion known as the "coffee-ring" effect. In this context, acoustic levitation appears as a genuine way to self-assemble liquid crystals in a substrate-less environment.

Here, we propose to take advantage of acoustic levitation coupled with Small Angle X-ray Scattering (LevSAXS) to follow in situ the self-organization of 1D and 2D swelling clay minerals in a single levitated droplet [3,4]. The advantage is to track fast non-equilibrium phenomena over a wide concentration range, while avoiding anchoring effects during drying. LevSAXS experiments are carried out during the drying of levitated droplets, revealing the nature of the crystal-liquid phases (columnar, nematic) and enable a complete exploration of the phase diagram with a limited sample volume (<10µL), in less than an hour, moving from a dilute to a highly concentrated state. Our results also reveal a gradual shift from osmotic to crystalline swelling, marked by a transition from a pure nematic glass to a coexistence zone where the nematic phase contracts and a saturated crystalline phase emerges (Figure). This transition occurs through a continuous process, forming interstratified structures ultimately progressing to an unsaturated crystalline state.

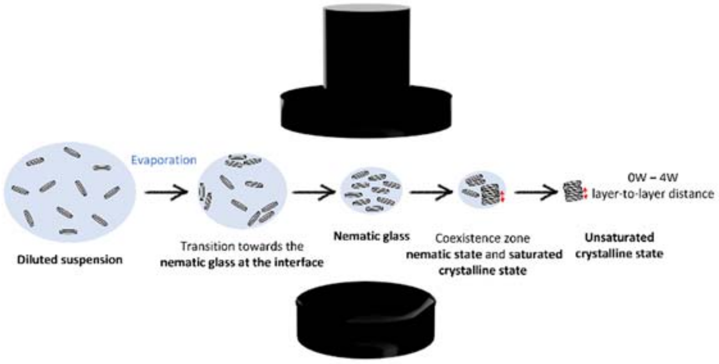

Figure. This scheme summarizes the evolution of the microstructure of smectites from dilute dispersions to the dry state probed by acoustic levitation.

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Formic Acid Production Via CO_2 Electroreduction Using CeO_2–Bi Catalysts Supported on Functionalized Carbon Nanotubes

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ABSTRACT

The declining cost of renewable energy sources such as wind and solar is accelerating the transition away from fossil fuels, enabling more sustainable economic growth. Initiatives like the EU Green Deal demonstrate the feasibility of this transition. Among emerging clean technologies, electrochemical CO_2 reduction (CO_2RR) offers a pathway to reduce emissions while generating valuable chemical products.

This study investigates the development of bismuth-based catalysts supported on functionalized multi-walled carbon nanotubes (MWCNTs)1, designed to facilitate the deposition of cerium oxide (CeO_2)2 from a metal alkoxide precursor. Bismuth was selected for its high selectivity toward formic acid (HCOOH), an important liquid organic hydrogen carrier (LOHC)3. Various Bi loadings were studied to assess the effect of CeO_2 compared with bare metal catalysts in CO_2RR.

Comprehensive characterization confirmed successful catalyst synthesis. Thermogravimetric analysis (TGA) showed that Tour-functionalized MWCNTs contained a controlled number of functional groups essential for CeO_2 deposition, with CeO_2 content aligning with theoretical predictions. Raman spectroscopy supported these findings, while X-ray diffraction (XRD) confirmed the presence of MWCNTs, CeO_2, and $Bi_2O_2CO_3$. BET analysis revealed a mesoporous structure with a high surface area.

Electrochemical testing in a three-electrode H-cell demonstrated that catalysts with 10% Bi achieved the best performance at –1.1 V vs RHE, reaching Faradaic efficiencies of 90% for HCOOH formation. A total of 60 mmol of product was obtained using only 0.25 mg of catalyst over a 0.5 cm2 electrode area in 2 hours, highlighting remarkable activity.

Finally, X-ray Absorption Fine Structure (XAFS) measurements conducted at the SOLEIL Synchrotron, including both ex situ and in situ analyses, confirmed substantial reduction of Ce and Bi under reaction conditions. Underlying the importance of the Bi^{3+}/Bi ratio for optimal HCOOH production. These results suggest a possible synergistic interaction between the two elements, enhancing CO_2 reduction performance.

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Evaluating Surface Properties on High-density Positive Electrodes for Li-batteries

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ABSTRACT

In a lithium-ion battery, the development of an improved positive electrode is crucial for achieving high energy density and superior electrochemical properties, which are prerequisites for high-voltage applications such as electric vehicles (EVs). Nickel-rich layered transition-metal oxides gained particular attention owing to their high operating voltage of 4.3 V and specific capacity of 220 mAh/g. However, the rapid capacity fade of NMC811 in the process of charge/discharge and inferior thermal stability have limited its extensive applications. To alleviate the capacity fade in high nickel cathodes, several surface modifications such as $LiNbO_3$, Li_3PO_4, Al_2O_3, etc., were reported elsewhere. These surface coatings were reported to be protecting the NMC cathode surface from HF reactivity, structural degradation, transition metal dissolution, etc., and stabilizing the interfacial reactions for long-term cyclability.

Herein, in this work, we will be preparing surface-modified high Ni-containing cathodes (NMC622, NMC811, and NMC85) with different coating percentages by sol-gel and electrospinning techniques and compare their electrochemical performance with pristine cathode materials. We will be exploring the effects of surface modification on the crystal structure with XRD, STM and XPS. HRTEM and SAED will be used to examine the coating uniformity and surface crystallinity. Operando X-ray analysis will be carried out at the ROCK beamline at Soleil to study the change in oxidation states of cathode elements and the surface-coated materials. These advanced characterizations will help us to deepen the knowledge on the advantageous effect of surface modification on the high-performance cathode materials and will be beneficial for their future developments.

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Formation of a Dense Liquid Precursor in Mineral Crystallization: Spinodal Decomposition Evidenced by Sub-millisecond Microfluidics Coupled to Time-resolved in situ SAXS

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ABSTRACT

Crystallization from solution often proceeds via a multi-step route, where dense liquid or amorphous precursors form before the crystalline phase emerges [1]. The nature and behavior of these precursors can play a crucial role in crystallization, ultimately shaping the formation and properties of the resulting nanocrystals [2]. Yet, they are not accounted for in the “classical” single-step theory (CNT), which remains the main framework for modelling and designing nanomaterials, underscoring the need for new theoretical tools.

Reactant-rich liquid droplets are the most challenging to investigate due to their labile and transient nature, complicating their characterization and the experimental differentiation between competing crystallization theories [3]. These droplets can arise from nucleation, spinodal decomposition or even kinetic-driven processes, making it crucial to identify their formation mechanism to select an appropriate theoretical model. However, experimental evidence is difficult to gather, especially in mineral systems [4], as distinguishing between these scenarios requires time-resolved and structural characterization at very small spatial (nanometer) and time (sub-milliseconds) scales.

Here, we show how we captured and tracked the formation of the reactant-rich liquid precursor of cerium oxalate, a well-known surrogate of actinide oxalates in the nuclear industry. By combining in situ X-ray scattering with ultrafast microfluidic mixers, we were able to probe this transient at the nanoscale, from 0.6 ms to 40 ms after mixing. With this setup we demonstrated that this liquid precursor is formed via an asymmetric spinodal decomposition, far from the classical framework, involving strong viscosity [5] and volume fraction contrasts between the newly formed phases.

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Fate of Self-assembled Squalene Nanoparticles in a Biomimetic Medium Assessed by Scattering Techniques

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ABSTRACT

Over the last 20 years, pharmaceutical industries gained interest towards therapeutic nanoparticles (NPs) so-called nanomedicines. The NP formulations demonstrated enhanced properties compared to the drug alone such as improved targeting, reduced toxicity, and enhanced pharmacokinetics. However, there is still a lack of data and understanding of the physicochemical properties of such compounds in particular after their injection in biological media leading to numerous failures in clinical trials[1].

