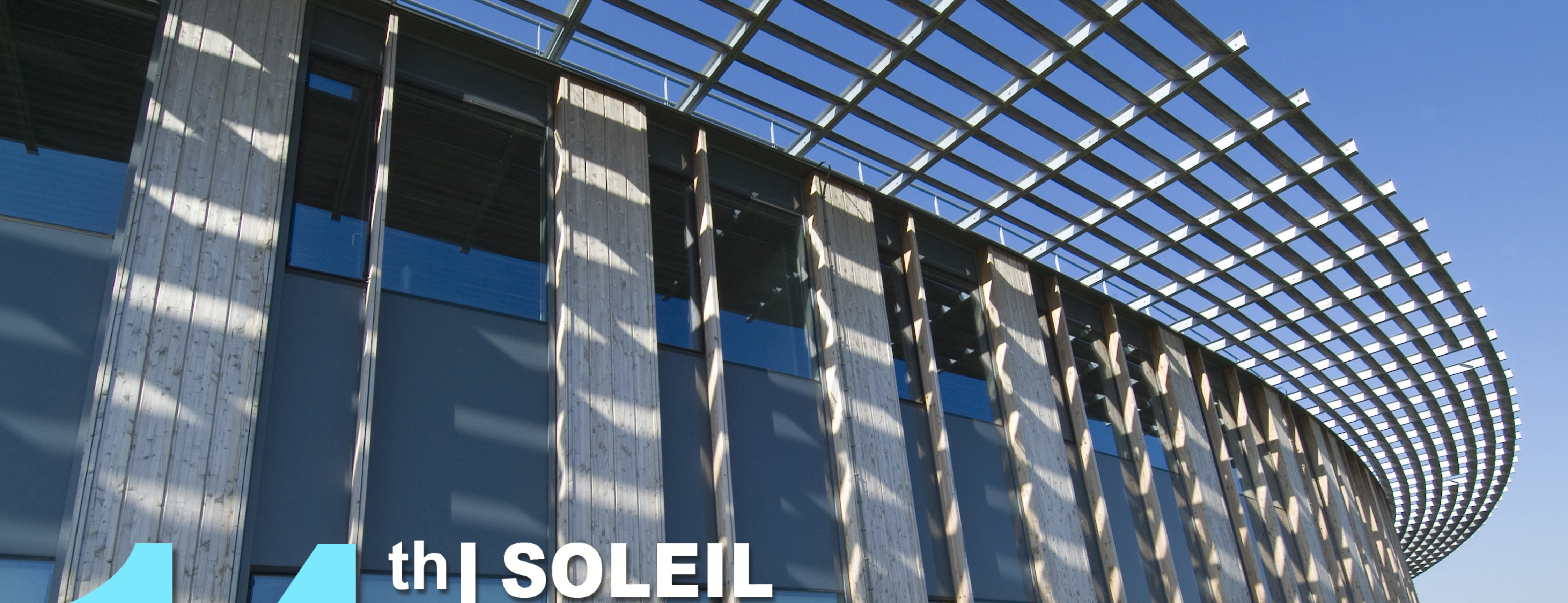


14th SOLEIL USERS' MEETING

JANUARY 17th & 18th, 2019

Centrale Supélec (Gif-s/-Yvette) & SOLEIL (Saint-Aubin)

SCIENTIFIC COMITTEE

Marie d'ANGELO (Institut des Nanosciences de Paris)
Vincent BOUDON (Lab. Interdisciplinaire Carnot de Bourgogne - Dijon)
Noemi CARMONA-TEJERO (Université Complutense - Madrid)
Frédéric DATCHI (IMPMC - Paris)
Nicolas DELSUC (ENS Département de Chimie - Paris)
Jean-Sébastien GIRARDON (Unité de Catalyse et de Chimie du Solide - Lille)
Yann GOHON (Institut Jean-Pierre Bourgin - Versailles)
Renaud GUILLEMIN (LCPMR - Paris)
Thomas MAROUTIAN (Université Paris-Sud)
Rémi MARSAC (Université de Rennes 1 - Rennes)
Benoît MASQUIDA (UMR7156 GMGM - CNRS - Université de Strasbourg)
Karine PROVOST (Institut de Chimie et des Matériaux de Paris-Est - Thiais)

Information and registration:
www.synchrotron-soleil.fr/en/events/sum-2019

SOLEIL
SYNCHROTRON

Welcome

The 14th SOLEIL Users' Meeting takes place on January 17th and 18th, 2019 at CentraleSupélec EIFFEL Building and at SOLEIL.

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

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

The 2 plenary lectures deal with different aspects related to recent and future synchrotron sources evolutions.

- Biology and Health,
- Surfaces/Interfaces/Electronic properties

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

The posters session and commercial exhibitions are held at CentraleSupélec - EIFFEL Building on the afternoon of January 17th.

Then a visit of DISCO, SAMBA and SEXTANTS beamlines is organized, as well as 2 forum/ discussions :

Data policy for users

Upgrade: "low energy" perspectives for users

The conference dinner takes place at SOLEIL.

Bienvenue

Le 14ème Colloque des Utilisateurs de SOLEIL se tiend les jeudi 17 et vendredi 18 janvier 2019, à CentraleSupélec - Bâtiment EIFFEL et à SOLEIL.

Ce rendez-vous incontournable pour la communauté des utilisateurs du rayonnement synchrotron est cette année l'occasion d'échanges et de restitutions 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 2 conférences plénières couvrent différents thèmes de recherche de la communauté des utilisateurs de SOLEIL:

- Biologie et Santé
- Surfaces/Interfaces/Propriétés électroniques

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

Un temps de convivialité et de discussion est organisé à CentraleSupélec - Bâtiment EIFFEL le jeudi 17 janvier après-midi avec la session posters et les stands d'entreprises.

A SOLEIL, sont organisés la visite des lignes DISCO, SAMBA et SEXTANTS, ainsi que deux forum/discussions :

Data policy for users

Upgrade: "low energy" perspectives for users

Le diner de la conférence a lieu à SOLEIL.

SOLEIL Users' Meeting

January 17th - 18th, 2019

Centrale-Supélec – Bâtiment Eiffel, Gif-sur-Yvette & Synchrotron SOLEIL, Saint-Aubin - France

CentraleSupélec - Bâtiment Eiffel, Gif-sur-Yvette - France
&
Synchrotron SOLEIL, Saint-Aubin - France

Programme

Thursday, January 17th

CENTRALE-SUPELEC-GIF-SUR-YVETTE - MICHELIN AUDITORIUM #2

09:00 - 10:00	Registration & coffee
10:00 - 10:10	Welcome / Introduction ***Jean-Sébastien Girardon*** *- ORGUES Chairperson*
10:10 - 10:20	The word of SOLEIL General Director ***Jean Daillant***
10:20 - 11:05	Biology: Biomimetic self-assemblies: 10 years of collaboration with SOLEIL ***Frank Artzner*** *- Institut de Physique de Rennes, France*
11:05 - 11:50	SOLEIL Evolution ***- Science directors*** *(Organisation of the Upgrade Project)* *-* ***Felisa Berenguer*** *(Opportunities exploiting the improved coherence of beam from SOLEIL 2)* *-* ***François Polack*** *(Optics for a high brilliance MBA source)*
11:50 - 12:10	Peer Review Committee Chairman 5 (5mn) - ***Thibaut Crépin*** Peer Review Committee Chairman 6 (5mn) - ***Jörg Göttlicher*** Questions 10mn
12:10 - 13:45	*Lunch*
13:45 - 15:15	Parallel sessions (see the detailed programme below) • Ancient & New Materials (Cultural heritage / Structure / Electronic Properties / Surfaces & Interfaces) • Dynamic, Reactivity & Chemical analysis (Diluted Matter & Chemistry) • Life & Earth Sciences (Biology / Health & Environment / Geoscience)
15:15 - 15:45	*Coffee break*
15:45 - 17:15	Parallel sessions (see the detailed programme below) • Ancient & New Materials (Cultural heritage / Structure / Electronic Properties / Surfaces & Interfaces) • Dynamic, Reactivity & Chemical analysis (Diluted Matter & Chemistry) • Life & Earth Sciences (Biology / Health & Environment / Geoscience)

17:15 - 18:45 Posters session / Commercial exhibition / ORGUES and AFURS Booth
and Coffee break

Transfer to SOLEIL 18:45

19:00 - 20:00 Visit of Beamlines (SAMBA / SEXTANTS / DISCO)
or
Forum – Discussion

- Data Policy for users – (***Amphitheatre SOLEIL***)
  B. Gagey, J-P. Itié (SOLEIL) K. Provost (ORGUES)
- Upgrade: "Low energy" perspectives for users – (***Bâtiment d'accueil***)
  A. Thompson, A. Taleb (SOLEIL), V. Boudon, N. Delsuc et R. Marsac (ORGUES)

20:00 - 21:30 *Buffet /* Award of the best student poster

Friday, January 18th

CENTRALE-SUPELEC-GIF-SUR-YVETTE - MICHELIN AUDITORIUM #2

9:00 - 09:45 Surfaces/Interfaces:
Magnetic skyrmions: When topology meets spintronics
***Vincent Cros** - Unité Mixte de Physique CNRS/Thalès, Palaiseau, France*

Parallel sessions (see the detailed programme below)

9:50 - 10:50
- Ancient & New Materials (Cultural heritage / Structure / Electronic Properties / Surfaces & Interfaces)
- Dynamic, Reactivity & Chemical analysis (Diluted Matter & Chemistry)
- Life & Earth Sciences (Biology / Health & Environment / Geoscience)

10:50 - 11:20 *Coffee break*

Parallel sessions (see the detailed programme below)

11:20 - 12:50
- Ancient & New Materials (Cultural heritage / Structure / Electronic Properties / Surfaces & Interfaces)
- Dynamic, Reactivity & Chemical analysis (Diluted Matter & Chemistry)
- Life & Earth Sciences (Biology / Health & Environment / Geoscience)

13:10 - 14:30 *Lunch*

Transfer to SOLEIL 14:45

2 tutorials at SOLEIL Synchrotron (see the detailed programme below)

15:00 - 18:00
- **Photoemission** - (***Salle Formation – Bât. T5***)
- **Coherence** - (***Salle Libra – Bât. Central***)

Parallel Sessions Schedule

Ancient & New Materials

(Cultural heritage / Structure / Electronic Properties /Surfaces & Interfaces)

Chairpersons:
Marie d'Angelo, Karine Provost, Noemi Carmona-Tejero, Thomas Maroutian & Frédéric Datchi

Thursday, January 17th

CENTRALE-SUPELEC-GIF-SUR-YVETTE - MICHELIN AUDITORIUM #3

13:45 - 14:15 (25'+5')	Dynamics in narrow band gap nanocrystals ***Emmanuel LHUILLIER*** *- INSP, Paris, France*
14:15 - 14:35 *(15'+5')*	Real time study of Si(111)-7×7 room temperature oxidation by near ambient pressure XPS ***Lucia Perez Ramirez*** *- LCPMR, Paris, France*
14:35 - 14:55 *(15'+5')*	A tunable and robust two-dimensional electron system at the (110) surface of SnO_2 ***Ji Dai*** *- CSNSM, Orsay, France*
14:55 - 15:15 *(15'+5')*	Defects investigation and engineering in 2D materials: A spectroscopic study ***Debora Pierucci*** *- ALBA Synchrotron, Barcelona, Spain*
15:15 - 15:45	*Coffee break*
15:45 - 16:15 (25'+5')	Self-assembled resonant nanostructured surfaces for optics: The precious role of X-rays ***Virginie PONSINET*** *- CRPP, Pessac, France*
16:15 - 16:35 *(15'+5')*	Structural resolution of inorganic nanotubes with complex stoichiometry ***Geoffrey Monet*** *- LPS, Orsay, France*
16:35 - 16:55 *(15'+5')*	Origin of the low value onset potential in nanostructured hematite photoanodes ***Stefan Stanescu*** *- Synchrotron SOLEIL, Saint Aubin, France*
16:55 - 17:15 *(15'+5')*	The formation of catalytically active interfacial Pt-NiO1-x nanostructures on $Pt_3Ni(111)$ under CO oxidation reaction ***Bongjin Simon Mun*** *- SOKENDAI, Tsukuba, Japan & GIST, Gwangju, Korea*

Parallel Sessions Schedule

Ancient & New Materials
(Cultural heritage / Structure / Electronic Properties /Surfaces & Interfaces)

Chairpersons:
Marie d'Angelo, Karine Provost, Noemi Carmona-Tejero, Thomas Maroutian & Frédéric Datchi

Friday, January 18th

CENTRALE-SUPELEC-GIF-SUR-YVETTE - MICHELIN AUDITORIUM #3

09:50 - 10:10 *(15'+5')*	An insider view on pressure induced amorphisation of molecular crystals ***Emiliano Fonda*** *- Synchrotron SOLEIL, Saint Aubin, France*
10:10 - 10:30 *(15'+5')*	Influence of applied pressure on the structural and magnetic properties of Y_1-xTbxFe$_2$D$_y$ compounds ***Valérie Paul-Boncour*** *- ICMPE, Thiais, France*
10:30 - 10:50 *(15'+5')*	Water/ammonia ice mixtures under high pressure and temperature ***Léon Andriambariarijaona*** *- IMPMC, Paris, France*
10:50 - 11:20	*Coffee break*
11:20 - 11:50 *(25'+5')*	X-ray diffraction and Cultural Heritage materials - Adaptive crystallography ***Catherine DEJOIE*** *- ESRF, Genoble, France*
11:50 - 12:10 *(15'+5')*	3D mapping by Laue micro-diffraction ***Loïc Renversade*** *- INAC Grenoble, France*
12:10 - 12:30 *(15'+5')*	Synchrotron based THz spectroscopy to probe magneto-electric effects in multiferroics ***Sophie Debrion*** *- Institut Néel, Grenoble, France*
12:30 - 12:50 *(15'+5')*	XMCD Spectroscopy at ultra-low temperature on DEIMOS beamline (SOLEIL) ***Weibin Li*** *- Synchrotron SOLEIL, Saint Aubin & IMPMC, Paris, France*
12:50 - 13:10	Conclusion

Parallel Sessions Schedule

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

Chairpersons:
Jean-Sébastien Girardon, Nicolas Delsuc, Vincent Boudon and Renaud Guillemin

Thursday, January 17th

CENTRALE-SUPELEC-GIF-SUR-YVETTE - MICHELIN AUDITORIUM $^{\#}$2

13:45 - 14:15 *(25'+5')*	Correlative X-ray fluorescence nano-imaging and optical microscopy to investigate chemical element compartmentalization in cells ***Richard ORTEGA** - CENBG, CNRS, University of Bordeaux, France*
14:15 - 14:35 *(15'+5')*	Irradiation of water ice in the O 1s region : Spectral and kinetic energy signatures of photodesorbed species ***Géraldine Féraud** - LERMA, PSL, CNRS, Paris, France*
14:35 - 14:55 *(15'+5')*	Progress around the High Resolution Heterodyne spectrometer of the AILES beamline ***Sophie Eliet** - IEMN, Villeneuve d'Ascq, France*
14:55 - 15:15 *(15'+5')*	State-selected ion-molecule reactions with VUV Synchrotron Radiation: The $O_2^+ + C_3H_6$ case ***Christian Alcaraz** - LCP, CNRS - Université Paris-Saclay, France*
15:15 - 15:45	*Coffee break*
15:45 - 16:15 *(25'+5')*	High resolution spectrometry at the AILES beamline ***Jean VANDER AUWERA** - Université Libre de Bruxelles,Brussels, Belgium*
16:15 - 16:35 *(15'+5')*	High-resolution analysis of the 12.6 µm absorption of the nitryl chloride $ClNO_2$ molecule ***Anusanth Anantharajah** - LISA, Institut Pierre Simon Laplace, Créteil, France*
16:35 - 16:55 *(15'+5')*	Role of hydrogen absorption in supported Pd nanocatalysts during CO-PROX: Insights from operando X-ray absorption spectroscopy ***Claudia Zlotea** - ICM Paris-Est, Thiais, France*
16:55 - 17:15 *(15'+5')*	Photoionization and dissociative photoionization of propynal in the gas phase: Theory and experiment. ***Imene Derbali** - MONARIS UMR 8233 CNRS, Sorbonne Université, France*