In this context, we proposed to study a particular case of “soft” NPs composed of a pro-drug which consists of a squalene (SQ) linked through an amide bond to Leucine-enkephaline (LENK). Feng et al. demonstrated that LENK-SQ NPs produced an analgesic effect comparable in duration to that of morphine, unlike LENK alone[2-4]. Moreover, contrary to the opioids currently used as painkillers, LENK allows to get rid of the development of an addiction over time by acting on peripherally localized receptors rather than central nervous system opioid receptors.

In this study, we characterized the assembly state of LENK-SQ bioconjugates in a biomimetic environment using physicochemical techniques focusing on small/wide angle X-ray scattering (SAXS/WAXS on SWING at SOLEIL) and small angle neutron scattering (SANS on D22 and SAM at ILL). Taking benefit of the BioSAXS sample changer, we were able to evidence and characterize the micellization of the bioconjugate in conditions that mimic physiological conditions of blood in terms of pH and ionic strength. The influence of different buffers was assessed across a range of concentrations, resulting in various pH and ionic strength conditions in the final suspension. These results were put into perspective with SANS analyses.

The study revealed an equilibrium between LENK-SQ bioconjugates, LENK-SQ NPs and micelles, which depended on buffer concentration[5]. Consequently, the relative proportion of each species appears to be primarily governed by the pH, highlighting its critical role in the relationship between drug efficacy and morphology of self-assembled bioconjugates. These findings provide key insights into how the physicochemical environment can influence NP formation and, ultimately, therapeutic performance.

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Radiation Damage with Soft X-rays in Organic and Hybrid Semiconducting Materials

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ABSTRACT

Radiation damage during soft X-ray characterization poses a challenge in the study of organic and hybrid electronic materials, especially in energy devices. Understanding dose limits and the nature of chemical degradation is essential for reliable interpretation. We focus on materials like PMMA (control), fullerene derivatives (PCBM, $PC_{71}BM$), and donor polymers (e.g., PTB7-Th, PDTS), which are commonly studied in the X-ray energy range of 280–320 eV [1, 2]. X-ray induced radiation damage in these key organic and hybrid photovoltaic materials is systematically investigated in this study. Using varied exposure times and exposure energies, we quantify spectral changes and damage thresholds in these materials. X-ray induced damage in hybrid metal halide perovskite solar cell materials is also presented.

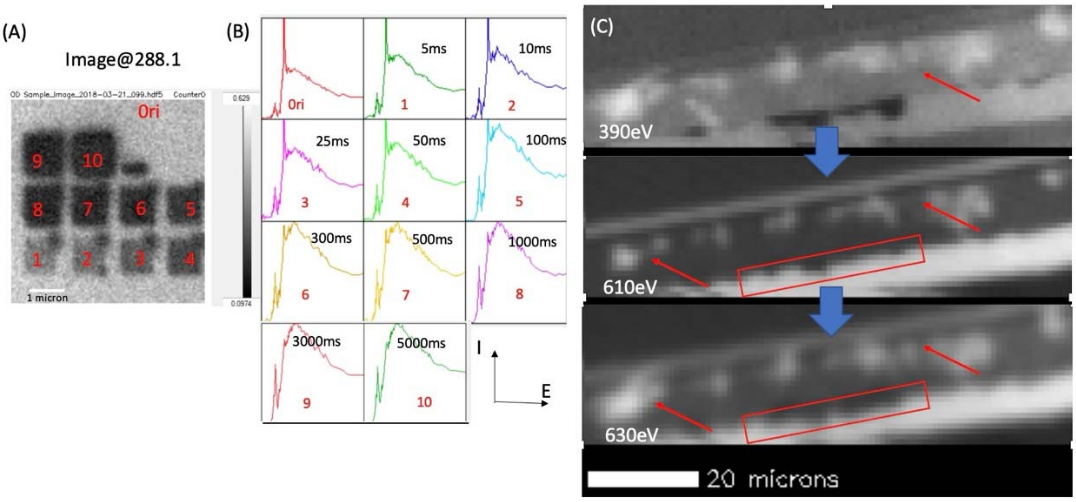

Figure 1. (A) STXM images at 288.1eV of PMMA thin film showing regions damaged at different exposure times. (B) C K-edge spectral changes corresponding to the different regions in (A). (C) STXM images of MAPI ($CH_3NH_3PbI_2$) perovskite layer showing evolution/damage of certain regions (red arrows and rectangles)

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Quantum Crystallographic Studies of Phase Transition in Minerals under Pressure

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ABSTRACT

Quantum Crystallography (QCr) uses various types of aspherical atomic electron densities (consequently aspheric atomic scattering factors) in the refinement of the structures of crystals and their electron densities against X-ray diffraction data. The main methods of QCr are: the refinement of multipole model of quantitative electron density distributions, the refinement of experimental wave functions and the refinement of the crystal structures using the Hirshfeld atom method (HAR). All these QCr methods provide better refinement results than the commonly used routine methods based on spherical atomic electron densities (IAM).
In this presentation, we will present the main ideas of quantum crystallographic methods along with their applications to the study of phase transitions in the structures of Calcite and Natrochalcite.

An important biomineral, Calcite (CaCO3)[1] is one of the primary carriers of carbon in geochemical reservoirs. Carbonate rocks serve as hosts to various natural resources, including ores, oil, and gas, and are transported deep into the deep mantle at subduction zones. We traced a reversible phase transformation of Calcite to Calcite-II, from R-3c to P21/c symmetry at pressure ranging from 0.85 GPa to 2.07 GPa. The reversible phase transition takes place at 1.5GPa. It involves twinning of crystals into two domains. The decrease of pressure removed twinning in all crystals which regained the quality suitable for multipole modelling. Will present detailed changes of electron density at atoms under pressure.

Natrochalcite is rare mineral possesing H3O2- (Fig. 1) [2] units and forming one of the shortest hydrogen bond (HB) reported so far in inorganic compounds. High pressure conditions can lead to the formation of an extremely short single-well HB in natrochalcite and to the phase transition connected with symmetry lowering above 2 GPa. It crystallizes in the monoclinic space group C2/m and it has usually emerald green colour. Natrochalcite gained ground in recent years as an anode material for lithium – ion batteries used in powering consumer electronics and vehicles. In this contribution, we will present details of changes of H-bonding in this mineral as a function of pressure as well as analyse variation of electronic parameters.

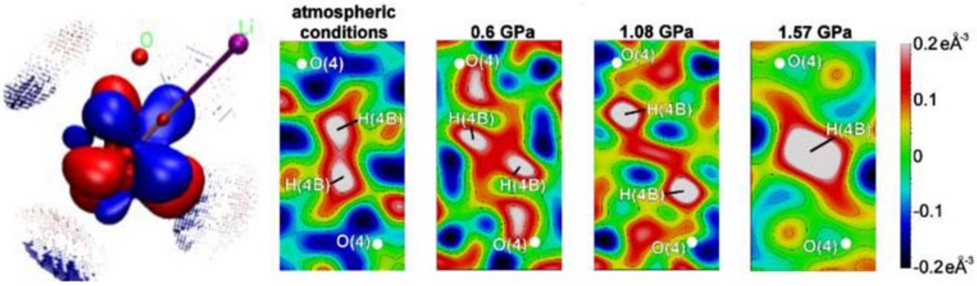

Fig. 1. (From the left) Relocation of electron density at F1 ion in hsiangualite, evolution of H-bonding in natrochalcite.