Parallel Sessions Schedule

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

Chairpersons:
Jean-Sébastien Girardon, Nicolas Delsuc, Vincent Boudon and Renaud Guillemin

Friday, January 18th

CENTRALE-SUPELEC-GIF-SUR-YVETTE - MICHELIN AUDITORIUM $^{\#}$2

09:50 - 10:10 *(15'+5')*	Line positions and intensities in the ν_2 band of sulfuryl fluoride using the C_{2v} Top Data System (C2vTDS) ***Maud Rotger*** *-GSMA, UMR CNRS 7331, Univ. de Reims Champagne Ardenne, France*
10:10 - 10:30 *(15'+5')*	In-situ XRD analysis of transient liquid assisted growth of $YBa_2Cu_3O_7$ superconducting films ***Juri Banchewski*** *- ICMAB-CSIC, Campus UAB, Bellaterra, Spain*
10:30 - 10:50 *(15'+5')*	First high resolution measurement and analysis of the 83.3 µm absorption of the chlorine nitrate $ClONO_2$ molecule ***Fridolin Kwabia Tchana*** *- LISA, Institut Pierre Simon Laplace, Créteil, France*
10:50 - 11:20	*Coffee break*
11:20 - 11:50 *(25'+5')*	Surface chemistry of colloidal surfactant-free gold nanoparticles generated by laser ablation ***Anna LEVY*** *- INSP Sorbonne Universités, Paris, France*
11:50 - 12:10 *(15'+5')*	Double inner-shell vacancies in molecules ***Dimitri Koulentianos*** *- LCPMR, Sorbonne Université Paris, France*
12:10 - 12:30 *(15'+5')*	The investigation of the ν_8 & ν_{21} bands of propane $CH_3CH_2CH_3$ at 11.5 & 10.9 µm: Evidence of large amplitude tunnelling effects ***Agnès Perrin*** *- LMD/IPSL, Ecole Polytechnique, Université Paris-Saclay, Palaiseau, France*
12:30 - 12:50 *(15'+5')*	Characterization of two-photon entanglement resulting from VUV photodissociation of H_2 ***Baptiste Fabre*** *- CELIA, Talence, France*
12:50 - 13:10	Conclusion

Parallel Sessions Schedule

Life & Earth Sciences
(Biology / Health & Environment / Geoscience)

Chairpersons:
Benoît Masquida, Yann Gohon and Remi Marsac

Thursday, January 17th

CENTRALE-SUPELEC-GIF-SUR-YVETTE - MICHELIN AUDITORIUM #1

13:45 - 14:15 *(25'+5')*	Structural basis of nucleotide sugar transport across the Golgi membrane ***Simon NEWSTEAD*** *- Department of Biochemistry, University of Oxford, UK*
14:15 - 14:45 *(25'+5')*	*In vitro, in cellulo and in crystallo* enzymatic reaction from APRT ***Pierre NIOCHE*** *- Université Paris Descartes, Centre Universitaire des Saints Pères, Paris France*
14:45 - 15:05 *(15'+5')*	Structure-function analysis of the photosynthetic ribulose epimerase CrRPE1 ***Julien Henri*** *- Laboratoire de Biologie Moléculaire et Cellulaire des Eucaryotes, Paris France*
15:05 - 15:45	*Coffee break*
15:45 - 16:15 *(25'+5')*	Cristal chemistry and stability of phyllosilicates: New approaches to solve old problems ***Benoit DUBACQ*** *- Institut des Sciences de la Terre, Paris, France*
16:15 - 16:35 *(15'+5')*	Calcium control on the size and organization of iron-organic matter nano-aggregates: Impact on their surface reactivity ***Anthony Beauvois*** *- Synchrotron SOLEIL, St-Aubin, France*
16:35 - 16:55 *(15'+5')*	Multimodal ultrastructural study of lipid droplet ***Marine Froissard*** *- INRA AgroParisTech, Paris, France*
16:55 - 17:15 *(15'+5')*	Investigations in the CaMoO$_4$ - Na$_{0.5}$Ln$_{0.5}$MoO$_4$ (Ln = La, Eu, Yb) solid solution series ***Nicolas Finck*** *- KIT-INE, Karlsruhe, Germany*

Parallel Sessions Schedule

Life & Earth Sciences
(Biology / Health & Environment / Geoscience)

Chairpersons:
Benoît Masquida, Yann Gohon and Remi Marsac

Friday, January 18th

CENTRALE-SUPELEC-GIF-SUR-YVETTE - MICHELIN AUDITORIUM #1

09:50 - 10:20 *(25'+5')*	Crystal chemistry of trace elements in sulfide minerals: environmental implications ***Guillaume MORIN*** *- IMPMC, Paris, France*
10:20 - 10:50 *(25'+5')*	Abiotic synthesis of amino acids in the recesses of the oceanic lithosphere ***Celine PISAPIA*** *- IPGP, Paris, France*
10:50 - 11:20	*Coffee break*
11:20 - 11:50 *(25'+5')*	Setting up an in-vivo crystallography platform at SOLEIL ***Pierre MONTAVILLE -*** *Synchrotron SOLEIL, St-Aubin, France*
11:50 - 12:10 *(15'+5')*	Looking deep inside the phloem and xylem cell wall composition by synchrotron FTIR and raman spectroscopy ***Rozenn Le Hir*** *- Institut Jean-Pierre Bourgin, Versailles, France*
12:10 - 12:30 *(15'+5')*	Structure of liquid crystalline nanocarriers for delivery of neuroprotective molecules ***Angelina Angelova*** *- Institut Galien Paris-Sud, Paris, France*
12:30 - 13:10	Conclusion

TUTORIALS

Friday, January 18th

Photoemission

Synchrotron SOLEIL - Salle Formation – Bât. T5

X-Ray Photoemission Spectroscopy: Processing, fitting and analyzing data acquired with synchrotron light

Julien Rault *&* ***Matthieu Silly*** *– Synchrotron SOLEIL, Gif-sur-Yvette, France*

15:00 - 15:30	**Introduction** • XPS at a synchrotron beamline • Data acquisition - Spectrometer • First data treatments - Softwares
15:30 - 16:45	**Low energy XPS: Graphene on SiC** • Peak fitting: Lineshapes & background • Energy dependence of surface & interface components
16:45 - 17:00	*Coffee break*
17:00 - 17:45	**High energy XPS** • Buried interfaces with HAXPES • Introduction to standing wave technique
17:45 - 18:00	**Closing words** • XPS at SOLEIL beamlines • Guidelines for XPS proposals

TUTORIALS

Friday, January 18th

Coherence

Synchrotron SOLEIL - Salle Libra – Bât. Central

15:00 - 15:55	Introduction générale à la cohérence et les techniques associées ***Felisa Berenguer*** *- Synchrotron SOLEIL, Gif-sur-Yvette, France*
15:55 - 16:05	*Coffee break*
16:05 - 16:35	Challenges of bio-inspired material science and perspectives in the - coherent - light of 4th generation Synchrotron sources ***Virginie Chamard*** *- Institut Fresnel, Marseille, France*
16:35 - 17:05	Bragg Coherent Diffraction Imaging benefits for materials science ***Stéphane Labat*** *- IM2NP, Marseille, France*
17:05 - 17:35	Benefits of coherence for imaging of complex natural and manufactured materials ***Laurent J. Michot*** *- Laboratoire Phenix, Paris, France*

PLENARY SESSION

PLENARY SESSION

CENTRALE-SUPELEC-GIF-SUR-YVETTE - MICHELIN AUDITORIUM #2

Thursday, January 17th

PT-01	Biomimetic self-assemblies: 10 years of collaboration with SOLEIL ***Frank Artzner***

Friday, January 18th

PT-02	Magnetic skyrmions: When topology meets spintronics ***Vincent Cros***

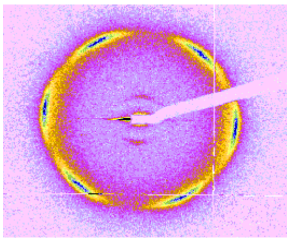
Biomimetic Self-assemblies:
10 Years of Collaboration with SOLEIL

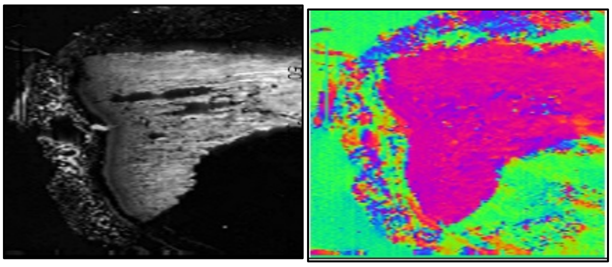
T. Bizien,[1] P. Legrand,[1] F. Meneau,[1] J. Perez,[1]
C. Mériadec,[2] M. Paternostre, F. Artzner[2]

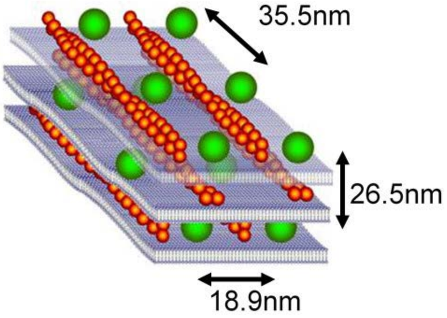
[1]*SWING & Proxima 1 BeamLine, Synchrotron SOLEIL, France*
[2]*Archi-Pex, IPR, UMR 6251, CNRS & Rennes University, France*

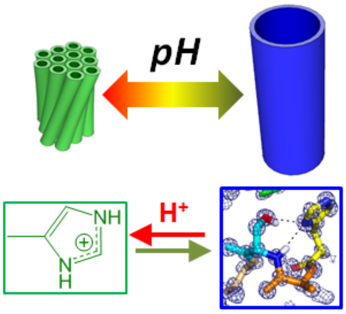
ABSTRACT

Building up hierarchical organizations is challenging because it requires the design of self-assembly mechanisms at various length scales and with similar time scales. Hijacking biological systems and self-assembly mechanisms are a unique opportunity to design such innovative mater. Two peptide nanotubes with well-defined organizations resolved at molecular or atomic scale will be presented. The diameter of the first nanotubes can be tuned by a single mutation of the peptides [1]. We recently studied a self-assembling pH sensitive peptide that forms either crystalline bundles of small nanotubes of 10nm width ($pH<6.5$) or large nanotubes of 50nm width ($pH>7.5$) [2]. Varied nanoparticle (NPs) crystals systems will be presented : by self-assembly between membranes, actin filaments and NPs and by drying processes at nanometric scale (colloidal crystallization). The other takes advantage of entropy effect during a controlled drying. Some recent experiments using small beam on SWING will complete the presentation.









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2] *Atomic view of the histidine environment stabilizing higher-pH conformations of pH-dependent proteins*, **Nature Communications** 6*: 7771* (2015).

3] *Crystallization of Fluorescent Quantum Dots within a Three-Dimensional Bio-Organic Template of Actin Filaments and Lipid Membranes*, **NanoLett.,** 2011, 11(12), 5543-5548.

4] *Three-Dimensional Self-Assembling of Gold Nanorods with Controlled Macroscopic Shape and Local Smectic B Order*, **ACS. Nano,** 2012, 6(5), 4137-4146.

Magnetic Skyrmions: When Topology Meets Spintronics

W. Legrand[1], D. Maccarriello[1], F. Ajejas[1], J.Y. Chauleau[1,2,*],
S. Collin[1], H. Popescu[2], K. Bouzehouane[1], N. Jaouen[2],
N. Reyren[1], V. Cros[1], A. Fert[1]

[1]Unité Mixte de Physique CNRS, Thales, Univ. Paris Sud, Université Paris-Saclay, Palaiseau
*[2]SOLEIL synchrotron, Gif sur Yvette, * Now at SPEC/CEA/CNRS, Gif sur Yvette*

ABSTRACT

Magnetic skyrmions are topological spin textures [1] that can be found in magnetic materials which break bulk or interface inversion symmetry, in which the skyrmions are stabilized by the Dzyaloshinskii-Moriya interaction (DMI) [2]. Due to their reduced size (as small as a few atomic lattices) and expected low depinning threshold for current-induced motion, magnetic skyrmions are expected to allow for improved scalability and be suitable for “abacus”-type applications in information and communication technologies [3].

Up to the last years, magnetic skyrmions were observed mostly at low temperature and under large magnetic fields in a few bulk non-centrosymmetric compounds and magnetic monolayers. In this talk, I will present experimental results at room temperature (RT) on small skyrmions (30-80 nm) in several types of multilayers associating magnetic layers of Co and nonmagnetic layers of heavy metals (Pt, Ir, Ru etc…) [4]. Then I will briefly describe i) the creation of skyrmions by current pulses and its mechanism [5], ii) the electrical detection of individual skyrmions [6], iii) the current-induced motion of skyrmions [5]. Then, I will present in more detail some recent results on shaping skyrmion profile and chirality in 3D by a control of the relative values of DMI and dipole interactions for a given number of layers [7]. I will show how we succeeded to experimentally determine by x-ray magnetic scattering (XRMS) the existence of a twisted chirality for the spin textures i.e. domain walls or skyrmions stabilized in multilayers [8,9]. Finally, I will describe how a fine engineering of the different magnetic interactions at play in these multilayers allows us to stabilize at RT spin spiral configuration or even small skyrmions in synthetic antiferromagnetic systems.

These advances made in technologically relevant materials open the way for the development of several concepts of skyrmion based devices going from race-track memory type to MRAM, from still highly silicon-compatible memories, such as multi-level MRAM or skyrmion racetrack memories to disruptive “beyond CMOS” technologies such as neuro-inspired architectures.

Ackn: ANR grant TOPSky (ANR-17-CE24-0025), FLAG-ERA SoGraph (ANR-15-GRFL-0005) and DARPA MIPR# HR0011831554.

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[3] A. Fert, N. Reyren, V. Cros, Nat. Rev. Mat. **2**, 17031 (2017);

[4] C. Moreau-Luchaire, VC *et al.*, Nat. Nanotech, **11**, 444 (2016);

[5] W. Legrand et al., Nano Letters 17, 2703 (2017); K

[6] D. Maccariello, VC *et al.*, Nat. Nanotech. (2018);

[7] W. Legrand, VC *et al.*, Science Adv. (2018);

[8] J.Y. Chauleau, VC *et al.*, Phys. Rev. Lett. **120**, 037202 (2018); [9] W. Legrand *et al.*, arXiv (2018).