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Structure of Assemblies of Nanospheres Confined in Smectic Liquid Crystal Defects

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ABSTRACT

Smectic liquid crystal 8CB, assembled on a rubbed polyvinyl alcohol (PVA) substrate, forms smectic layers curved into hemicylinders. Within these periodic flattened hemicylinders, ribbonlike grain-boundary topological defects are created. These defects can confine nanoparticles (NPs), such as gold or semiconductor nanospheres. At sufficiently high NP concentrations, the confined particles self-assemble into ribbon-like monolayers with hexagonal ordering 1 . GISAXS measurements reveal two symmetric intensity maxima on the upper part of the scattering ring, demonstrating that the central smectic layers of the hemicylinders are not strictly flat. Instead, two symmetric regions of straight but tilted smectic layers form, producing a central chevron of width W that joins the straight and tilted layers with a characteristic dihedral angle 2 . This inclination is transmitted to the NP assembly, leading to a corresponding tilt of the NP monolayer. Recent experiments on the SIXS beamline show that when NPs exceed a threshold diameter of approximately 4 nm, they form ordered hexagonal monolayers aligned with the hemicylinder axis. In contrast, smaller NPs form an average disordered hexagonal lattice. This size-dependent behaviour arises because larger NPs protrude partially from the defect core, inducing elastic distortions in the surrounding liquid crystal that impose orientational constraints. Smaller NPs remain fully trapped within the defect core and do not perturb the neighbouring liquid crystal, allowing the hexagonal lattice to rotate freely and lose long-range orientation. Within liquid-crystal defects, the interparticle spacing is reduced relative to pure NP monolayers and decreases further with increasing NP concentration, indicating compression of the smectic environment. We will continue to use GISAXS and TSAXS to quantify NP arrangements and interparticle distances. Future work will focus on synthesising a broader range of chemical ligands and exploring the assembly behaviour of diverse nanoparticles within liquid-crystal topological defects.

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Contribution of Infrared Spectrometry to the Understanding of Calcareous Biominerals

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ABSTRACT

Calcareous mollusk shells are complex biocomposites of minerals and organic matter (up to 5%). Their principal component is typically present as the mineral polymorphs calcite and aragonite (1). However, as biocomposites, their structures are governed by this organic matter, present at the micro- and nanoscale (2). It is observed as an envelope surrounding the structural units (e.g., prisms or tablets) and is also integrated within the units themselves. Given that the organic matter composition and distribution are species-dependent, determining its precise spatial distribution is a key factor for an accurate understanding of biomineralization processes.

Previous studies have shown that when the shells consist of only one polymorph (either calcite or aragonite), the microstructural change between them is progressive. Conversely, when calcite and aragonite co-exist, they are separated by an organic layer. The chemical composition differs at the end of the prismatic calcitic layer, and the first stages of the aragonite layer do not exhibit the nacre structure (3- 5) .

Several Infrared (IR) techniques are now available for mapping the distribution of organic molecules and phases at a micro and nanoscale. This allows a direct correlation of the structural organization and the composition of the components. So, this study employed a sequence of techniques: classical FTIR observations were succeeded by super-resolved Optical-Photothermal Infrared Spectroscopy (OPTIR). The analysis culminated in the use of scattering-Scanning Near-Field Optical Microspectroscopy (s-SNOM) to achieve nanoscale examination, focusing on the interface between the outer and inner shell layers. The shells of *Pinctada*, owing to their simple and large structures, serve as optimal specimens (6-7).

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Characterization & First Performance Evaluation of LEAPS-INNOV HPGe Detector for Spectroscopy Applications

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ABSTRACT

We present the first operational prototype of a high-purity Germanium (HPGe) detector developed within the framework of the European LEAPS-INNOV project. This prototype features a monolithic, multi-element sensor optimized for high-resolution X-ray spectroscopy in the hard X-ray regime. The study includes a comprehensive laboratory-based characterization of the detector's spectral and spatial performance, and an on-beam evaluation at the BM05 beamline of the ESRF synchrotron facility using monochromatic X-rays in the 20–50 keV energy range. Detailed characterization results are reported, including sensor performance metrics such as energy resolution, count rate, and spatial response uniformity.

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Irradiation Passport for Art (IPA)

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ABSTRACT

Objects of art are increasingly exposed to ionizing radiation as analytical techniques using intense photon, electron and ion beams produced by particle accelerators, synchrotrons, microscopes and other sources, are increasingly being applied for their study. Modern analytical techniques use the interactions of photons, electrons and ions with materials to identify the materials in the object. But interaction means that there is a chance of visible or invisible alterations, either permanent or temporary. The consequences of radiation in terms of long-term effects are not fully known. Several recent studies have shown that interactions between pigments and binding media are likely to significantly influence material response under irradiation (1 and 2). As is well known, exposure to radiation is of a cumulative nature. This fact is important for everyone involved in cultural heritage research and treatment, as this means that previous exposure of objects or environments may change the sensitivity of objects or research samples in future examinations, or may even alter the material characteristics if certain thresholds are surpassed. Therefore, it is important for the cultural heritage field to record and document the exposure of art objects as well as research samples to irradiation. This idea is the starting point of the project, the Irradiation Passport for Art (IPA), a database in which can be recorded the location, total exposure and circumstances of use of radiation. There is also space to monitor the irradiate spot afterwards. With such a passport, the field can work towards safer and more controlled use of radiation for the examination and treatment of cultural heritage. The passport can be used for research into the long-term effects of irradiation of objects of art. The information on earlier exposures is crucial for the selection of future areas of investigation and prevents double exposure. Finally, when a restoration treatment is planned it is of importance to know if and where an object was irradiated. The IPA project is led by conservation scientists, a physical chemist and a conservator and has the support of an international team with different irradiation expertise, in which important synchrotron-institutes and research institutes involved in research in cultural heritage are represented. The IPA database has been developed as a password-protected website that institutes can register for, which holds information on the exposure, all the relevant parameters that were used during the measurement and information on changes if they occurred. We hope that putting the information in the website will become part of the regular documentation process. The website is meant to be used by conservation scientists and conservators. It will not hold the actual data, this stays with the partner institutes that have uploaded the parameters. Partners can contact each other if they wish to have detailed information and would like to request examination results to be shared.

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Redox Speciation of Cerium in the Presence of Natural Organic Matter

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ABSTRACT

Understanding the interactions between trace metals and natural organic matter (NOM) is crucial due to its significant influence on metal speciation, mobility, toxicity, and bioavailability. Cerium (Ce), a lanthanide element, is of particular interest because of its abundance and unique redox properties, since it exists in both Ce(III) and Ce(IV) oxidation states. This redox flexibility makes Ce a powerful proxy for paleo-environmental reconstructions.1 However, distinguishing between Ce(III) and Ce(IV) in complex natural matrices like organic matter remains challenging, especially at environmentally relevant concentrations. X-ray absorption spectroscopy (XAS) at the Ce $M_{4,5}$-edges may offer a robust analytical approach to directly resolve Ce oxidation states under these conditions.

XAS measurements were performed at the DEIMOS beamline, which offers a perfect sample environment for redox sensitive elements, with its Ar-glovebox connected to the end station. Ce redox speciation was investigated across a 5-10 pH range in the presence of NOM under both aerobic and anaerobic conditions. To highlight the role of NOM, parallel experiments were performed without NOM under aerobic conditions. Linear combination fitting with Ce(III) and Ce(IV) references was applied to determine Ce redox speciation.

The results showed a strong pH dependent Ce oxidation in the presence of organic matter under aerobic conditions, with negligible Ce(IV) at pH 5 and nearly complete oxidation (~94%) at pH 10. Dissolved oxygen (O_2) was identified as the primary oxidant, as anaerobic conditions lead to negligible Ce oxidation. At pH 6, in the absence of NOM, ~50% Ce(IV) formed, whereas the Ce-NOM system showed only ~25% Ce(IV). This finding is consistent with preferential complexation of Ce(III) by organic matter, which stabilizes the reduced state and limits the oxidation. At higher pH (8–10), more than 80% Ce(IV) formed, where oxidation is driven by hydrolysis and precipitation as CeO_2 nanoparticles, independent of organic matter.

Overall, this study clarifies the mechanisms controlling Ce redox behavior in the presence of organic matter across different pH conditions. These findings can be directly used in developing risk assessment and management strategies for Ce in aquatic environments. Longer term, they can also be incorporated into predictive models of Ce redox speciation, improving our ability to evaluate and manage Ce contamination in natural systems.

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Lacquer Coatings on Carriages: The Possibilities of Synchrotron-based µFTIR Spectroscopy for the Study of Multilayered Historical Samples

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ABSTRACT

Before being progressively replaced by cars at the beginning of the 20th century, horse-drawn vehicles such as carriages and sledges played a central role in society. Thus, several aspects of their manufacturing, including the materials and techniques involved, reflect the scientific, technological and societal development of their time.