PARALLEL SESSIONS

PARALLEL SESSION

Ancient & New Materials

(Cultural heritage / Structure / Electronic Properties / Surfaces & Interfaces)

CENTRALE-SUPELEC-GIF-SUR-YVETTE - MICHELIN AUDITORIUM #3

Thursday, January 17th

Chairpersons:

Marie d’Angelo, Karine Provost, Noemi Carmona-Tejero, Thomas Maroutian
& Frédéric Datchi

IT-01	Dynamics in narrow band gap nanocrystals ***E. Lhuillier***
OC-01	Real time study of Si(111)-7×7 room temperature oxidation by near ambient pressure XPS ***L. Perez Ramirez***
OC-02	A tunable and robust two-dimensional electron system at the (110) surface of SnO_2 ***J. Dai***
OC-03	Defects investigation and engineering in 2D materials: A spectroscopic study ***D. Pierucci***
IT-02	Self-assembled resonant nanostructured surfaces for optics: The precious role of X-rays ***V. Ponsinet***
OC-04	Structural resolution of inorganic nanotubes with complex stoichiometry ***G. Monet***
OC-05	Origin of the low value onset potential in nanostructured hematite photoanodes ***S. Stanescu***
OC-06	The formation of catalytically active interfacial Pt-NiO_{1-x} nanostructures on $Pt_3Ni(111)$ under CO oxidation reaction ***B. S. Mun***

PARALLEL SESSION

Ancient & New Materials

(Cultural heritage / Structure / Electronic Properties /
Surfaces & Interfaces)

CENTRALE-SUPELEC-GIF-SUR-YVETTE - MICHELIN AUDITORIUM $^{\#}$3

Friday, January 18th

Chairpersons:

Marie d’Angelo, Karine Provost, Noemi Carmona-Tejero, Thomas Maroutian
& Frédéric Datchi

OC-07	An insider view on pressure induced amorphisation of molecular crystals ***E. Fonda***
OC-08	Influence of applied pressure on the structural and magnetic properties of Y_1-xTbxFe$_2$Dy compounds ***V. Paul-Boncour***
OC-09	Water/ammonia ice mixtures under high pressure and temperature ***L. Andriambariarijaona***
IT-03	X-ray diffraction and cultural heritage materials - Adaptive crystallography ***C. Dejoie***
OC-10	3D mapping by Laue micro-diffraction ***L. Renversade***
OC-11	Synchrotron based THz spectroscopy to probe magneto-electric effects in multiferroics ***S. Debrion***
OC-12	XMCD spectroscopy at ultra-low temperature on DEIMOS beamline (SOLEIL) ***W. Li***

Dynamics in Narrow Band Gap Nanocrystals

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ABSTRACT

Carrier dynamics is driving key parameters in semiconducting nanocrystals such as the luminescence efficiency of the power conversion efficiency for nanocrystal based solar cell. In the visible range of wavelength, many methods, mostly based on time resolved have been developed. On the other hand, when narrower energy transition are involved, typically in the mid infrared, method such as time resolved photoluminescence can no longer be used. New methods have to be developed.

I will illustrate how in the case of narrow band gap nanocrystals of HgTe which optical feature are in the 1 to 5µm range [1-3], we have developed new methods based on transient photocurrent [1-2] and time resolved photoemission [3]. Beyond the device characterization, I will show how it is possible to unveil band structure parameters from this time resolved method [2].

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Real Time Study of Si(111)-7×7 Room Temperature Oxidation by Near Ambient Pressure XPS

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ABSTRACT

The study of silicon oxidation has attracted considerable interest since the 1960s as silicon dioxide is the gate oxide of MOS technology. Phenomenological interpretations of the kinetics of silicon oxidation were accompanied by atomic transport studies and physicochemical analyzes of the Si/SiO2 interface, in which synchrotron radiation X-ray photoemission spectroscopy (XPS)8,9 had the most significant role. With the advent of near ambient pressure photoemission (NAP-XPS), real-time monitoring of the oxide growth was finally made possible.

Here, we present a NAP-XPS study of the oxidation of the Si(111)-7×7 surface under O2 atmosphere using the set-up of the LCPMR (Sorbonne Université) installed at TEMPO beamline, SOLEIL. The clean reconstructed surface was exposed to dry oxygen at room temperature under pressures ranging from 10–7 to 1 mbar, and the Si 2p core-level (suboxide distribution and Fermi level position in the gap) and secondary electron energy distribution curve (work function) were monitored as a function of time. Two regimes are observed: a regime of low oxygen coverage where O2 adsorption and decomposition on surface adatoms dominates the process, and a regime where a continuous SiO2 layer has formed and O2 seeks to fit into the free interstices of amorphous silica inducing a change of surface dipole probably due to ozonyl species stabilized by the dense SiO2 network10. By solving longstanding questions that had previously been addressed only by theoretical calculations, this real-time XPS experiment illustrates the interest of giving a complete electron energy scheme of a surface being oxidized under “realistic” NAP conditions.

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A Tunable and Robust Two-dimensional Electron System at the (110) Surface of SnO_2

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ABSTRACT

Tin oxide (SnO_2) is an important transparent binary oxide widely used as a gas sensor material and believed to remain insulating even in the presence of oxygen vacancies[1]. We report the discovery of a metallic two-dimensional electron system (2DES), see Figure 1, at the (110) surface of the transparent bulk insulator SnO_2, with the exciting possibility to tune its carrier density at will by means of external parameters[2]. We characterize its electronic structure using angle resolved photoemission spectroscopy (ARPES), and show that it is formed out of the bulk s-like conduction band minimum of SnO_2 confined at the surface. This 2DES is robust with respect to surface preparation, insensitive to surface reconstructions, and exhibits clear signatures of electron phonon coupling.

Furthermore, our experimental data show that the emergence of the metallic 2DES is related to the presence of surface oxygen vacancies, providing crucial input to the possible origin of n-type conductivity in SnO2 that is at the basis of a wide range of technological applications. Taken together with previous results on other oxide templates[3], our study proves that the emergence of a 2DES depends on the delicate interplay of the crystal structure and the orbital origin of the conduction electrons.

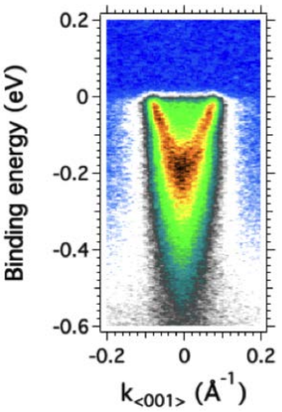

Figure 1: Energy-momentum ARPES intensity map at the SnO_2(110) surface, along the in plane $k_{<001>}$ direction. The measurement temperature is T = 15 K.

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Defects Investigation and Engineering in 2D Materials: A Spectroscopic Study

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ABSTRACT

As a result of thermal equilibrium and the kinetics of processing, all real materials contain structural defects which could significantly affect their properties.
However, most of the richness of material science can be attributed to defects. As Ashcroft and Mermin state in their famous book on solid state physics: *“Like human defects, those of crystals come in a seemingly endless variety, many dreary and depressing, and a few fascinating.”* This statement is best represented by the development of semiconductor industry over 50 years. In fact, engineering defect in 3D semiconductors materials constitutes a key approach to tailor electronic properties and enable modern electronics.

In the past decade, new two-dimensional (2D) materials have attracted much interest due to their unique physical and chemical properties as well as potential applications in electronics, optoelectronics, energy storage and catalysis[1]. Like 3D materials the structure of 2D materials always contains different type of defects, such as vacancies, adatoms, edges, grain boundaries and substitutional impurities. Moreover, due to reduced degrees of freedom compared to bulk materials, 2D materials properties are also more strongly influenced by defects. Therefore, understanding the role of defects in 2D layers represents a main challenge to materials research and offers a great opportunity to control electronic properties and functionalities of these materials. In this talk, I will show that x-ray photoemission spectroscopy is a valid non-destructive technique to uncover the nature of defects in 2D materials as MoS_2[2] and h-BN[3–5]. I will also present an effective strategy of defect engineering to control MoS_2 doping.

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Self-assembled Resonant Nanostructured Surfaces for Optics: The Precious Role of X-rays

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ABSTRACT

The control of light propagation and refraction in thin layers of materials is crucial for the development of optical and optoelectronic devices for high-resolution imaging and lithography, enhanced photovoltaic and Raman substrates, or optical communication[1,2]. Such control can be obtained by nanostructured metal/dielectric composite thin films, due to their localized surface plasmon resonances (LSPR). This has encouraged, in the recent years, active research efforts towards the fabrication of nanostructured metal-dielectric materials and surfaces. This presentation will show how we use self-assembling block copolymers for the "bottom-up" fabrication of original plasmonic nanostructures in bulk and at surfaces[3-5].

In such nanomaterials, in which the structuration results at least partly from self-assembly processes and presents some degree of disorder, the extraction of accurate optical responses from experimental data and the understanding of the underlying physical principles critically rely on the precise knowledge of the sample structure. X-ray small-angle scattering in transmission and grazing-incidence geometries, as well as X-ray specular reflectivity constitute invaluable tools, along with spectroscopy, microscopy and other techniques.

We will present the fabrication and study of periodic cylindrical and lamellar assemblies composed of nanometric domains of pure polymer and domains of composite of polymer and gold, which can lead to either thin anisotropic nanocomposites films or ultra-thin nanostructured gold layers, of various patterns and scales. The occurrence of specific nanostructure-related optical properties such as high refractive index, hyperbolic propagation or optical magnetism will be discussed.

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Structural Resolution of Inorganic Nanotubes with Complex Stoichiometry

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ABSTRACT

Single-walled nanotubes (SWNT) constitute an appealing class of materials in which new synthesis strategies recently emerged. Determination of the atomic structure of single-walled nanotubes with complex stoichiometry remains elusive due to the too many atomic coordinates to be fitted with respect to X-ray diffractograms inherently exhibiting rather broad features. Here we introduce a new approach, which enables resolution of their structure [1]. It is based on the use of helical symmetries allowing one to consider the smallest unit cell followed by semi-empirical energy minimization leading to a reduction of the number of structural parameters to be fitted.

We applied this method to recently synthesized methylated alumino-silicate and alumino-germanate imogolite nanotubes of nominal composition $(OH)_3Al_2O_3Si(Ge)CH_3$ [2]. Thanks to their chemical versatility, imogolite nanotubes (INT) are promising candidates for applications in molecular storage, recognition and separation [3]. Fit of wide-angle X-ray scattering (WAXS) diagrams of methylated INTs enabled us to determine their atomic structure. Unlike their (N,0) zigzag hydroxylated analog, methylated INTs roll up into a (N,N) armchair structure (Figure).

The authors acknowledge Erik Elkaim from beamline CRISTAL, where WAXS diagrams were recorded.

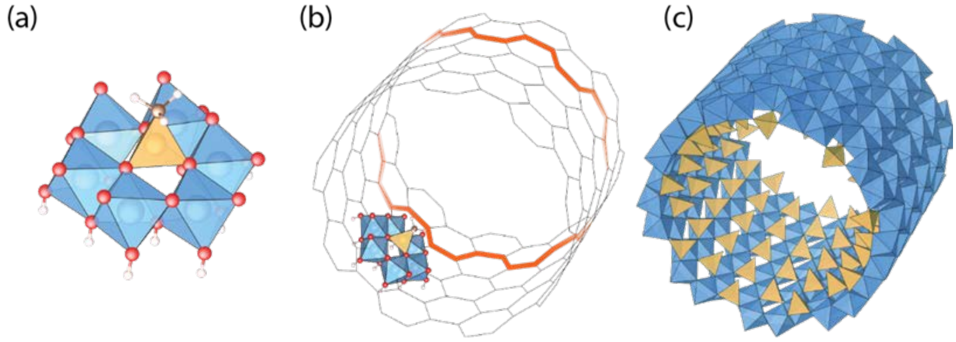

Figure: (a) An-octahedral gibbsite-like layer (in blue) with isolated $(Si(Ge)O_3)CH_3$ tetrahedron units (in yellow). (b) and (c) The methylated INT structure. Its armchair character is highlighted by the thick orange line in (b).

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Origin of the Low Value Onset Potential in Nanostructured Hematite Photoanodes

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ABSTRACT

Solar-to-hydrogen conversion offers a clean, viable and sustainable approach for hydrogen production, replacing at long term the use of fossil fuels[1]. Semiconducting oxide photoanodes can be employed in photo-electrolysis cells to efficiently drive the water splitting reaction[2]. Under sunlight radiation, electron-hole pairs are created at the photoanode: the holes participate in the oxidation reaction, while electrons from the cathode are involved in the reduction reaction. In such systems the hydrogen production is generally quantified through the measured photocurrent generated under sunlight illumination upon applying an external voltage. Another parameter, the onset potential, which is the minimum voltage necessary to generate non-zero photocurrent, is directly related to the gain from solar energy conversion relative to standard electrolysis. This onset potential has a value of 1.6 V for simple electrolysis using two Pt electrodes, but reaches values as low as 0.6 V in the present study. Hematite photoanodes were fabricated using aqueous chemical growth[3], a simple method for generating films composed of organized nanostructures. Film thickness and morphology are tuned by adjusting the aqueous solution pH, which in turn controls the photo-electrochemical activity, the photocurrent density and the quantum efficiency. Low onset potential values characterize all our samples. We relate these low values to the Brønsted acidification of the photoanode, arising from the presence of a proton rich phase. Soft X-ray Scanning Transmission X-ray Microscopy (STXM) at the Soleil HERMES beamline was used to characterize the hematite photoanode. An additional hexahydrated iron chloride ($FeCl_3.6H_2O$) phase was identified. Fitting STXM 3D datasets (X, Y, photon energy) with reference spectra recorded from commercial hematite and the $FeCl_3.6H_2O$ used as a precursor for aqueous growth, results in quantitative chemical speciation maps where spatial distribution of both phases (hematite and precursor) is clearly established.

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The Formation of Catalytically Active Interfacial Pt-NiO_{1-x} Nanostructures on $Pt_3Ni(111)$ under CO Oxidation Reaction

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ABSTRACT

In the research of surface catalysis, the interaction between metal and metal oxides plays critical role in catalytic reaction. Especially, the role of interfacial states of strong metal-support interaction has been investigated for many years. In this presentation, with the combination of ambient pressure STM and ambient XPS, we unveiled the presence of catalytically active interfacial Pt-NiO_{1-x} nanostructures during *operando* condition. Under elevated pressure of oxygen, NiO_{1-x} clusters segregates to the surface of Pt-skin surface layer on $Pt_3Ni(111)$. Under CO oxidation condition, the coexistence of NiO_{1-x} clusters on the Pt skin is observed. DFT calculation of $Pt_3Ni(111)$ also support that a CO molecule adsorbed on Pt-NiO_{1-x} nanostructures has a lower surface energy barrier than Pt surface.

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An Insider View on Pressure Induced Amorphisation of Molecular Crystals

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ABSTRACT

Pressure induced amorphisation (PIA) has been observed in various materials, but the mechanism of the order-disorder transition can differ. It can imply coordination change, like in GeO2 [1] or in nano-anatase [2] (nTiO2).

AX4 molecular compounds where A= Sn or Ge and I = Cl, Br, I exhibit also reversible PIA [3,4], accompanied by metallization as for GeI4 and SnI4. The mechanism proposed to explain the phase transformation is a charge transfer from intramolecular bonds (Sn-I) to intermolecular bonds (I-I). At ambient pressure, these compounds crystallize in a cubic structure with SnI4 molecules interacting through Van der Waals forces. At high pressure, charge transfer leads to the creation of Sn-I-I-Sn-I chains [5] and conductivity increases. Such mechanism can effectively explain the amorphisation and the metallization, but it has not been fully demonstrated.

Previous studies employed mostly X-ray scattering to determine the structure. Now, thanks to the advent of nano polycrystalline diamonds [6,7], we are able to combine EXAFS and XRD at high energies up to 27GPa; we applied recent advances in Reverse Monte Carlo [8] EXAFS analysis to obtain a more comprehensive picture than traditional analysis.

XRD data indicate a progressive amorphisation that takes place above 15 GPa. EXAFS reveals a more complex picture where Sn-I compression is followed by expansion and splitting in two sub shells well before amorphisation. I atoms of different SnI4 tetrahedrons quickly approach and between 10 and 15 GPa we observe the formation of I-I bonds by the elongation of Sn-I distance and a redistribution of the number of intra and intermolecular I-I bonds. Sn-I and I-I distances remain different even after complete amorphisation that occurs above 22.6 GPa. GeI4 shows a similar behavior, but with some peculiarities that could be related to the greater strength of the shorter Ge-I bond.

Our results are in agreement with the percolation model of Pasternak and Taylor [4], and provide a new understanding on this process of amorphisation. We clearly evidence the deformations of the high pressure structures before and after amorphisation.

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Influence of Applied Pressure on the Structural and Magnetic Properties of $Y_{1-x}Tb_xFe_2D_y$ Compounds

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ABSTRACT

The magnetocaloric effect (MCE) can be used for various applications ranging from adiabatic demagnetization at very low temperatures to magnetic refrigeration near room temperature. Much work has been done in recent decades to develop new magnetocaloric materials suitable for these applications as well as systems operating on a magnetic heat pump principle [1]. The RCo_2 and RNi_2 Laves phases exhibit intense MCE at low temperatures, which decrease relatively quickly when the temperature increases [2]. Cubic RFe_2 are ferrimagnet with Curie temperatures ranging from 540 to 730 K and have a low MCE around T_C. Hydrogen insertion induce a cell volume increase, a lowering of crystal symmetry and of the Curie temperature. For an H(D) content near 4.2 H(D)/f.u. monoclinic distortions accompanied by various metamagnetic transitions are observed [3,4]. These magnetic transitions are attributed to a weakening of the *R*-Fe interactions and an instability of the Fe moment due to large H content. A large MCE effect has been found near a ferrimagnetic-antiferromagnetic transition (F-AF) which temperature T_{F-AF} depends on the nature of the *R* element and H isotope [5].

In order to determine the influence of the structural changes on the magnetic and magnetocaloric properties of these compounds we have studied $Y_{1-x}Tb_xFe_2(H,D_y$ compounds using complementary methods such as high magnetic field, neutron diffraction and XMCD. As T_{F-AF} is very sensitive to the volume changes induced by the Tb substitution and (H,D) isotope effect, we have also followed these variations by applying an external pressure. The structural changes were followed by X ray diffraction under pressure (PSICHE beam-line) for x=0 and 0.5. The influence of the pressure on the magnetic properties was followed by magnetic and XMCD measurements (ODE beam line). These results will be presented and discussed in order clarify the critical parameters for both fundamental understanding and magnetocaloric application.

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Water/Ammonia Ice Mixtures under High Pressure and Temperature

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ABSTRACT

Water and ammonia are major components of the interior of giant icy planets such as Neptune and Uranus, where they are submitted to a wide range of pressure and temperature conditions. Studying the mixtures of these ices under high P-T conditions is therefore required to model the inner structure of these planets. Unlike for pure ices, the properties of binary mixtures remain to date widely unknown at high density. Three types of exotic phases have been observed in the pure ices, namely the symmetric phase of water ice [1], the ionic phase of ammonia [2, 3] and the superionic phase for both ices [4, 5]. These exotic states could be reached under more moderate conditions in the mixed ices. Indeed, we recently observed a partially ionized state in ammonia monohydrate at a pressure ten times lower than the molecular-ionic transition in pure ammonia [6].

This presentation will report on our experimental investigations of two different ammonia/water compounds, ammonia hemihydrate $H_2O(NH_3)_2$ and ammonia dihydrate $(H_2O)_2NH_3$ under high P-T conditions. Using synchrotron x-ray diffraction and Raman spectroscopy up to 30 GPa and 700 K, we have discovered several new phases of these compounds and mapped their phase diagrams. In particular, we have observed a simple body-centered cubic phase stable at high pressures and temperatures which is a good candidate for a superionic conductor.

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X-ray Diffraction and Cultural Heritage Materials – Adaptive Crystallography

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ABSTRACT

Cultural Heritage materials are often complex and heterogeneous materials with a multi-scale architecture. Several phases of different crystalline forms in a wide grain size distribution co-exist, each of these phases keeping in their long-range and/or short-range structural arrangement a memory of the transformations that occurred to the material. In addition, global position/dispersion of these phases in the material is also closely related to its properties (optical, mechanical, …), its manufacturing process, functionality or long-term conservation. X-ray diffraction methods are often the methods of choice to perform advanced structural analyses. By mapping the material with a micron-sized beam and combining several X-ray diffraction modes (Laue and monochromatic), it becomes possible to retrieve 2-dimensional and 3-dimensional structural information, with single-crystal/powder amorphous/crystalline phases taken into account. This is going to be illustrated through the study of galena-based and carbon-based black pigments used in Ancient Egypt in cosmetics and ink. Under heating, an oxidation layer emerges at the surface of galena single crystals, and this effect has been monitored in situ by switching between Laue and monochromatic diffraction modes. On the other hand, carbon-based pigments used in the preparation of inks are mostly amorphous. A diffraction-tomography experiment has been carried out on papyrus fragments, and the signal from both crystalline and amorphous phases extracted. If our first motivation is to gain insight into the manufacturing process of black pigments in ancient time, Cultural Heritage materials, because of their intrinsic heterogeneity, are often good candidates for pushing towards special developments, which can benefit to other area of materials science.

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Cartographie 3D par Micro-diffraction Laue

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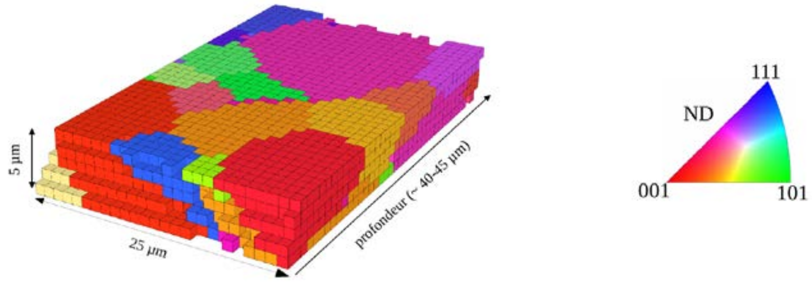
ABSTRACT

La micro-diffraction Laue est une technique établie de caractérisation des microstructures basée sur la diffraction sur monocristal en faisceau blanc et résolue spatiallement [1]. Utilisant un faisceau X synchrotron polychromatique micro-focalisé, elle permet de cartographier les champs d'orientations et de déformations élastiques, ainsi qu'étudier les défauts liés à la plasticité avec une résolution spatiale de plusieurs 100 nm et une résolution angulaire pouvant atteindre 10^{-4}.



Cartographie d'orientation de la microstrucure par microscopie 3D Laue de zircone yttriée polycristalline (electrolyte SOFC). Les couleurs correspondent aux orientations cristallines en figure de pôle inverse. Dans chaque voxel (1x1x1 μm^3) sont déterminés l'orientation et les paramètres structuraux cristallins.

L'analyse standard des diagrammes de Laue fournit une information de surface moyennée sur toute la longueur de pénétration du faisceau. La microscopie 3D par micro-diffraction Laue, ou « Differential Aperture X-Ray Microscopy » [2], permet de résoudre en profondeur l'analyse des microstructures, avec une résolution submicrométrique. Plusieurs centaines de clichés sont mesurées à différentes positions d'un fil absorbant (e.g, en tungstène) placé entre l'échantillon et le détecteur, et pouvant masquer graduellement l'intensité diffracté. Par triangulation, l'intensité diffractée par n'importe quels plans cristallin en profondeur peut être reconstruite.

Un tel outil d'imagerie 3D est aujourd'hui accessible aux utilisateurs de la ligne CRG-IF BM32 à l'ESRF, suite notamment à l'apport de nombreuses améliorations aux méthodes de calibration et de reconstruction, au développement d'un logiciel destiné au traitement des données, ainsi qu'à la récente acquisition d'une caméra rapide. Dans cette présentation, nous décrivons ces diverses avancées et les illustrons au travers de quelques exemples d'application.

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Synchrotron Based THZ Spectroscopy to Probe Magneto-electric Effects in Multiferroics

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ABSTRACT

Electromagnetic waves are particularity well suited to probe characteristic excitations associated to both magnetic and electric orders as for instance in multiferroics where they lie in the THz range. Since the magnetic response is several orders of magnitude smaller than the electric response, an intense and stable source is required that is available on the AILES beam line at SOLEIL. We have studied hexagonal manganites $RMnO_3$ with R=Er, and Ho. In these multiferroics, ferroelectricity and magnetic orders are quite decoupled: ferroelectricity occurs at much high temperature ($T_C \approx 800K$) than the ordering of the Mn magnetic moments ($T_N \approx 80K$). Despite these different energy scales, non-negligible coupling between the electric and magnetic degrees of freedom are present, in their static as well as dynamical properties. In this study, we report on the THz dynamical properties of these two compounds and bring new insight on the coupling effects between the 3d (Mn) and 4f elements (R) that lead to new form of elecromagnons [1] as well as hybridized R-Mn magnetic excitations [2].

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XMCD Spectroscopy at Ultra-low Temperature on DEIMOS Beamline (Synchrotron SOLEIL)

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ABSTRACT

X-ray magnetic circular dichroism (XMCD) spectroscopy is a very powerful technique which characterizes the magnetic properties of advanced materials. XMCD is based on X-ray absorption spectroscopy (XAS) which allows measurements with element selectivity and high sensitivity. It is thus most adapted to the studies of the magnetic properties of very diluted system such as Single Molecular Magnets (SMM) isolated on surface.

The DEIMOS beamline is a soft X-ray beamline located at Synchrotron SOLEIL and dedicated to the study of magnetic and electronic properties of samples. Recently a new cooling system based on ^{3}He-^{4}He dilution principle has been installed in the Cryo-magnet of the DEIMOS beamline allowing for XMCD measurements from room temperature down to 180 millikelvins.

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PARALLEL SESSION

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

CENTRALE-SUPELEC-GIF-SUR-YVETTE - MICHELIN AUDITORIUM #2

Thursday, January 17th

Chairpersons:

Jean-Sébastien Girardon, Nicolas Delsuc, Vincent Boudon and Renaud Guillemin

IT-04	Correlative X-ray fluorescence nano-imaging and optical microscopy to investigate chemical element compartmentalization in cells ***R. Ortega***
OC-13	Irradiation of water ice in the O 1s region : Spectral and kinetic energy signatures of photodesorbed species ***G. Féraud***
OC-14	Progress around the high resolution heterodyne spectrometer of the AILES beamline ***S. Eliet***
OC-15	State-selected ion-molecule reactions with VUV Synchrotron Radiation: The O_2^+ + C_3H_6 case ***C. Alcaraz***
IT-05	High resolution spectrometry at the AILES beamline ***J. Vander Auwera***
OC-16	High-resolution analysis of the 12.6 µm absorption of the nitryl chloride $ClNO_2$ molecule ***A. Anantharajah***
OC-17	Role of hydrogen absorption in supported Pd nanocatalysts during CO-PROX: Insights from operando X-ray absorption spectroscopy ***C. Zlotea***
OC-18	Photoionization and dissociative photoionization of propynal in the gas phase: Theory and experiment ***I. Derbali***

PARALLEL SESSION

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

CENTRALE-SUPELEC-GIF-SUR-YVETTE - MICHELIN AUDITORIUM $^{\#}$2

Friday, January 18th

Chairpersons:

Jean-Sébastien Girardon, Nicolas Delsuc, Vincent Boudon and Renaud Guillemin

OC-19	Line positions and intensities in the ν_2 band of sulfuryl fluoride using the C_{2v} Top Data System (C_{2v}TDS) ***M. Rotger***
OC-20	In-situ XRD analysis of transient liquid assisted growth of $YBa_2Cu_3O_7$ superconducting films ***J. Banchewski***
OC-21	First high resolution measurement and analysis of the 83.3 µm absorption of the chlorine nitrate $ClONO_2$ molecule ***F. Kwabia Tchana***
IT-06	Surface chemistry of colloidal surfactant-free gold nanoparticles generated by laser ablation ***A. Levy***
OC-22	Double inner-shell vacancies in molecules ***D. Koulentianos***
OC-23	The investigation of the ν_8 & ν_{21} bands of propane $CH_3CH_2CH_3$ at 11.5 & 10.9 µm: Evidence of large amplitude tunnelling effects ***A.Perrin***
OC-24	Characterization of two-photon entanglement resulting from VUV photodissociation of H_2 ***B. Fabre***

Correlative X-ray Fluorescence Nano-imaging and Optical Microscopy to Investigate Chemical Element Compartmentalization in Cells

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ABSTRACT

Synchrotron X-ray fluorescence imaging holds the potential for fundamental breakthroughs in the understanding of biological systems because chemical element distributions can be evidenced at the sub-cellular level. What is the distribution of trace metals in cells? Do some elements accumulate within sub-cellular organelles? What is the local chemistry of the elements in these organelles? These are some of the fundamental questions that can be addressed using synchrotron radiation X-ray nano-probes. Such direct detection of chemical elements in single cells, and their speciation analysis, is a challenging task that requires sophisticated analytical developments. Improvements to obtain submicron X-ray beam sizes have been made in the last few years allowing chemical imaging at high lateral resolution. SR-XRF (Synchrotron Radiation X-ray Fluorescence) with hard X-ray beams can now provide chemical element imaging with less than 30 nm spatial resolution. Moreover, synchrotron radiation offers the unique capability of spatially resolved chemical speciation using micro-XAS (X-ray Absorption Spectroscopy). In order to localize precisely the distribution of the elements within the cell organelles, their identification is prerequisite and fluorescence labeling is a tool of choice. As this will be discussed, this approach imposes some limitations for sample preparation. Organelle localization can however be performed using various specific fluorescent dyes or fluorescent proteins, on living cells prior to cryogenic fixation allowing the preservation of element distribution [1-2]. The potential of these methods for biomedical investigations will be illustrated with examples of application in the field of neurosciences [3-4].

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Irradiation of Water Ice in the O 1s Region : Spectral and Kinetic Energy Signatures of Photodesorbed Species

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ABSTRACT

In the colder parts of the interstellar medium, dust grains are covered with molecular ices, whose major component is water. They act as the main molecular reservoir of these regions and are therefore of high interest in astrochemistry. Among many radiative processes that occur into these icy mantles, the ones induced by X-rays may play an important role, for example in protoplanetary disks [1], but their effects remain poorly known. In particular, they can release molecules or radicals into the gas phase, by so-called photodesorption processes, and thus have an important role in the gas-to-ice abundance ratio measured by the most recent radiotelescopes. Besides this astrophysical context, X-ray induced desorption can also bring useful information on the physico-chemical properties of water ice, for example regarding the structure of the ice surface [2].