As such vehicles were meant to be used outdoors, they were systematically exposed to extremely harsh environmental conditions, which included extensive exposure to rain, high humidity and direct light. Hence, the sensitive wooden parts constituting these objects required to be constantly protected against the effects of the environment, which was achieved by applying several layers of impermeable coatings, also known as lacquers. However, the composition and chemical properties of such lacquers for outdoor applications remain largely unknown today. This knowledge gap hinders appropriate restoration and conservation of the coatings, resulting in severe degradation issues that negatively impact the overall appearance and integrity of the historical vehicles.

This preliminary study focuses on five green carriages from the hippomobile heritage collection of the Royal Museum of Art and History located in Brussels. The aim of this investigation is to identify the main ingredients involved in the confection of these coatings and to look for recurring materials/trends within this list of ingredients.

However, one challenge encountered when working with such lacquers is the superposition of numerous extremely thin layers (<10 µm), not easily distinguished by conventional laboratory-based instruments. Thus, after the preliminary identification of key ingredients present in the lacquers thanks to benchtop FTIR and SEM-EDX analyses, synchrotron-based µFTIR measurements were performed in order to get a better understanding of the repartition of the identified components within the stratigraphy of our samples. These first results allowed us to shed light on the structure and composition of the complex multilayered coatings of five case studies, allowing the identification of possible trends regarding the pigments and layering techniques used for the manufacture of green lacquers on carriages.

Following the conclusive results of this preliminary study, the next step of this research will be to expand the corpus to a more significant number of horse-drawn vehicles in order to confirm the possible trends, along with considerations to the time period, geographical area and type of vehicle involved.

Fragmentation of Plastics Induces Cr(VI) Release : Implications upon Environmental Degradation

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ABSTRACT

Metallic additives are widely used in the formulation of plastics to give them different properties. Although the use of hazardous substabces is now largely restricted in the EU, numerous metal(oid)s, such as lead, arsenic or chromium(VI), were incorporated into the composition of plastic formulation[1,2] before these restrictions entered into effect. However, such legacy plastics which contain metal(oid)s are still present in landfills or dispersed in natural environments. Under environmental weathering, plastics can be altered leading to fragmentation into micro- and nanoplastics (i.e., < 5 mm and < 1 µm, respectively)[3]. However, the fate of such metal(loid)s additives during environmental degradation of plastics remains poorly understood.

To assess the behavior of such additives during plastics degradation, environmental macroplastics were collected from the banks of the the Yvette river in Gif-sur-Yvette (France) and altered through UV-C irradiation followed by mechanical fragmentation. The distribution of elements in the different size fractions obtained (i.e. macro-, micro- and nanoplastics) was characterized by micro- and nano-XRF mapping at the LUCIA and Nanoscopium beamlines. Chromium (Cr) speciation was determined collecting XANES and EXAFS spectra at the LUCIA beamline[4]. These analyses permitted to quantify the distribution of Cr and determine its speciation in plastics through the degradation process. Macroplastic revealed significant concentrations of Cr, in which Cr(VI) dominates in the form of micrometric aggregates of crocoite ($PbCrO_4$) homogeneously distributed within the polymer matrix. These distribution and speciation are not altered by fragmentation into microplastics. By contrast, a dramatic decrease in total chromium content is observed in nanoplastics, which is associated with the shift of the main chromium species from Cr(VI) to Cr(III) bound to the polymer matrix.

The drastic decrease in Cr content associated with its speciation change from Cr(VI) to Cr(III), as the main species in the final stage of plastics, highlights the release of Cr(VI) during fragmentation. This study demonstrates that the fragmentation of macroplastics and microplastics into nanoplastics that can occur in the environment leads to their leaching and to the release of potentially toxic microparticulate Cr(VI) when contained from the formulation.

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Localisation Spatiale 2D et 3D de Microsphères de Polyéthylène chez la Moule par Techniques Synchrotron

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ABSTRACT

Le polyéthylène (PE) est l'un des contaminants microplastiques les plus abondants trouvés dans les espèces marines. Des composés métalliques sont souvent associés aux plastiques pour leur conférer des propriétés comme la couleur pour le dioxyde de titane (TiO_2) ou peuvent s'adsorber au cours du cycle de vie des plastiques, en milieu aquatique notamment. Nous avons tiré profit de la présence de titane (Ti) associé à du PE pour localiser des microsphères de PE dans des moules exposées à ces microsphères. La distribution du Ti mais également les distributions des éléments constitutifs du tissu animal (P, S, Cl, Ca, K) sont obtenues sur des cryo-coupes de moules entières avec une résolution spatiale de 3 µm, par cartographie de fluorescence X (figure 1a) sur la ligne de lumière LUCIA au Synchrotron SOLEIL. La méthode est suffisamment sensible pour détecter avec un fort contraste toutes microsphères ou fragments et pour discriminer du Ti dans les microsphères de PE de particules de Ti venant d'autres contaminations.

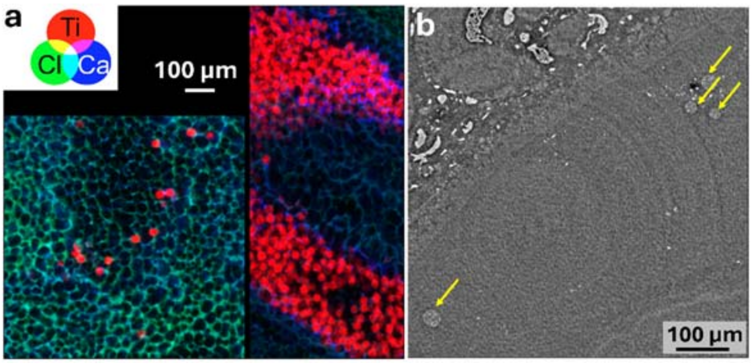

Figure 1a. Cartographie de fluorescence X sur une coupe cryogénique de moule, montrant les microsphères en rouge (Ti), le Cl en vert et le Ca en bleu. **b**. Slide virtuelle obtenue par tomographie X ; les flèches indiquent les microsphères.

La distribution spatiale 3D des microsphères de PE sur la moule entière, sans aucune coupe physique de l'échantillon, a été obtenue par tomographie par rayons X sur la ligne ANATOMIX avec une résolution spatiale de 1.5 µm. Les microsphères sont observées dans différentes zones du tractus digestif (figure 1b). En segmentant les microsphères sur l'ensemble du volume de la moule, il sera ensuite possible d'obtenir un bilan de matière sur la répartition et la quantité de microsphères de PE dans les différents compartiments digestifs de la moule.

Structures of Ices by Quantum Crystallography and PDF

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ABSTRACT

Ice is the solid form of water (H_2O), a substance fundamental to life on Earth. The most familiar form of ice is the hexagonally structured ice Ih, which forms in our everyday environment in the form of snowflakes and ice cubes. However, water can crystallize into at least 21 distinct phases, unique in structure, depending on the temperature/pressure and route of formation. The different phases are denoted by Roman numerals (e.g., Ice Ih, II, III etc.), and have found relevance across a diverse range of different research areas, from geology and planetary science to fundamental physics.

At pressures exceeding 2–3 GPa, water molecules arrange themselves into cubic ice VII (Fig. 1a, space group Pn-3m)[1,2]. This is one of the densest ice structures (ca. 1.50g/cm3) with ices X and XI (2.51g/cm3 and >2.51g/cm3, respectively). Ice VII plays a role in the water-rich interiors of Jupiter's moon Europa and Saturn's moon Enceladus and other planetary bodies. This high-pressure polymorph of ice, is known for its disordered hydrogen positions, yet the nature of this disorder has remained unresolved.

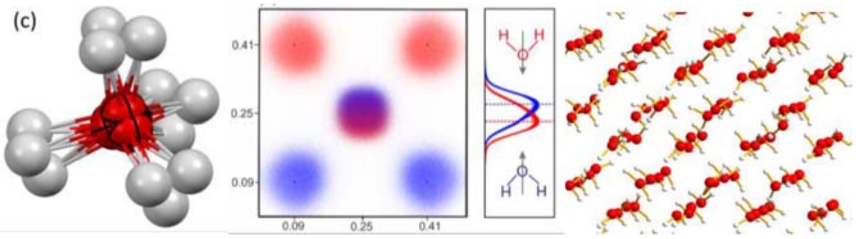

***Figure 1** (from the left); Disordered model of ice VII refined by HAR (the average structure), distribution of oxygen atoms in ice VII from PDF and RMC refinement and unique positions of water molecules in ice VII (local structure).*

In this contribution will present details of structures of ices (VI[3], VII[1,2], Ih [4]) obtained with quantum-crystallographic Hirshfeld Atom Refinement against single crystal X-ray and electron diffraction data. We will also present the first quantitative characterisation of disorder in D2O ice VII and VI obtained through a combination of Pair Distribution Function (PDF) analysis, Reverse Monte Carlo (RMC) modelling, and high-pressure neutron scattering. Our results provide a detailed decomposition of both the average and local atomic structures of Ice VII, revealing a previously unquantified level of structural disorder. These findings are corroborated by density functional theory (DFT) calculations, offering a comprehensive understanding of the structural behaviour of Ice VII under extreme conditions.

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Structural Phase Transition in Epitaxial Lead-free $Bi_{0.5}Na_{0.5}TiO_3$-$BaTiO_3$ Ferroelectric Relaxor Thin Films

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ABSTRACT

Perovskite ferroelectric materials have diverse functionalities and are widely used in various kinds of modern electronic devices, such as sensors and actuators, but have also great significance for high-power dielectric energy storage. Environmental concerns and RoHS directives have given rise to extensive research in the past two decades into lead-free ferroelectric materials, among them the lead-free relaxor $(Bi,Na)TiO_3$ [1]. The (x) $Bi_{0.5}Na_{0.5}TiO_3$ – (1-x) $BaTiO_3$ (BNT-BT) solid solution has been thoroughly investigated because of its significant potential as piezoelectric material [2] and as a ferroelectric material for energy storage [3,4]. This system exhibits a morphotropic phase boundary (MPB) around x = 0.06, which separates a ferroelectric tetragonal phase (P4mm) from a ferroelectric rhombohedral phase (R3c) associated to a large mechanical response [5]. In the vicinity of the MPB, the R3c ferroelectric phase coexists with the P4bm phase which is characterized as a weakly polar ferrielectric phase resulting from an uncompensated antiferroelectric order [6]. This P4bm phase acts as a depolarization field and restrains the domain boundary, giving rise to a complex polar nanodomain structure. The coexisting R3c/P4bm symmetries induce a disorder which influences the structural as well as the electrical properties.

Recently, temperature-dependent studies of dielectric and ferroelectric properties of (001) and (111) BNT-BT epitaxial thin films with a composition in the vicinity of the MPB evidenced the coexistence of both R3c and P4bm phases, in relation with an electric field induced phase switching [7]. Dielectric studies revealed anomalies that are closely linked to structural phase transformations in BNT-BT which were studied in bulk but, to our knowledge, never in thin films so far.

Here, we present temperature-dependent structural studies of 200-nm thin BNT-BT (001) thin films deposited by pulsed laser deposition on $LaAlO_3$ (LAO) (a_0 = 3.787 Å) substrates using synchrotron X-ray diffraction. The BNT-BT thin films were integrated between a $La_{0.5}Sr_{0.5}CoO_3$ (LSCO) bottom electrode and circular Pt top electrodes of 250 µm diameter sputter deposited through a shadow mask for electrical characterisations at the home laboratory. The samples were heated up to 700 °C using an Anton Paar furnace and X-ray diffraction patterns of the BNT-BT **002, 003, 103, 104,** and **204** Bragg reflections were *in-situ* recorded using a 2D XPAD hybrid pixel detector at the DiffAbs beamline. While the diffraction intensity of the **002**, **103**, and **204** BNT-BT reflections seem not to be strongly affected, the **003** and **104** BNT-BT Bragg peaks become less intense with increasing temperature. All 5 Bragg reflections exist for the P4bm, P4mm, and R3c crystal structure. However, in the case of the Pnma phase, which has been identified only by transmission electron microscopy in pure BNT, the **003** and **104** reflections are absent. The variation in intensity thus might indicate a phase transition.

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Micro-fabrication using Synchrotron Radiation

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ABSTRACT

LIGA, the German acronym for Lithography, Electroplating, and Moulding, enables the fabrication of structures with sub-micrometer lateral resolution, high aspect ratios (heights of several hundred micrometers), and complex shapes in a wide range of materials (polymers, metals and ceramics). This technology relies on synchrotron radiation to provide the X-ray flux, extreme precision, and depth of field that are required for such fabrication.

Since 2009, a dedicated deep X-ray photolithography (LIGA) station has been available on the Metrology beamline at SOLEIL. This station is open to both academic and industrial research projects and can operate with either polychromatic (white) or monochromatic beams. Its versatility makes it suitable for standard microfabrication while also supporting higher-resolution and more demanding structures.

Interest in specific and highly accurate X-ray optical components is steadily increasing at synchrotron facilities, driven by the growing demands of advanced X-ray beam shaping, characterization, and imaging techniques. Examples include knife-edge structures for beam characterization, pinholes with diameters from submicron to a few microns serving as defining apertures for X-ray Coherent Diffraction Imaging or X-ray Ptychography experiments, Hartmann grids or amplitude/phase gratings for accurate wavefront measurement and phase imaging. Such structures require micrometer to submicrometer resolution, thicknesses of up to tens of microns, and millimeter-scale fields of view – specifications that can only be achieved by LIGA technology.

One active research area concerns MetaMaterials (MM), whose unique structural design possibilities make them suitable for constructing optical devices (such as lenses, switches, and modulators) operating in the THz regime with unusual properties, as negative refraction and sub-wavelength focusing. LIGA technology, ultrasonic manufacturing, and ICP-DRIE machining for micrometric structural dimensions within tens of micrometers depth were used to demonstrate resonances in the THz regime using dielectric materials thanks to their low losses and isotropic properties [1], and for focusing THz emission from a spintronic emitter device (STE) [2].

Some recent developments will also be presented, including the fabrication of higher-resolution LIGA masks, and the upgrades to the LIGA station carried out since 2018 to improve experimental conditions (double-cooled 200 µm-thick IF1 beryllium windows, efficient sample thermalization, and autonomous control of the station via the Tango software environment).

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Structural Investigations of HfO_2-based Transistor Stacks During Annealing and Electric Field Cycling by In-situ XRD

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ABSTRACT

Ferroelectric (FE) hafnium-oxide (HfO_2) materials are emerging as highly promising candidates for next-generation memory and logic technologies, including ferroelectric random-access memory (FeRAM), ferroelectric field-effect transistors (FeFETs), negative-capacitance FETs, and neuromorphic computing devices. Fully leveraging these technologies requires a clear understanding of HfO_2 thermodynamics across multiple length scales and in contact with various metal electrodes. Originally introduced as a high-κ dielectric for DRAM and later adopted in the 45-nm CMOS node in 2007, HfO_2 now serves widely as a transistor gate oxide. Ferroelectricity was first discovered in Si-doped HfO_2 (HSO) [1] and subsequently in $Hf_{0.5}Zr_{0.5}O_2$ [2], sparking major interest due to the material's Complementary Metal Oxide Semiconductor (CMOS) compatibility and strong FE behavior even at ~ 10-nm thicknesses. Although chemical doping can stabilize the FE phase, optimal performance still requires a capping electrode, crystallization annealing, and wake-up cycling, adding process complexity.