We irradiated H_2O ices between 520 and 600 eV using the SPICES 2 set-up connected to the SEXTANTS beamline. Following O 1s core excitation or ionisation, photodesorption of many species are detected and the efficiency of the photodesorption for each species is quantified. Neutral species are the most abundant, whereas positive or negative ions are much weaker [3]. The comparison between photodesorption spectra, *ie* the intensity of photodesorbed species as a function of the excitation energy, and absorption spectra measured in-situ gives information on the various processes involved in the photodesorption (Fig.1). Secondary electrons produced in the ice mainly lead to desorption of neutral molecules, whereas the dissociation of H_2O ejects protons for example. Measurement of the kinetic energy of desorbed ions gives valuable insights on the photodesorption processes but also on the ice structure at the surface.

All these data show the complexity of processes linked to core excitations, and the richness of information that can be retrieved, from chemical to structural ones, for physical-chemistry or astrophysical studies.

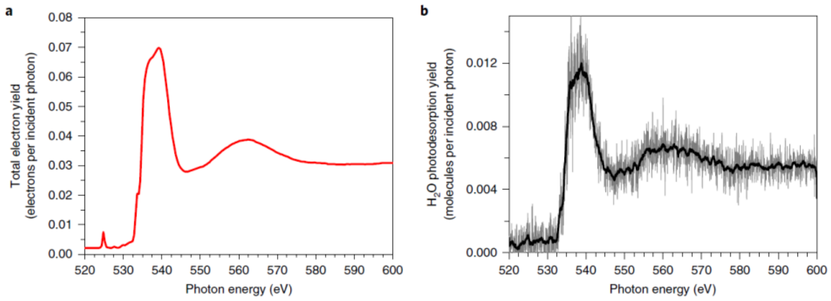

Figure 1 ***a.*** *Absorption of an amorphous H_2O ice at 15 K*

b. *Photodesorption of H_2O [3]*

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Progress around the High Resolution Heterodyne Spectrometer of the AILES Beamline

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ABSTRACT

Far infrared beamlines around the world exploiting the brightness of the synchrotron radiation for high resolution investigations are exclusively using Fourier-transform spectrometers, usually Bruker IFS 125 instruments, which exhibit a nominal resolution of about 30 MHz (0.001 cm^{-1}) limited by the mechanical path difference. Although "high" by standard definition, this resolution is the limiting factor in the gas phase investigation of many molecules as it is larger than their natural linewidth in many studies.

To overcome such purely instrumental limitation and exploit the far-infrared synchrotron radiation at its full capacity, the HEROES consortium is currently developing a new spectrometer on the AILES beamline at SOLEIL allowing to achieve a sub-MHz resolution [1]. This spectrometer is based on the heterodyne detection technique for which the synchrotron radiation extracted by the AILES beamline is mixed with a bright local oscillator in the terahertz domain. The principle of the spectrometer, together with the first experimental results, will be presented.

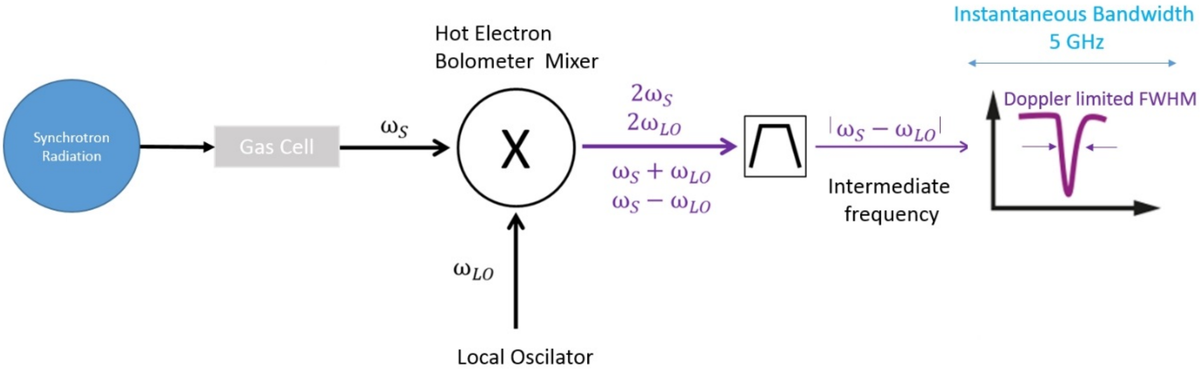

Figure 1. Principle of the heterodyne detection of the synchrotron radiation mixed with a local oscillator

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State-selected Ion-molecule Reactions with VUV Synchrotron Radiation : The O_2^+ + C_3H_6 Case

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ABSTRACT

In this contribution, we will present recent results on state-selected ion-molecule reactions obtained with the CERISES set-up: a guided ion-beam experiment [1]. In these experiments, the photoionization of a neutral precursor by VUV synchrotron radiation from the DESIRS beamline [2] and the TPEPICO technique are used to prepare state-selected cations before reaction. Absolute reaction cross sections are measured as a function of the cation excitation and collision energy.

Recent developments of the setup allow for the production of new types of neutral precursors such as hydrocarbon radicals ($C_xH_y^\bullet$) and clusters (A_n) opening the possibility of new studies on the reactivity of their cations, $[C_xH_y^\bullet]^+$ and $[A_n]^+$, which include the comparison of the reactivity of different isomers or the effect of solvatation on the reactivity of cations. This enhances the offer on the chemistry of ions to external users of SOLEIL who can apply for beamtime with the CERISES setup through an association between our team and SOLEIL.

The measurements that will be presented here are needed to refine the description of reactive astrophysical or industrial plasmas. The present results were recorded at SOLEIL synchrotron in spring 2018 in the framework of a collaborative project aiming at a better description and optimization of industrial plasmas used for depollution of factory exhaust. To this end, the chemistry of ionic form of the major atmospheric species with main industrial pollutants has to be described.

Here, molecular oxygen, O_2, has been used to produce O_2^+ molecular ions by photoionization. By means of TPEPICO coincidence methods and using the 1-bunch mode of operation of SOLEIL, they were prepared in selected, long-lived vibrational and electronic states ($X^2\Pi_g$, v=0-15 and $a^4\Pi_u$, v=0-4). Their reactivity with the propene molecule (CH_2=CH-CH_3) has been studied by varying the excitation energy and the collision energy and recording the absolute reaction cross sections for all ionic products.

Very contrasted results have been obtained, and, though they can be described in terms of charge transfer and dissociative charge transfer, specific sensitivity to the ionic state as well as to the collision energy has been observed, and will be discussed.

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High Resolution Spectrometry at the AILES Beamline

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ABSTRACT

Molecular lines observed in high resolution far infrared spectra are associated with pure rotation transitions or belong to low-energy vibrational bands. Together with other parameters characterizing them, the intensities and broadening coefficients of these lines are required for example to determine the physical and chemical properties of planetary atmospheres, to monitor the operation of industrial facilities using optical remote sensing techniques or to gain insight into the physics of the studied molecules or intermolecular interactions. These spectroscopic parameters are measured in the laboratory.

This lecture will deal with the measurement of the intensities and broadening coefficients of molecular lines observed in high resolution far infrared absorption spectra. It will focus on high resolution Fourier transform spectroscopy associated with synchrotron radiation carried out at the AILES beamline of SOLEIL. Taking advantage of the high brightness and highly collimated nature of synchrotron radiation, which are big advantages at low energies over conventional sources [1], the AILES beamline can indeed provide high signal-to-noise ratio, high resolution spectra of very weak molecular absorptions. The lecture will present and discuss some recent [2-6] and ongoing measurements carried out relying on high resolution absorption spectra recorded at the AILES beamline, highlighting some aspects specific to these retrievals.

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High-resolution Analysis of the 12.6 µm Absorption of the Nitryl Chloride $ClNO_2$ Molecule

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ABSTRACT

Nitryl chloride ($ClNO_2$) is a molecule of great interest for atmospheric chemistry since it is produced by heterogeneous reactions, in the marine troposphere, between NaCl sea-salt aerosols and gaseous N_2O_5 [1,2], and on polar stratospheric clouds, between N_2O_5 and solid HCl [3,4].

Despite its atmospheric importance and to the best of our knowledge, there is no tentative detection of $ClNO_2$ using infrared techniques. Due to their sharp *Q* branches falling into an atmospheric "window", the detection of the ν_2 bands might be an advantageous route for future attempts to detect atmospheric $ClNO_2$.

For this purpose, the 12.6 µm region of $ClNO_2$ has been recorded at high resolution (0.00102 cm^{-1}) using a Fourier transform spectrometer and the SOLEIL synchrotron light source. $ClNO_2$ was found during our studies of chlorine nitrate and, after fractional distillation at –77°C was introduced into a multipass White cell made of inert materials, with an optical path length of 5.4 m. 320 scans were recorded for the range 715-850 cm^{-1} at a total pressure of 0.23 mbar and a temperature of 250 K.

A thorough analysis of the ν_2, $2\nu_6$ and $2\nu_3$ bands of $^{35}ClNO_2$ and of the ν_2 band of $^{37}ClNO_2$ which fall in this region, has been carried out using a Hamiltonian model which takes explicitly into account the numerous resonances affecting the ro-vibrational energy levels; especially the C-type Coriolis resonance between the mode ν_2 and the mode $\nu_3 + \nu_6$. These two modes are only separated by less than 20 cm^{-1} and they are thoroughly mixed.

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Role of Hydrogen Absorption in Supported Pd Nanocatalysts during CO-PROX: Insights from *operando* X-ray Absorption Spectroscopy

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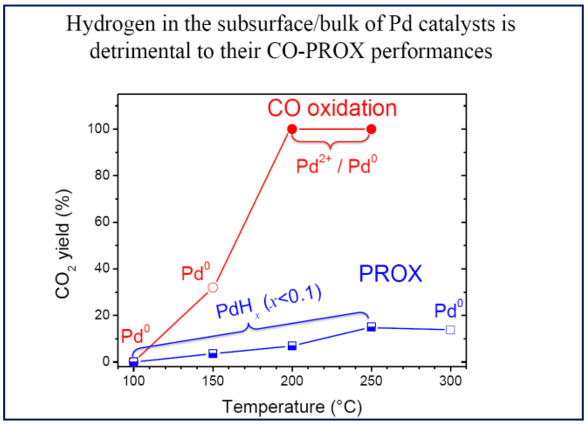
ABSTRACT

The nature of the active phase (metallic *vs.* oxidic, metal phase *vs.* concentrated hydride/ diluted solid solution with hydrogen) in heterogeneous catalysis by supported metals is still a matter of high debate.[1] Here, we have monitored for the first time oxide-supported Pd nanocatalysts (average particle size 4.5 nm) during both CO oxidation (in H_2-free atmosphere) and preferential oxidation of CO in H_2 excess (PROX) by *operando* X-ray absorption spectroscopy (Rock beamline at Soleil). Under our conditions, the CO conversion in the absence of H_2 is around 30% at 150 °C and reaches 100% at 200 °C, whereas in the presence of H_2 the conversion reaches a maximum of 15% (at 250 °C), in agreement with our previous works using a conventional flow-fixed bed reactor.[2] The active phase for CO oxidation below 200 °C is metallic Pd, whereas it is a solid solution of Pd with hydrogen during PROX below 300 °C (Figure). This presentation will clarify the role of hydrogen in supported Pd catalysts during the PROX reaction.[3]



Hydrogen in the subsurface/bulk of Pd catalysts is detrimental to their CO-PROX performances

Figure: CO_2 yield during CO oxidation and PROX over Pd/ASA, as measured by MS during XAS experiments. Empty, half-filled and full symbols stand for metallic Pd, solid solution PdH_x ($x < 0.1$) and mixed Pd^{2+}/Pd^0 species, respectively, as determined from EXAFS refinements.

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Photoionization and Dissociative Photoionization of Propynal in the Gas Phase: Theory and Experiment

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ABSTRACT

Propynal, as well as some of its isomers and fragments have been detected in the interstellar medium in several objects.[1] In addition laboratory experiments have shown that propynal can be formed on interstellar ice analogues.[2] In order to further understand the observed abundances and chemical reactions that may take place in these dilute media, investigations on the single photon ionization of the propynal molecule in the gas-phase, in the 10.00-15.75 eV energy range, are particularly relevant. Experiments have been carried out using the DELICIOUS3 spectrometer,[3] in connection with the DESIRS beamline at SOLEIL. Mass spectra, PEPICO and TPEPICO spectra have been interpreted using ab-initio and DFT calculations similar to those presented in ref.[4] The fragmentation mechanisms of the $H_2C_3O^+$ parent cation have been also studied. The calculated appearance energies of all the fragments are in excellent agreement with the experimental findings. The theoretical characterization of the electronic excited states was used to interpret the TPEPICO spectra. The present results will be useful to interpret astrophysical abundances of propynal and its cation in the various interstellar environments where it is observed.

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Line Positions and Intensities in the ν_2 Band of Sulfuryl Fluoride using the C_{2v} Top Data System (C_{2v}TDS)

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ABSTRACT

Sulfuryl fluoride (SO_2F_2) is a widely used insecticide and an atmospheric pollutant. It is also of a fundamental interest due to its nearly tetrahedral symmetry, making it, thereby, an intermediate case between spherical and asymmetric-top molecules. For this reason, an oriented tensorial formalism adapted to almost tetraheral XY_2Z_2 asymmetric top with C_{2v} symmetry has been developped [1].

A new high-resolution infrared spectrum of the ν_2 band of SO_2F_2 centered at 849.4 cm^{-1} has been recorded with a resolution of 0.00102 cm^{-1} at the AILES beam line of SOLEIL Synchrotron facility. A global frequency and intensity analysis was carried out. Analysis has been performed in the $O(3) \supset T_d \supset C_{2v}$ group chain thanks to the C_{2v}TDS program suite [2].

A total of 2407 line positions and 72 line intensities have been assigned and fitted with global root mean square deviation RMS of 0.19×10^{-3} cm^{-1} and 2.98 %, respectively.

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In-situ XRD Analysis of Transient Liquid Assisted Growth of $YBa_2Cu_3O_7$ Superconducting Films

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ABSTRACT

To date, a broad commercial market of applications based on High Temperature Superconductivity (HTS) is kept from emerging due to the high manufacturing costs of superconducting tapes, also referred to as Coated Conductors (CCs) [1]. Performance-wise, such tapes reach remarkable current values of 400 A at 77 K in 1 cm width, however, the fabrication throughput and cost-effectiveness is limited by small growth rates of the superconducting layer in the order of ~1-5 nm/s [2]. To address this challenge, we are developing a novel growth approach, entitled Transient Liquid Assisted Growth (TLAG), which combines the technological feasibility and upgradability of Chemical Solution Deposition (a low-cost technique consisting of metalorganic layer deposition, pyrolysis and superconducting phase crystallization at elevated temperatures) with ultrahigh growth rates of liquid-mediated techniques. Through experiments realized at Soleil we have been able to demonstrate growth rates of 100 nm/s which, in turn, has drawn much attention of the applied superconductivity field towards this new prosess.