At the DiffAbs beamline, we examined crystallization and phase evolution in industrial Front-End-of-Line (FEoL) HSO-based Metal-Ferroelectric-Insulator-Semiconductor (MFIS) transistor stacks (grown at the 300 mm clean room facility of STMicroelectronics, Crolles, France) during thermal annealing and electrical cycling using *in situ* XRD. Annealing experiments were conducted from 450 to 1000 °C under slow-ramp, flash-anneal (300 °C/min), and fast-ramp with dwell time at the targeted temperature. Tracking the 111, 002, and 022 Bragg peaks enabled quantification of monoclinic, tetragonal, and orthorhombic phase fractions. A key result is that crystallization begins at ~ 450 °C when the stack is held at this temperature for several minutes before cooling down, demonstrating Back-End-of-Line (BEoL) compatibility (< 500 °C). Electric cycling studies on patterned devices (with 1 or 2 nm SiO_xN_y as the insulating layer, and annealed at 750 or 1000 °C) revealed that samples annealed at 750 °C show a progressive shift of the o(111)/t(101) peak toward lower 2θ values, indicating a tetragonal-to-orthorhombic phase transformation with cycling up to 10^5 cycles. In contrast, stacks annealed at 1000 °C displayed no structural evolution.

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Study of the Phase Composition in $Hf_xZr_{1-x}O_2$ Depending on Field-cycling via X-ray Diffraction

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ABSTRACT

Ferroelectric hafnium oxide (HfO_2) has been widely investigated thanks to its compatibility with CMOS. The HfO_2 thin film is deposited as amorphous and crystallizes to polycrystalline upon annealing, possessing several phases, including ferroelectric (o-phase, Pca21) and non-ferroelectric phases. Therefore, the ferroelectricity of HfO_2 can be improved by stabilizing the orthorhombic phase, which can be adjusted by five root causes: doping, oxygen vacancies, surface/interface/grain boundary energy, electrical field, and stress [1]. Among them, the electric field is an indirect factor of phase change, exhibiting both an increase and a decrease in ferroelectricity during electrical field cycling. Specifically, in $Hf_xZr_{1-x}O_2$ (HZO), the contents of Hf and Zr of the thin film affect the phase composition, increasing m-phase (t-phase) for Hf-rich (Zr-rich) HZO [2] respectively. In addition to this, HZO exhibits different preferences for phase composition depending on film thickness due to changes in Gibbs free energy [3].

In this research, we analyzed HZO thin films with three different thicknesses (5, 7, and 9 nm) and three different Hf:Zr ratios (1:2, 1:1, and 2:1) manufactured by NaMLab (Dresden) within the framework of the D3PO project. The samples were fabricated *via* atomic layer deposition (ALD) in a TiN/HZO/TiN capacitor structure. Later, the HZO thin film is structured with small-sized capacitors (100 x 100 μm^2 lateral size) at CEA Saclay. Each capacitor was field cycled at 4 MV/cm and 100 kHz with a different number of cycles ($1\text{-}10^6$ cycles). Crystalline phase composition was analyzed by X-ray diffraction (XRD) at DiffAbs in synchrotron Soleil using 8.048 keV ($\lambda \sim 1.5405$ Å) x-ray beam energy. The o(111)/t(101), m(-111), and m(111) peaks were investigated. The o(111)/t(101) peak shift to lower 2θ angles was observed with increasing number of cycles, indicating an increase of the ferroelectric o-phase, which is located at a lower angle than the t-phase. The phenomenon was most pronounced in the Hf:Zr=1:2 composition. This research on the phase composition of HZO with various thicknesses, compositions, and electrical fields will help to comprehensively understand the effects of each parameter and find an optimal condition for high-performance HZO thin film.

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A Unique Experimental End-Station Enabling Correlative RIXS and XEOL Spectroscopies under Electric and Magnetic Fields

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ABSTRACT

In this poster we present a unique experimental end-station developed at the inelastic branch of the SEXTANTS beamline, enabling correlative resonant inelastic X-ray scattering (RIXS) and X-ray excited optical luminescence (XEOL) spectroscopies under combined electric and magnetic fields. Since early 2020, this novel sample environment, named MAGELEC, has been available to users for advanced RIXS experiments. MAGELEC consists of a sample holder equipped with 12 electrical contacts combined with a compact quadrupolar magnet delivering a rotatable magnetic field up to 0.45 T. Owing to its specific design, entirely developed at SOLEIL, the full scattering plane is accessible, allowing magnetic dichroism RIXS (RIXS-MD) experiments over a wide temperature range from 400 K down to 18 K.

In addition, in collaboration with researchers of the Laboratoire de Physique des Solides an optical detection system compatible with MAGELEC has been conceived and installed, enabling the correlation of RIXS(-MD) measurements with XEOL spectroscopy under magnetic field. The main characteristics of this experimental station are presented together with representative results obtained on ferromagnetic transition metal compounds and two-dimensional van der Waals materials.

This worldwide unique platform opens new perspectives for fundamental research on magnetic materials through RIXS magnetic circular and linear dichroism (RIXS-MCD/MLD) spectroscopies, enabling investigations beyond the sensitivity of conventional X-ray magnetic circular and/or linear dichroism techniques. Furthermore, it allows RIXS experiments to be performed under operando conditions and enables a precise correlation between electronic excitations and luminescence response, of primary interest for spintronic and optoelectronic applications.

ACKNOWLEDGEMENTS

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1s2p Resonant Inelastic X-ray Scattering Natural Circular Dichroism

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ABSTRACT

Measurements from a recently developed, bulk-sensitive, element specific, photon-in photon-out, hard x-ray spectroscopic technique “Resonant Inelastic X-ray Scattering Natural Circular Dichroism (RIXS-NCD)” are presented. 1s2p RIXS-NCD spectra of two cobalt and manganese based chiral compounds demonstrate clear circular dichroism arising from the metal centre chirality and resulting valence orbital mixing. Additional dependence on the incident photon wavevector orientation relative to the crystal structure, as well as the scattering angle of the emitted photons is also demonstrated. Finally, constant emission energy cuts of the RIXS-NCD spectra are compared with DFT calculations demonstrating strong agreement.

Epitaxial Growth of Ultra-thin Film on Chiral Substrates

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ABSTRACT

Crystals with low symmetry are of renewed interest in the field of spintronics as it can induce asymmetric effects such as spin-orbit torque field free switching[1]. Here, we propose to reduce the symmetry of the interface between any kind of materials by using what is called chiral substrates. In the case of a face centered cubic material, a surface with terraces, steps and kinks is chiral, where (hkl) corresponding to the surface is such that h≠k≠l≠0.

By using grazing incidence x-ray diffraction, we have started studying the epitaxial growth of metallic ultra-thin films (mainly Co and Au) on different chiral substrates, namely Cu(643), Cu(523) and Si(763). To study their epitaxial relationship, we have determined the orientations of the substrates and the ultra-thin films. The diffraction diagrams obtained for the analysis are represented in the form of stereographic projections consisting of a particular family of poles, thus called as pole figures. It has been observed that the thin films retain the chirality. However, the orientation of the epilayer can be significantly modified and we have even found that it can be of opposite handedness as compared to the substrate. The results are discussed in the framework of magic epitaxy[2], which considers the mesoscale distances between steps and between kinks of both the substrate and the epilayer as the key misfit parameters that should be minimized.

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Synchrotron-assisted HPHT Annealing of Quantum Nanodiamonds: In Situ Control of Phase Stability

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ABSTRACT

Group-IV color centers in nanodiamond, such as silicon-vacancy (SiV) defects, are promising quantum emitters for sensing and photonics due to their bright and narrow zero-phonon line (ZPL) emission, representing up to 80% of their total luminescence [1–3]. However, in as-grown CVD nanodiamonds, residual lattice strain induces significant spectral broadening, preventing access to the fine electronic structure of SiV centers even at cryogenic temperatures. To mitigate this effect, we carried out a controlled high-pressure and high-temperature (HPHT) annealing process using the Paris–Edinburgh press, performed in situ at the PSICHE beamline of Synchrotron SOLEIL [4].

The synchrotron X-ray diffraction and tomography measurements were crucial for the precise calibration of pressure and temperature conditions within the assembly, enabling us to finely tune the HPHT parameters to promote strain relaxation while avoiding the onset of graphitization. These in situ synchrotron investigations provided real-time insight into nanodiamond phase stability and strain-release mechanisms, which were confirmed ex situ by optical measurements, leading to the first observation of resolved fine-structure transitions in SiV centers after HPHT treatment.