In this presentation, we introduce *in-situ* growth experiments implemented and performed in two consecutive years at the DiffAbs beamline, synchrotron Soleil. In particular, we want to share our experience on how a precise control of growth parameters (total pressures, PO_2 partial pressures, temperatures, heating ramps, etc.), XRD imaging with a time resolution of 100ms and sophisticated data handling allowed us to explore complex nucleation processes, to follow intermediate phase reactions and to demonstrate ultrahigh growth rates up to 100 nm/s. Thin epitaxial layers of 300-500 nm are grown with an Anton-Paar DHS1100 heating stage. Hard x-ray photons of 18keV in combination with a 2D area pixel detector are used to follow all process reactions in two different geometries: Gracing incidence diffraction for initial precursor and intermediate phases and ω-2θ geometry for the epitaxial, superconducting phase. We will conclude with a brief summary on the relevance of the novel process and motivate possible experiments and upgrades in the near future.

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First High Resolution Measurement and Analysis of the 83.3 µm Absorption of the Chlorine Nitrate $ClONO_2$ Molecule

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ABSTRACT

Chlorine nitrate ($ClONO_2$) is a very important atmospheric “reservoir” of ClO and NO_2, destroying stratospheric ozone through catalytic cycles [1, 2]. It was detected for the first time by IR spectroscopy [3], a detection confirmed by MIPAS and the ATMOS experiment [4]. However, the measurements have permitted to confirm the poor quality of the spectroscopic database, particularly for the 12.8 µm region. An accurate restitution of its vertical profile was not possible [5, 6] due to the lack of absolute intensities and the numerous non-modelled hot bands.

Many high-resolution spectroscopic studies in the microwave and mid-infrared regions are available [7 and therein]. However, chlorine nitrate present four fundamentals in the far-infrared region below 600 cm^{-1}, with the lowest which corresponds to the torsional mode, ν_9 around 83.3 µm. Two previous studies deal with the $v_9 = 1$ state of $ClONO_2$. This torsional band exhibiting at least 7 peaks has been observed at low resolution (0.3 cm^{-1}), near 120 cm^{-1} by Fleming in 1977 [8] and was reexamined at 0.06 cm^{-1} resolution (showing a single, regularly spaced series of Q branches) by Chance and Traub in 1982 [9] without any precise determination of the band center. More recently, the analysis of the mid-infrared ν_8 and $\nu_8 + \nu_9$ band spectral regions of $^{35}ClONO_2$ lead to an indirect determination of the ν_9 band center at 123.7219 (20) [10].

In this work, the 83.3 µm region of $ClONO_2$ has been recorded at high resolution (0.001 cm^{-1}) using a Fourier transform spectrometer and the SOLEIL synchrotron light source. Spectrum analysis is ongoing and will determine the molecular parameters of this spectral region. In turn, this will enable an analysis of the hot bands involving low energy levels in the mid-infrared region.

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Surface Chemistry of Colloidal Surfactant-free Gold Nanoparticles Generated by Laser Ablation

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ABSTRACT

A promising nanoparticle synthesis technique widely developed in the past few years is based on laser irradiation of a solid target in a liquid environment. The Pulsed Laser Ablation in Liquids (PLAL) method results in the formation of ligand-free nanoparticles. These bare nanoparticles in organic or non-organic solvents are well-suited for the development of different technological applications[1] usually requiring subsequent surface functionalization, which can be subsequently tailored on bare particles. In addition, the surface chemical composition of these nanoparticles is expected to take part in the colloidal stability of the PLAL product. The resulting surface charge could be responsible of the electrostatic repulsion impeding their aggregation. However, no consensus[2-6] has been drawn so far on these questions and thus a precise knowledge of their surface properties and composition is mandatory. An experimental investigation of the surface chemistry occurring at the PLAL nanoparticle surface will be presented based on experiments conducted at SOLEIL synchrotron facility on the PLEIADES beamline. X-ray photoelectron spectroscopy measurements performed on free-standing[7,8] gold nanoparticles will be reported addressing the question of (i) their surface oxidation state and (ii) the chemical composition of their first's surface atomic layers. Signatures of halide-ions and possible gold oxidized atoms on the nanoparticle surface have been evidenced, demonstrating that this technique provides a promising new way to study bare gold surfaces and a complementary insight to colloidal stability.

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Double Inner-shell Vacancies in Molecules

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ABSTRACT

Electronic states of matter, where both 1s electrons have been simultaneously ejected to the continuum[1,2], referred as double-core-hole (DCH) continuum states, attract great scientific interest due to the unique properties they posses, as discussed more than thirty years ago by Cederbaum *et al.*[3] More specifically for the case of molecules, $1s^{-2}$ DCH states, where both vacancies have been created on the same atomic site, known as single-site (ss) DCH states, will exhibit great orbital relaxation effects, whilst creation of the vacancies in two different atomic sites, referred as two-site (ts) DCH states and noted as $1s^{-1}1s^{-1}$, will result in increased chemical shifts allowing for a detailed probe of the chemical environment of an atom in a molecule. The formation of DCH states through a core-ionization core-excitation mechanism, referred as DCH pre-edge states and noted as $1s^{-2}V$, with V referring to the molecular orbital where the excited electron has been promoted to, has been discussed by Carniato *et al.*[4,5] and can lead to final states of different symmetries, forbidden in conventional $1s^{-1}$ or $1s^{-1}V$ spectroscopies. Since their initial description, several works concerning the formation of DCH pre-edge states in atoms and molecules have been published[6,7,8].

The experimental observation of $1s^{-2}V$, $1s^{-1}(2s,2p)^{-1}V$, as well as $1s^{-1}1s^{-1}V$ pre-edge states, has been achieved by our group using the Hard X-ray Photoelectron Spectroscopy (HAXPES) endstation of the GALAXIES beamline at SOLEIL Synchrotron[9,10]. In particular, the formation of $1s^{-1}2p^{-1}(^{1,3}P)V$ and $1s^{-1}2s^{-1}(^{1,3}S)V$ DCH states in HCl[11] has been observed and the related spectral features have been interpreted based on a fit model, taking into account Rydberg series within the different spin-orbit terms and the results from *ab initio* quantum chemical calculations. From the experimental data the different double ionization thresholds have been extrapolated and the values of quantum defects have been estimated. Furthermore, photoelectron spectra showing the formation of $1s^{-2}V$ DCH states of CH_3CN[12] have been measured and the experimental spectra have been simulated by high-level *ab initio* calculations considering the direct (dipolar ionization-monopolar excitation) and conjugate (monopolar ionization-dipolar excitation) nature of each transition. In addition, the different processes contributing to the chemical shift between the two non-equivalent carbon atoms have also been explored. The formation of $1s^{-2}V$ states at the O site of CO has also been observed and the experimental data are currently analysed[13].

Regarding the ts-DCH pre-edge states of the form $1s^{-1}1s^{-1}V$, such states have unambiguously been recorded for the first time for N_2 and CO molecules and will be the subject of a forthcoming publication[14].

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The Investigation of the ν_8 & ν_{21} Bands of Propane $CH_3CH_2CH_3$ at 11.5 & 10.9 µm: Evidence of Large Amplitude Tunnelling Effects

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ABSTRACT

We present detailed investigations of the ν_8 band (C-C symmetric stretch at 870 cm^{-1}), and ν_{21} band (CH_3 rock at 921 cm^{-1}) of propane (C_3H_8). For this analysis we used a high resolution (0.0015 cm^{-1}) infrared spectrum of propane, recorded at 142 K using the SOLEIL-LISA cryogenic cell, with synchrotron radiation at the SOLEIL French light source facility coupled to a Bruker IFS-125 Fourier transform spectrometer. For both bands the rotational energy levels in the upper states are split because of interactions with the internal rotations of the methyl groups, leading to the identification of AA, EE, AE and EA torsional components. We show that these torsional splittings are due to the existence of anharmonic and Coriolis resonances, coupling the 21^1 and 8^1 rotational levels to nearby highly excited levels of the two internal rotations of the methyl groups. An effective "vibration – torsion- rotation" Hamiltonian model was built in the G_{36} symmetry group which accounts for both types of resonances. In parallel, a code computing the line intensities was developed to allow unambiguous torsional component assignments.

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Characterization of Two-photon Entanglement Resulting from VUV Photodissociation of H_2

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ABSTRACT

Excitation of the dihydrogen molecule can lead to the emission of two Lyman-α photons via the following processes:

$$\begin{aligned}\mathrm{H}_2 + h\nu_{\mathrm{VUV}} &\rightarrow \mathrm{H}_2^{**}\left(\mathrm{Q}_2\ {}^1\Pi_u\right)\\ &\rightarrow \mathrm{H}(2p) + \mathrm{H}(2p)\\ &\rightarrow \mathrm{H}(1s) + \mathrm{H}(1s) + 2h\nu_{\ \mathrm{Ly}\text{-}\alpha}\end{aligned}$$

Entanglement of these two Lyman-α photons emitted during the deexcitation of a pair of H(2p) atoms have attracted a lot of interest since the end of the eighties. In particular, in recent publications authors reported a shortening of the lifetime of the H(2p) states produced during the dissociation of excited H_2 molecules due to the two-atom entanglement[1,2]. This statement was furthermore supported by the analysis of the angular dependence of the emission of the produced two Lyman-α photons.

In this communication, we will present the experimental results obtained at the SOLEIL synchrotron facility on the DESIRS beamline using single bunch mode. In order to characterize the influence of entanglement on the decay dynamics of the pair of H(2p) atoms, we have setup a complete experiment where the initial time t_0 and the arrival times t_1 and t_2 of the two Lyman-α photons were measured in coincidence. The absolute decay time of each H(2p) atom was first measured as a function of pressure to ensure that the two Lyman-α photons came from the same molecule. In the appropriate pressure range, we then measured the coincident photon yield for 0, 45 and 90°-tilt angle of the VUV excitation photon polarization and the associated t_0, t_1, and t_2 times. Comparison of these measurements with previously published theoretical models[2,3,4] seems to show that, (i) the angular probability distribution is a clear signature of entanglement and (ii) the absolute decay time of each photons does not allow to draw any conclusion about the role of entanglement in the decay dynamics of two entangled H(2p) atoms.

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PARALLEL SESSION

Life & Earth Sciences
(Biology / Health & Environment / Geoscience)

CENTRALE-SUPELEC-GIF-SUR-YVETTE - MICHELIN AUDITORIUM $^{\#}$1

Thursday, January 17th

Chairpersons:

Benoît Masquida, Yann Gohon and Remi Marsac

IT-07	Structural basis of nucleotide sugar transport across the Golgi membrane ***S. Newstead***
IT-08	*In vitro, in cellulo and in crystallo* enzymatic reaction from APRT ***P. Nioche***
OC-25	Structure-function analysis of the photosynthetic ribulose epimerase CrRPE1 ***J. Henri***
IT-09	Cristal chemistry and stability of phyllosilicates: New approaches to solve old problems ***B. Dubacq***
OC-26	Calcium control on the size and organization of iron-organic matter nano-aggregates: Impact on their surface reactivity ***A. Beauvois***
OC-27	Multimodal ultrastructural study of lipid droplet ***M. Froissard***
OC-28	Investigations in the $CaMoO_4$ – $Na_{0.5}Ln_{0.5}MoO_4$ (Ln = La, Eu, Yb) solid solution series ***N. Finck***

PARALLEL SESSION

Life & Earth Sciences
(Biology / Health & Environment / Geoscience)

CENTRALE-SUPELEC-GIF-SUR-YVETTE - MICHELIN AUDITORIUM #1

Friday, January 18th

Chairpersons:

Benoît Masquida, Yann Gohon and Remi Marsac

IT-09	Crystal chemistry of trace elements in sulfide minerals: Environmental implications ***G. Morin***
IT-10	Abiotic synthesis of amino acids in the recesses of the oceanic lithosphere ***C. Pisapia***
IT-11	Setting up an in-vivo crystallography platform at SOLEIL ***P. Montaville***
OC-29	Looking deep inside the phloem and xylem cell wall composition by synchrotron FTIR and Raman spectroscopy ***R. Le Hir***
OC-30	Structure of liquid crystalline nanocarriers for delivery of neuroprotective molecules ***A. Angelova***

Structural Basis of Nucleotide Sugar Transport across the Golgi Membrane

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ABSTRACT

Glycosylation is a fundamental cellular process that, in eukaryotes, occurs in the lumen of both the Golgi apparatus and the endoplasmic reticulum. Nucleotide sugar transporters (NSTs) are an essential component of the glycosylation pathway, providing the diverse range of substrates required for the glycosyltransferases. NSTs are linked to several developmental and immune disorders in humans, and in pathogenic microbes they have an important role in virulence. How NSTs recognize and transport activated monosaccharides, however, is currently unclear. In this talk I will present crystal structurea of an NST, the GDP-mannose transporter Vrg4, in both the substrate-free and the bound states[1]. A hitherto unobserved requirement of short-chain lipids in activating the transporter supports a model for regulation within the highly dynamic membranes of the Golgi apparatus. Our results provide a structural basis for understanding nucleotide sugar recognition, and provide insights into the transport and regulatory mechanism of this family of intracellular transporters.

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In Vitro, *In Cellulo* and *In Crystallo* Enzymatic Reaction from APRT

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ABSTRACT

We have investigated the human adenine phosphoribosyltransferase (APRT) that produces AMP from adenine and PRPP in the purine salvage pathway (1–5). We show that a single oxygen atom from the Tyr105 side chain is responsible for selecting the active conformation of the 12 amino acid long catalytic flexible loop. Using *in vitro*, *in cellulo* and *in crystallo* approaches, we demonstrate that Tyr105 is key for the fine-tuning of the kinetic activity efficiencies of both the forward and reverse reactions. Our results reveal an evolutionary pressure on the strictly conserved Tyr105 and on the dynamic motion of the flexible loop in phosphoribosyltransferases that is essential for purine biosynthesis in cells (6).

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Structure-function Analysis of the Photosynthetic Ribulose Epimerase CrRPE1

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ABSTRACT

Photosynthesis is the primary carbon source for the biosphere. The Calvin-Benson cycle fixes atmospheric CO_2 into organic trioses through 11 reaction steps[1]. Transketolase (TRK)[2], ribulose-5-phosphate-3-epimerase (RPE), ribose-5-phosphate isomerase (RPI) and phosphoribulokinase (PRK)[3] individually contribute to the regeneration of ribulose-1,5-bisphosphate, the substrate of Rubisco mediated carboxylation.

We solved the crystal structure of RPE1 from the model, single chloroplast, unicellular alga *Chlamydomonas reinhardtii* at a resolution of 1.96 Å in space group $P2_1$. The protein folds as a $(\beta\text{-}\alpha)_8$ barrel of the triose-phosphate isomerase family. Crystal packing analysis suggests a homo-hexameric quaternary structure that was confirmed in solution by SEC-SAXS experiments. Epimerase active site is centered on a zinc ion bound by two histidines and two aspartates side chains. Three loops constrain the access to zinc, hence conditionning the formation of the enzyme-substrate complex.

Whole proteome analysis[4] identified in CrRPE1 two phospho-serines and a phospho-threonine, which side chains map at the entrance of our modelled active site. CrRPE1 was also identified in the global thioredoxin interactome[5]. Our crystal structure localizes the four cysteines thiols in positions accessible to solvent, supporting RPE1 modification by redox signals. In vitro assays of epimerase activity were developed to calculate enzymatic parameters.

Surprisingly however, neither redox treatments nor phospho-mimicking mutations significantly impacted in vitro reaction rates. Furthermore, at measured K_M and k_{cat}, enzyme and substrate concentrations cause a thermodynamic bottleneck in the Calvin-Benson cycle metabolic flux[6]. According to the substrate channeling hypothesis[7] multi-enzymatic complexes maximize metabolic efficiency. Hence, we now aim to integrate TRK-RPE-RPI-PRK structure-function relationships to probe the higher order organization of photosynthetic enzymes.

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Cristal Chemistry and Stability of Phyllosilicates: New Approaches to Solve Old Problems

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ABSTRACT

Phyllosilicates (mica, chlorite, serpentine, clays) are minerals widespread in Earth’s continental and oceanic crust and at their surface. They are ubiquitous products of metamorphism, alteration of magmatic rocks and hydrothermal processes, owing to large stability fields and wide compositional ranges. Phyllosilicates are of particular interest for metamorphic petrology because their composition reflects their pressure and temperature of crystallization: they are used as paleo-thermobarometers and help understand the history of rocks buried towards Earth’s interior and exhumed back to the surface via plate tectonics.

Analysis of rock textures and measurement of the structure and composition of rock-forming minerals are necessary to reconstruct the pressure-temperature-time history of these rocks, and are traditionally carried out with electron microscopy and mass spectrometry techniques. Thermodynamics allows for quantitative modelling of reactions between minerals and geological fluids at varying pressure, temperature and composition of the system.

Because minerals like phyllosilicates often show changes of composition (zoning) over small scales (typically a few micrometres), *in-situ* analyses are necessary, and crystal-scale mapping is very useful for understanding how reactions take place and equilibrium is reached, or not reached, in rocks. An additional challenge is the measurement of the oxidation state of Fe, which varies in phyllosilicates, including within single crystals. This talk will show how synchrotron radiation techniques (μ-XRF and μ-XANES at the K-edge of Fe) shed light on lingering problems and offer exciting perspectives for metamorphic petrology.

Calcium Control on the Size and Organization of Iron-organic Matter Nano-aggregates: Impact on their Surface Reactivity

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ABSTRACT

Natural colloids are known to control the dynamic of many pollutants in the environment. They are heterogeneous, composed of minerals, organic matter (OM) or a combination of these phases. Their small size and their high functional group density allow natural nanoparticles to trap and transport pollutants [1]. Among natural colloids, the one composed of iron oxides and OM (Fe-OM) are of major importance because of their high surface reactivity and their high abundance in natural systems.

In a previous study [2], we demonstrated that Fe is distributed as oligomers and ferrihydrite (Fh) nanoparticles organized as a fractal network bound to a spherical and compact OM nano-aggregate. With the Fe/OM ratio increases, the nanoparticle/oligomer ratio and the size of the nanoaggregates increases while their compactness decreases. For associated element such as arsenic (As), the consequence is an increase of its sorption with the increasing Fe/OM ratio (note that As/Fe were identical for each tested Fe/OM). Sorption capacities of Fe-OM nano-aggregates are thus not only related to their size but also to their structural organization. This organization depends on the physico-chemical conditions of the nano-aggregates formation, such as the pH, the ionic strength or the presence of other elements in natural system. Calcium (Ca) is one of the most abundant cations in the environment and it exhibits a high affinity for OM.

We therefore studied the impact of Ca on the size and the structural organization of Fe-OM associations. Thanks to XAS experiments at both Ca and Fe K-edge combined with SAXS and A4F-UV-MALS measurements, we observed that Ca is bound to OM as outersphere complexes. For a given Fe/OM ratio, adding Ca does not modify the oligomer/Fe nano-particles ratio but the nanoparticles size increases with the increasing Ca/Fe ratio.. Arsenic adsorption experiments (coupling ultra-filtrations, DOC and ICP-MS measurements) demonstrate that, for a given As/Fe ratio, the As adsorption increases with the increasing Ca/Fe ratio.

These results show that cations such as Ca must influence the OM organization which, dramatically influences the Fe phases structure and Fe-OM organization. As a consequence, their adsorption capacity towards As increases with the increasing Ca/Fe ratio. A next step is to determine how the organic matter organization is modified by Ca.

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Multimodal Ultrastructural Study of Lipid Droplet

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ABSTRACT

In all organisms, storage lipids are maintained in the cytoplasm in specialized organelles called lipid droplets (LDs). These nanoparticles consist mainly of a core of neutral lipids (triacylglycerols and/or steryl esters) enclosed in a monolayer of phospholipids, and contain a number of proteins which vary considerably with the species. More than inert fat balls, LDs are complex organelles and their abnormal dynamics is associated with several diseases (virus-induced steatosis, diabetes, atherosclerosis and myopathies). In the context of green chemistry, LDs are promising sources of lipid-derived molecules for chemistry, food, medicine and cosmetics. For these reasons, understanding LD structure and way of life is of major importance.

Combination of synchrotron radiation techniques enable us to go deeper into the comprehension of LD biology. First, we investigated the structure of a peculiar class of highly hydrophobic LD proteins called Class I LD proteins. These proteins exhibit structural convergence with a hairpin folding that target and anchor the protein to the LD. We developed a genetic approach using heterologous expression in yeast to perform comparative functional and structural study of seed oleosins [1 , 2], mammalian caveolin and hepatitis C virus core protein. We obtained circular dichroism spectra of oleosin AtOle1 inserted in LD [3]. Second, we investigated the ultrastructure of the LD core using label-free imaging techniques, deep ultra violet on living yeast and transmission X-ray microscopy on cryo-fixed cells. We confirmed the ultrastructural lipid heterogeneity of LD and its concentric layer organization

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Investigations in the $CaMoO_4$ – $Na_{0.5}Ln_{0.5}MoO_4$ (Ln = La, Eu, Yb) Solid Solution Series

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ABSTRACT

High-level nuclear waste (HLW) is foreseen to be encapsulated in steel containers and placed in deep geological repositories to isolate it from the biosphere. However, during the evolution of the repository system, groundwater may migrate through the barriers and contact the waste packages. Upon contact with water under repository relevant conditions HLW glass will alter and secondary phases, such as powellite[1] ($CaMoO_4$), will form in the alteration layer. The neoformation of secondary phases establishes a new geochemical barrier for re-immobilization of radionuclides, such as the long-lived actinides, dissolved from the waste matrices. Structural incorporation by formation of solid solution can arguably result in long-term efficient immobilization.

Powellite was synthesized in the presence of trivalent lanthanides, used as non-radioactive chemical surrogates for actinides, whereby Ca^{2+} was substituted by mono- and trivalent cations. Structural analysis by X-ray powder diffraction showed the presence of only powellite-like structures, no other phase could be detected. Furthermore, fits to the diffractograms indicated the formation of complete solid solution series between the $CaMoO_4$ and $Na_{0.5}Ln_{0.5}MoO_4$ (Ln = La, Eu, Yb) endmembers with significant negative excess volume, positive excess volume and almost no excess volume for the La, Yb and Eu series, respectively. These findings were further corroborated by Raman spectroscopy where bands systematically broaden with the Ca substitution rate as a consequence of increasing structural disorder. Information on local ordering was obtained by X-ray absorption spectroscopy. In all series, pre-edge features in the Mo *K*-edge XANES show that Mo tetrahedra are hardly affected by the substitution and EXAFS data suggest random Ln distribution within the powellite structure. The absence of local Ln clustering is also corroborated by fits to the Ln L_3-edge EXAFS data. Finally, the increasing Debye-Waller terms with increasing size of the substituting Ln suggests increasing structural disorder, in agreement with Raman spectroscopy data. Since powellite is able to accommodate the large Ln^{3+} ions at Ca structural site provided charge is balanced by co-insertion of Na^+, actinides may as well be incorporated within powellite, as indicated by reported luminescence data[2]. However, structural data are still missing for powellite containing actinides, but are planned to be obtained in future investigations.

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IT-09

Crystal Chemistry of Trace Elements in Sulfide Minerals: Environmental Implications

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ABSTRACT

The mechanisms of metal sulfide mineral formation in low temperature environments and their role in trace metal biogeochemistry remain incompletely understood. Among research questions still open in this field, a major challenge concerns the understanding of the molecular scale mechanisms underlying the biotic and abiotic formation of pyrite in natural systems, such as marine and continental sediments, flood plains and hydromorphic soils.

In this context, we used synchrotron-based Extended X-ray Absorption Fine Structure (EXAFS) spectroscopy to elucidate some key steps of pyrite nucleation at ambient temperature [1] and to unravel the mechanisms of trace metal incorporation in this mineral [1,2]. We have also investigated the molecular-level structure and chemistry of poorly- and nano-crystalline sulfide minerals in natural settings and in engineered bioremediation processes. We will especially focus on the role of pyrite to mitigate trace metals transfers to the great New Caledonian lagoon, based on a detailed understanding of the formation and long-term evolution of metal-bearing pyrite in mangroves [3,4] (Coll. KNS, New Caledonia). In a similar context, we will highlight some key steps of nickel sequestration in biogenic iron sulfides produced by indigenous bacteria [5]. Finally, we will give some evidences for the major role of sedimentary pyrite in the long-term arsenic cycle in South Asian deltas [6] (coll. EPFL, Switzerland, University of Technology, Ho Chi Minh City, Vietnam) and we will demonstrate that arsenic sulfides formation by acidophilic sulfate reducers appears as a promising water treatment process at heavily contaminated mining sites [7] (Coll. BRGM, Orléans, HSM, Montpellier).

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Abiotic Synthesis of Amino Acids in the Recesses of the Oceanic Lithosphere

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ABSTRACT

The hydrothermal alteration of mantle rocks, namely serpentinization, is known to generate favourable conditions for abiotic organic synthesis. Yet, identifying the pathways leading to the production of complex organic molecules is a challenging problem that has critical implications for prebiotic chemistry, the origin of life and the functioning of modern rock-hosted life. This potential for abiotic synthesis was confirmed by the analysis of hydrothermal vent fluids, as well as laboratory and thermodynamic modelling, but remains underexplored in deep natural rocks. In order to further investigate serpentinizing environments as a critical venue for prebiotic chemistry and life activity, we used a correlative microscopy approach, notably including Synchrotron-based Deep-UV fluorescence and Fourier Transform Infrared microspectroscopies, supported by chemometrics analysis [1].

This approach was applied to serpentinized peridotites from the Atlantis massif (30°N, Mid-Atlantic ridge; IODP Expeditions 304/305) to track organic compounds at the pore level in rocks. We highlighted in these rocks the occurrence of aromatic amino acids formed abiotically and preserved at depth in the hydrating oceanic crust [2]. They were found in the nanoporosity of a highly reactive iron-rich saponite clay, which would have catalyzed Friedel-Crafts type reactions and thus promoted amino acids formation during a low-temperature alteration stage of the rocks. Demonstrating the potential of fluid-rock interactions in the oceanic lithosphere to generate amino acids abiotically gives credence to the hydrothermal theory for the origin of life, and may shed light on the functioning of the present-day deep biosphere.

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Setting Up an In-vivo Crystallography Platform at SOLEIL

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ABSTRACT

The combined use of modern microfocus synchrotron beamlines in conjunction with serial crystallography approaches allows the exploitation of a reasonably low number of micron-sized protein crystals for structure determination. Such micro-crystallography techniques open the door to the investigation of new protein crystallography methods such as the *in vivo* crystallography.

In vivo crystallography is a phenomenon during which naturally or heterologously expressed proteins crystallize within the living cell. This process has been observed to occur in the cytoplasm or within specific subcellular compartments [1]. Such crystals are limited in size but, unlike classical *in vitro* crystallography, are produced in a native-like environment. Anticipated benefits of such system are an alternative way to obtain crystals of proteins for which classical *in vitro* crystal growth revealed unsuccessful as well as the opportunity to study functionally important post-translational modifications. Additionally, *in vivo* crystallography could, when successful, minimize the efforts provided in optimizing purification of samples, currently presenting one of the main bottlenecks of the technique [2]. The investigation of the full potential of *in vivo* crystallography requires an understanding of the parameters underlying the process. The commonly admitted prerequisite is the accumulation of high concentration of the target protein in a restricted location within the living cell. Little is known, however, about the influence of the specific biochemical environment on protein crystal nucleation and growth.

We propose a strategy to explore the possibility to turn cells into elaborated "crystal screens" by addressing multiple protein targets toward specific subcellular compartments (cytoplasm, nucleus, ER, peroxysomes) through a microplate based small scale cell culture setup. In addition, the screens can be further extended by coupling the protein overexpression with the cellular uptake of chemical compounds acting as crystal nucleators such as specific caged lanthanides [3]. The use of such chemical compounds is moreover envisioned to be a way to solve the inherent phase problem of *in vivo* crystallography. Second harmonic generation microscopy (SHG) is a key method to evaluate the "*in vivo* screens", and to get insight of the *in vivo* crystallogenesis process.

The ultimate goal of the project is to build a semi-automated *in vivo* crystallography platform within a synchrotron facility using microfluidics to couple the *in vivo* crystallography screens to the SHG-based scoring step and ultimately to the data collection step through serial crystallography.

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Looking Deep Inside the Phloem and Xylem Cell Wall Composition by Synchrotron FTIR and Raman Spectroscopy

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ABSTRACT

Plants are of primary importance for human being since they provide directly or indirectly raw materials for food, clothing and energy. A majority of these products are coming from components of the plant cell wall, especially the secondary cell wall that is composed of lignin, cellulose and hemicelluloses. Therefore, studying the factors involved in the secondary cell wall formation is of importance to improve the yield and quality of the plant biomass. Plant cell walls are highly complex structures that are modified during plant growth and development[1]. In addition, a highly tissue-specific composition is observed, which confers biophysical properties to the cell walls depending on their function. For example, the cell wall of xylem vessels and fibers that transport water and provide mechanical support for erected organs is lignified, whereas the cell wall of the phloem cells that participate in the long-distance allocation of sugars, is enriched in polysaccharides. However, additional information about the cell wall composition of such tissues at the cell-level is still needed to better understand the relationship between the cell wall structure and the function of phloem and xylem. Additionally, little is known about the factors acting on sugar allocation to supply carbohydrates skeletons in secondary cell wall formation.

To tackle these points, we used synchrotron radiation-based Fourier-transform infrared (SR-FTIR) and Raman spectroscopy to probe the cell wall composition of the floral stem vascular tissues of wild-type Arabidopsis and the double-mutant *sweet11-1xsweet12-1*, which has impaired sugar cell-to-cell transport[2,3]. In addition to confirming modifications in the xylem cell wall composition, the SR-FTIR spectra allowed highlighting modified hemicellulose composition in the phloem cell walls of the double mutant. Combining Raman spectroscopy with a classification and regression tree (CART) method, we identified combinations of Raman shifts that could distinguish xylem vessels and xylem fibers. In addition, the disruption of the *SWEET11* and *SWEET12* genes impacted on xylem wall composition in a cell-specific manner, with changes in hemicelluloses and cellulose observed at the xylem vessel interfaces[4].

These results suggest that the facilitated sugar transport by transporters situated between vascular parenchyma cells and conducting cells is important for ensuring correct phloem and xylem cell wall composition.