Importantly, the calibrated HPHT setup can now be reliably operated off-beam, enabling systematic post-annealing studies on different types of nanodiamonds and color centers. This methodology establishes a robust experimental reference for future off-beam HPHT annealing treatments and serves as a benchmark for the broader quantum diamond research community.

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Circuit Map Visit Beamlines

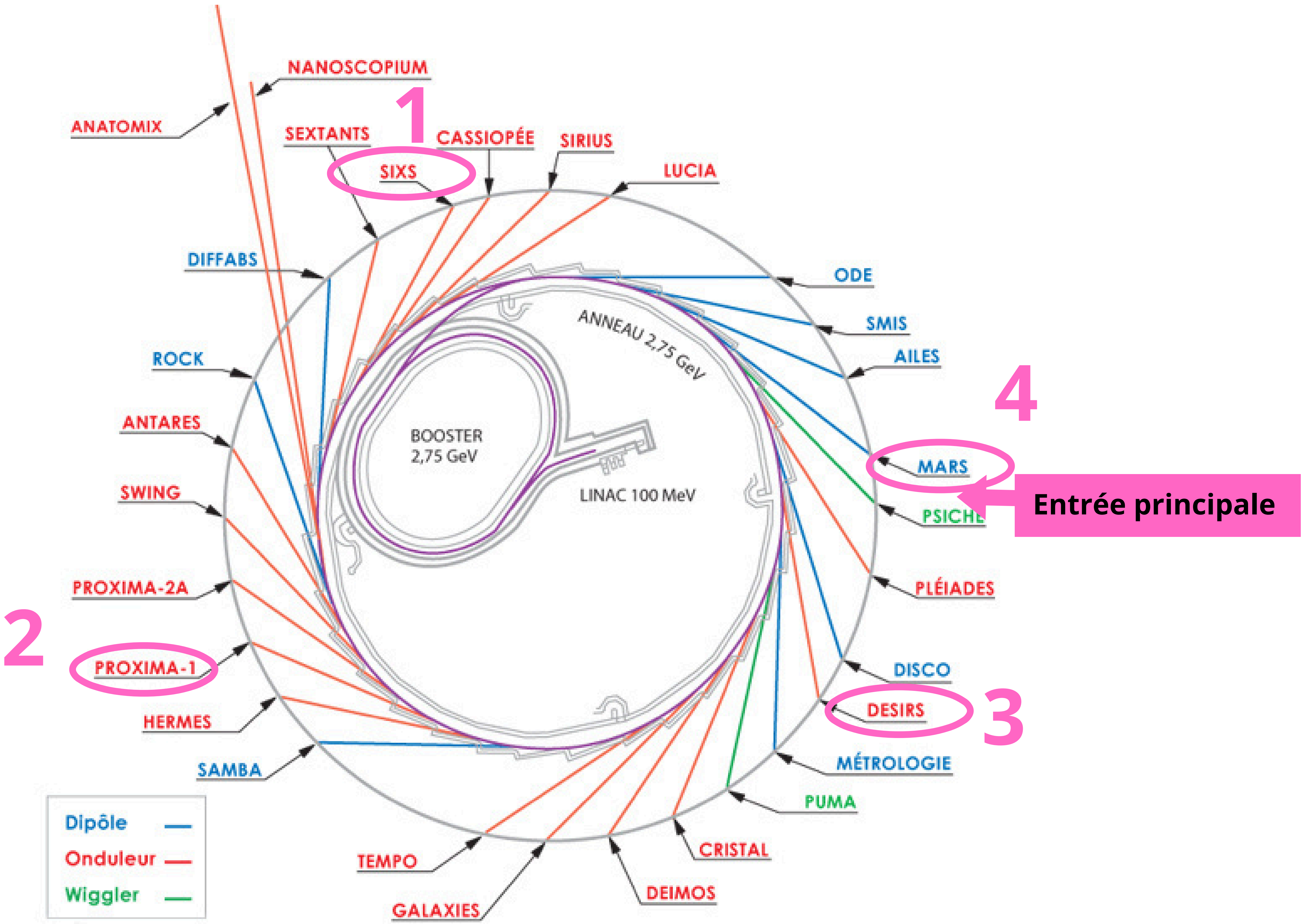
DESIRS

MARS

PROXIMA 1

SIXS

GROUPE 1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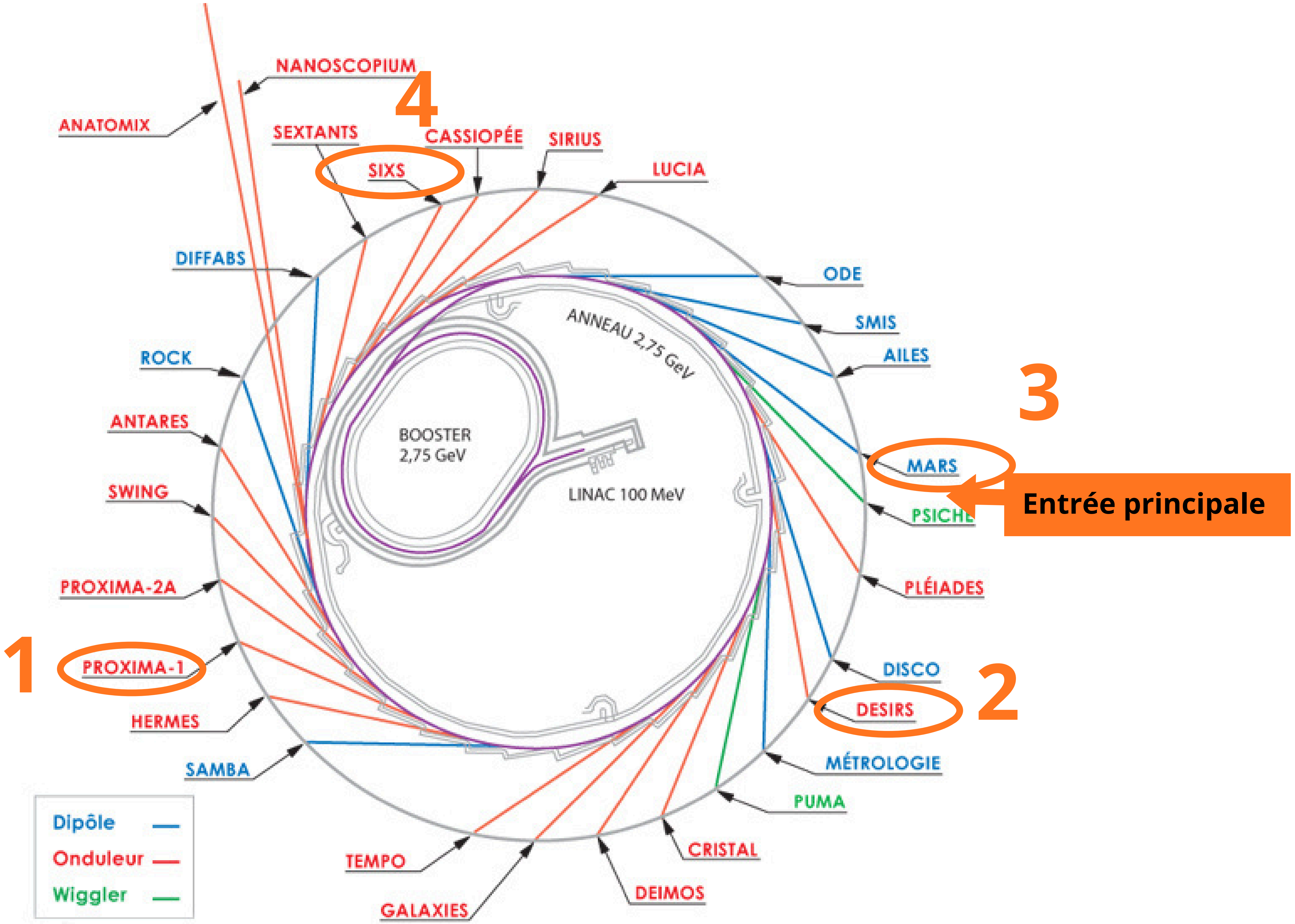
GROUPE 2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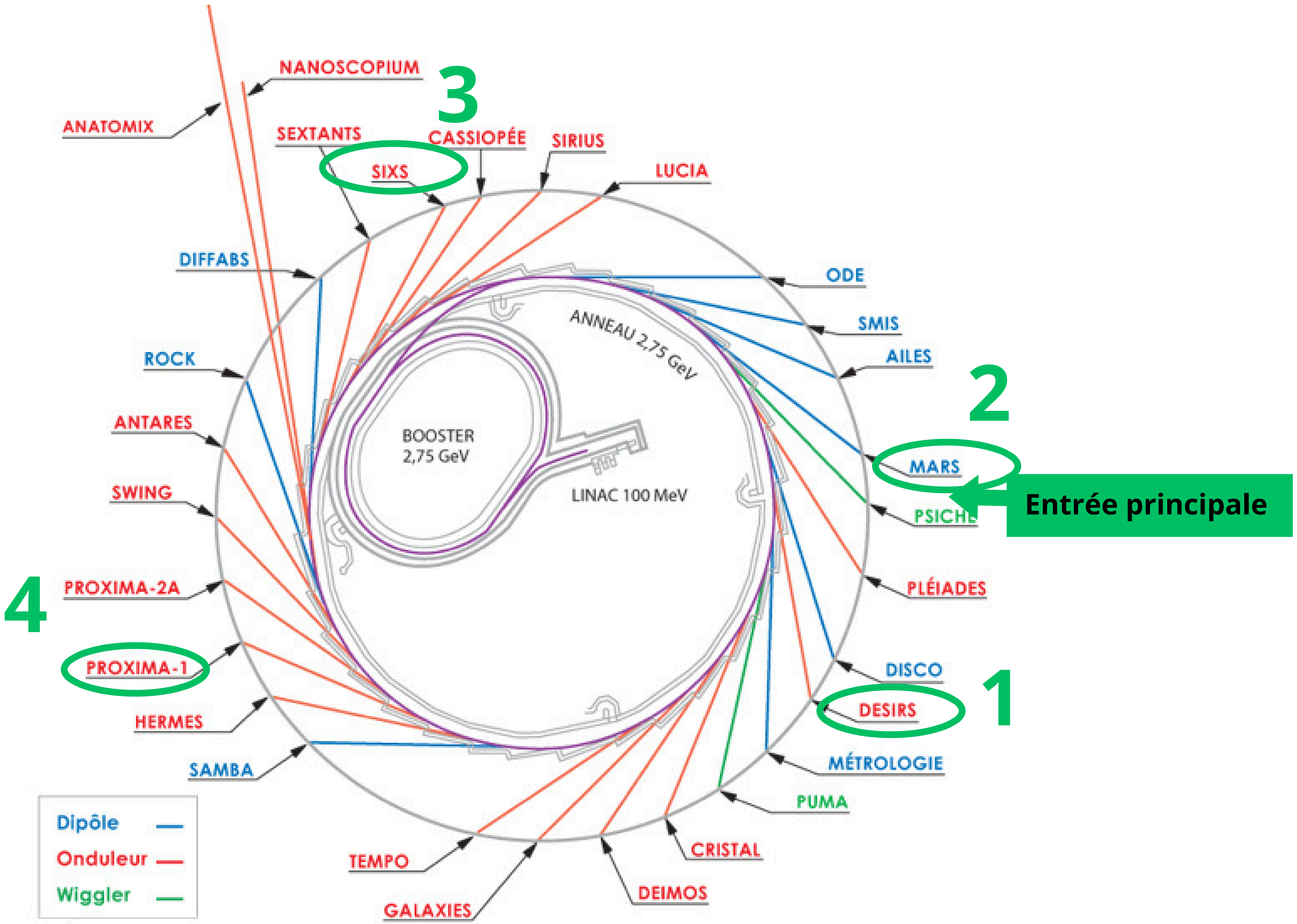
GROUPE 3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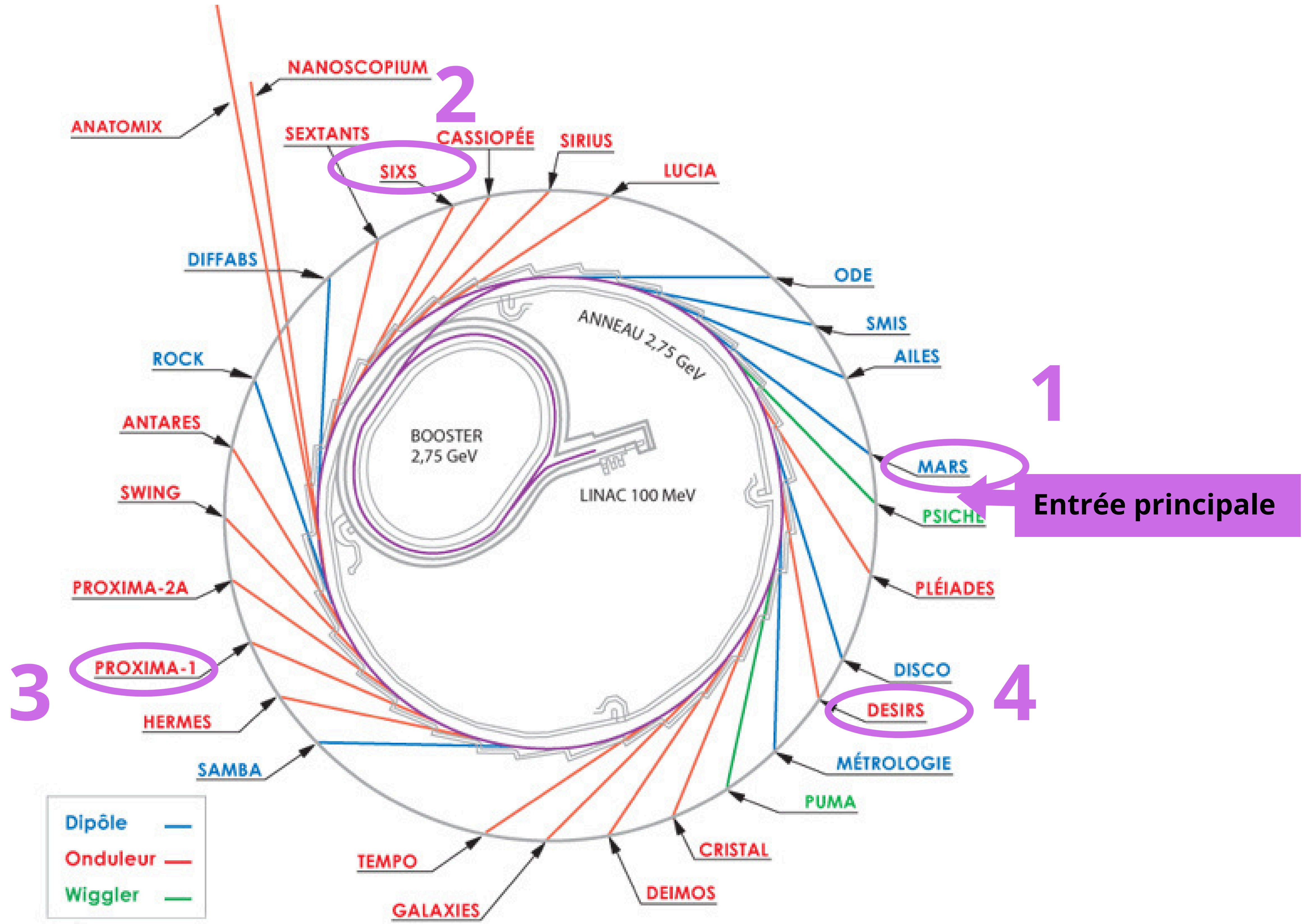
GROUPE 4



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LIST OF COMMERCIAL EXHIBITORS

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