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Structure of Liquid Crystalline Nanocarriers for Delivery of Neuroprotective Molecules

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ABSTRACT

Neuronal cell loss and dysfunction are involved in a number of pathologies such as Alzheimer's disease (AD), Parkinson's disease (PD), Hungtington's disease (HD), depression, hearing impairment, stroke, spinal cord injury, Rett syndrome, and amyotrophic lateral sclerosis (ALS). The activity of neurotrophic proteins and phytochemicals in preventing neuronal damage attracts current interest in view of the necessity of combination therapies of neurodegenerative diseases [1,2]. On the other side, omega-3 polyunsaturated fatty acids (ω-3 PUFA) are bioactive lipids with considerable impact in medicine and nutrition [3]. These compounds exert structuring effects on the cellular membrane organization, regulate the gene expression, and modulate various signaling cascades and metabolic processes.

Nonlamellar phases, formed by lyotropic lipids, display several advantages for the design of drug delivery carriers of neuroprotective molecules [3-6]. They may produce densely packed self-assembled nanochannel-type architectures in addition to vesicular membranes. Our research focuses on understanding of the mechanism and dynamics of formation of self-assembled nanocarriers of amphiphilic building blocks and time-resolved structural studies of the assembly and loading of therapeutic biomacromolecules. The lyotropic liquid crystalline assemblies are investigated by small-angle X-ray scattering (SAXS) and cryo-transmission electron microscopy (cryo-TEM). The quasi-elastic light scattering (QELS) technique is also applied in order to get insights into the mechanism of formation of stable nanodispersions.

By mixing ω-3 PUFA with the lyotropic lipid MO we accomplished tuning of the average critical packing parameter of the binary mixtures, which provoked the induction of intermediate liquid crystalline states between 3D cubic and 3D sponge-like lipid membrane organizations. A phase transition from a periodic to a random organization of the lipid membranes was evidenced at high ω-3 PUFA content. The obtained multiarchitecture assemblies comprise topological features of double membrane vesicles, cubosomes, spongosomes, and their precursors. This demonstrated the strong influence of ω-3 PUFA on the inner liquid crystalline organization of the carriers at the nanoscale.

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POSTERS SESSION

List of Student Posters

PO-AN-01	Determination of the role of titanium in the structure of amorphous blast-furnace slag by micro-Xanes at Ti K-edge ***D. Le Cornec***
PO-AN-02	Excited electronic states in thiophene and thiolane using resonant Auger spectroscopy ***J.B. Martins***
PO-AN-03	A multi-beamlines study of bimetallic Prussian Blue analogs for methodological developments in transition metal K-edge XMCD ***A. N'Diaye***
PO-AN-04	Polymerization of nitrogen in ammonium azide at high pressures ***G. Zhang***
PO-DR-05	A combination of FAIMS separation with Synchrotron UV-photo activation for the tandem MS analysis of synthetic polymers ***I. Aloui***
PO-DR-06	Solution chemistry meets ultrafast crystallization: An in-situ XRD line broadening approach ***J. Banchewski***
PO-DR-07	NH_3 ultrafast dissociation probed by energy-selected resonant Auger electron-ion coincidence measurements ***F. Hosseini***
PO-DR-08	Quantifying water ionization by soft X-rays ***L. Huart***
PO-LH-09	Preliminary analysis of the interacting Pentad bands (v2+2v4, v2+v3, 4v2, v1+2v2, 2v1) of CF_4 in the [1600-1800] cm-1 region ***M. Mattoussi***
PO-LH-10	Structure of a multiprotein assembly of the DNA double-strand breaks repair pathway ***S. Zahid***

Determination of the Role of Titanium in the Structure of Amorphous Blast-furnace Slag by Micro-Xanes at Ti K-edge

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ABSTRACT

Glass alteration is of large interest, from materials to Earth and environmental sciences. Ground Granulated Blast-furnace Slag (GGBS) is a glassy by-product of pig iron and steel manufacturing. This amorphous solid is a porous and textured calcium aluminate glass with an unusual silica-poor composition (about 35 wt.% SiO_2). It is a hydraulic binder: the dissolution of the vitreous structure in water leads to the formation of various products including a calcium silicate hydrate (CSH) gel which is responsible for the setting of the material. When the GGBS is mixed with cement or another activator, this dissolution takes place within a few days. GGBS has been used in cement for a hundred years as it improves its resistance to chloride and sulfate attacks and contributes to reduce the CO_2 footprint by limiting the use of clinker.

Various studies have tried to better understand and predict GGBS reactivity in water. However, the structural control of glassy slag to binder transformation is poorly understood. In particular, the role of the cations in the starting glass is still unknown. It has also been noticed that above 1 wt.% TiO_2 in the pristine glass, the reactivity of the slag drops drastically but there is no understanding of the structural origin of this variation.

We present here the first results on the role of titanium in the structure of granulated blast-furnace slag. XANES at Ti K-edge was performed with a micrometer-large beam on the LUCIA beamline of the SOLEIL synchrotron. Energy dispersive X-ray spectroscopy was used on the beamline to probe the heterogeneities of the samples and locate precisely the hydrated and non-hydrated areas of interest. The coordination of Ti is determined by analysis of the pre-edge peak of the XANES spectra and its role on the glassy structure is discussed.

Excited Electronic States in Thiophene and Thiolane using Resonant Auger Spectroscopy

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ABSTRACT

In this work, we present an experimental and theoretical study of the high-resolution high-energy resonant Auger spectroscopy in thiophene and thiolane gas-phase molecules around the resonant excitation of the Sulphur *K*-shell to the lowest unoccupied molecular orbital (LUMO) and further beyond the ionization threshold. Such detailed tuning of the photon energy allows monitoring the Auger spectra both as a function of Auger electron kinetic energy and the photon energy. Data visualization in the form of two-dimensional (2D) Auger maps enables the analysis and highlights the qualitative difference in the behavior of various spectral lines. The change in the order of the two lowest orbitals in thiophene when compared to thiolane was observed from 2D maps.

To improve the interpretation of the experimental measurements, theoretical chemistry models were applied to obtain an explanation for the differences between the spectral lines in 2D Auger maps. We chose the multi configurational wave functions to describe the excited states, applying a specific routine for inner-shell states (IS-CASSCF) [2]. In this method, high energy states can be reached by constraining the occupation of the core orbitals and optimizing them during an isolated SCF step. Relaxation effects are included in our description and they play an important role in the accurate description of excitations from S 1s to σ^* and π^* orbitals, as well their correlate states in Auger S $2p^{-1}$ states.

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A Multi-beamlines Study of Bimetallic Prussian Blue Analogs for Methodological Developments in Transition Metal K-edge XMCD

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ABSTRACT

Prussian Blue Analogs (PBA) of general formula $Y_xA_4[B(CN)_6]_{(8+x)/3}$ (Y = alkali cation; A,B = transition metal (TM); x = 0-4) are studied for their (photo)magnetic property, which is interesting for high-density information storage. For some stoichiometry, a reversible metal-metal charge transfer along the A—NC—B cyanide bridge can indeed be photoinduced, but it is observed at a temperature that is too low to be used in real applications. The cyanide bridge structural distortion appears to be the key to control and adjust this property. As they are too small to be quantified with classical structure-characterization techniques, we are working on the development of a methodology based on X-ray Magnetic Circular Dichroism (XMCD) at the TM K-edge. First measurements for NiFe PBAs indeed showed significant variations of the Fe and Ni K-edges signals related to pressure-induced structural distorsion[1,2]. Nevertheless, the XMCD signals at the TM K-edge are not well understood yet, and it is mandatory to (i) develop a methodology to quantify small structural distortions from the signals and (ii) disentangle the physical effects originating TM K-edge XMCD.

To develop this methodology, we are conducting a systematic investigation of non-photomagnetic PBAs ($A_4[B(CN)_6]_{2.7}$) at the K-edge of the A and B transition metals. In addition to XMCD measurements, XAS is also performed to characterize in details the electronic structure and local environment of the transition metals in the model PBAs. This requires to couple experiments on three beamlines: FAME-UHD (CRG beamline), ODE and SAMBA. FAME-UHD offers highly-resolved spectra thanks to their analyser-crystals spectrometer, thus bringing information on the electronic structure and site symmetry thanks to the pre-edge analysis. On SAMBA, we measure the EXAFS signal in order to have quantitative information on the local environment of each TMs (coordination number, distance between the TM and its neighbours…). Finally, ODE is the beamline dedicated to TM K-edge XMCD and all our XMCD experiments are performed there. By combining the information obtained from the 3 beamlines measurements, the variations observed on the XMCD signals can be related to variations in the electronic and structural parameters.

We will present our first results of this multi-beamlines study. A series of $A_4[Fe(CN)_6]_{2.7}$ PBAs (A=Mn, Co, Ni, Cu) was studied at the A and Fe K-edges, as well as a first series of $(Ni_{1-x}Co_x)_4[Fe(CN)_6]_{2.7}$ trimetallic PBA. We will focus on the interest of combining the three beamlines to develop our methodology and on the first electronic information obtained on these model PBAs thanks to the pre-edge analysis from the FAME-UHD data.

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Polymerization of Nitrogen in Ammonium Azide at High Pressures

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ABSTRACT

Hydronations at ambient conditions display a rich variety of molecules including NH_3, N_2H_4, N_3H and NH_4N_3. Pressure is expected to enhance the diversity of hydronitrogen's chemical associations. A variety of compounds, calculated stable on the formation enthalpy-composition convex hull of the N-H system, are relevant to planetary sciences and as possible metastable high energy density polynitrogen material. By ab initio molecular dynamics simulations, ammonium azide is predicted to be an effective precursor to form polynitrogen, such as N_5^{-1}, N_8[2] and N_8H[3].

The sample of ammonia azide was synthesized by Professor Zhu Hongyang of Jilin University[4]. We used high pressure Raman and X-ray diffraction experiments to detect the synthesis reaction of NH_4N_3 with nitrogen at high temperature and pressure (300K-700K, ambient to 50 GPa). We found that there is a phase transition around 25GPa and 650K and the new phase is stable at room temperature and is metastable on decompression up to 6GPa where it reverts to ammonium azide. The new phase of the sample may be a nitrogen chain structure containing $N = N - N$ and $\equiv N - N$.

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A Combination of FAIMS Separation with Synchrotron UV-photo Activation for the Tandem MS Analysis of Synthetic Polymers

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ABSTRACT

Synthetic polymers are used throughout many areas such as health industry, energy, or communication. The physicochemical properties of synthetic polymers are closely dependent on their structure. Their characterization is often delicate because a polymer is generally a heterogeneous mixture, since polymerization reactions lead to the formation of molar masses distributions. Polymers can exhibit a chemical heterogeneity, various topologies, (linear, grafted, cyclic, star-shaped...). In this context, it is necessary to develop powerful analytical techniques. Mass spectrometry of synthetic polymers can be performed to obtain characteristic information of each macromolecular chain individually present in a polymer sample. Characterization of synthetic polymers can be performed by single-stage mass spectrometry but tandem mass spectrometry is required for more detailed information.

In order to obtain detailed structural information, tandem mass spectrometry, which consists in deliberately inducing gas phase decomposition reactions from previously selected precursor ion, is necessary. The main technique used to perform tandem mass spectrometry analysis is collision-induced dissociation[1] (CID). However, other activation techniques have been developed more recently such as electron-transfer dissociation[2,3] (ETD) and UV irradiation of trapped ions[4,5].

The goal of this work was to study the effect of wavelength-tunable UV synchrotron irradiation of synthetic polymer ions, combined or not with field asymmetric waveform ion mobility. Precursor ions produced by ESI (positive mode) from different model polymers have been stored in an ion trap mass spectrometer coupled to the DISCO beamline (52-221 nm), and then activated by UV synchrotron irradiation during a variable time period and over a range of wavelengths. For the highest mass polymers, UV activation was combined with field asymmetric waveform ion mobility spectrometry. Synchrotron UV beam for tandem MS experiments from polymers and the combined use of ion mobility for multiply charged precursor ions selection creates new opportunities for the characterization of polymers.

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Solution Chemistry Meets Ultrafast Crystallization: An *in-situ* XRD Line Broadening Approach

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ABSTRACT

Superconductivity is one of the most profoundly studied fields in modern physics and yet still the subject remains of global interest. At present, Low Temperature Superconductors (LTS) govern the major part of market applications (e.g. Nuclear Magnetic Resonance Spectroscopy (NMR) and High Magnetic Fields) although High Temperature Superconductors (HTS) exhibit better performance in their superconducting state. What is still limiting HTS to enter a broad market of applications is its high cost/performance ratio. To address this issue, we are developing a novel growth technique, entitled transient liquid assisted growth (TLAG), to fabricate low-cost, high throughput Coated Conductors (CCs) incorporating $YBa_2Cu_3O_{7-x}$ (YBCO) as superconducting layer. The idea of TLAG relies on the capability of a ternary system composed of $BaCuO_2$, CuO and Y_2O_3 to form a eutectic $BaCuO_2$-CuO(l) liquid phase in the presence of dispersed Y_2O_3 solid nanoparticles. Upon dissolution of Y_2O_3 in the liquid the epitaxial substrate interface is used to promote heterogenous nucleation of the $YBa_2Cu_3O_7$ (YBCO) superconducting layer at growth rates beyond present technologies.

At Soleil, *in-situ* growth experiments were carried out following the epitaxial layer in ω-2θ geometry with a beam energy of 18 keV. XRD area scans with acquisition times per scan of 100 ms were recorded with a hybrid pixel area detector. A first stage analysis of the growth process revealed the complex reaction paths of all involved phases and ultrahigh film growth rates up to 100 nm/s. But what can be learned about the initial growth stage of heterogenous nucleation and how can that knowledge be useful for the design of high throughput film manufacturing?

In this presentation we focus on the initial stage of nuclei formation and observe rapid line broadening changes in the out-of-plane and in-plane component of the symmetrical reflection of YBCO. Such changes are solely caused by crystallite size increase [1] in the proximity of fast convertion rates. The analysis of particle size broadening is applied to study the evolution of two chemically deposited layers that were expected to create different supersaturation conditions. We show that initial solution stoichiometry is key to tune nucleation density and liquid kinetics, two essential parameters in liquid-mediated growth techniques. A discussion on rate-limiting processes [2] as well as 2D-XRD imaging as a potential tool to study ultrafast nucleation processes is given.

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NH_3 Ultrafast Dissociation Probed by Energy-selected Resonant Auger Electron-ion Coincidence Measurements

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ABSTRACT

Resonant excitation of a core electron to an anti-bonding molecular orbital may lead to ultrafast nuclear dynamics and even dissociation, which occurs on the same time-scale and, therefore, competes with radiative or non-radiative Auger decay [1].

For this study we used ES-AEPICO (energy-selected resonant Auger electron-ion coincidence) which is a unique complementary tool to high-resolution photoelectron spectroscopy as it allows the measurements of the UFD phenomenon and the determination of fragmentation mechanisms [2]. This is because the observed resonant Auger final states can be directly correlated to the fragment ions, which are expected to be formed by UFD, their behavior can be tracked as a function of the photon energy. For this research we used the state-of-the-art EPICEA setup which is permanently installed at PLEIADES beamline of the SOLEIL synchrotron.

Narrow bandwidth photon energies across the N_{1s}->$4a_1$ resonance is used to produce dissociative N 1s core-excited states. ES-AEPICO spectra is recorded at several energies across the resonance. Detuning the photon energy allows varying the effective lifetime [3] and then the competition between resonant Auger and ultrafast fragmentation.

The data analysis provide the two-dimensional resonant Auger electron–photoion coincidence maps for the process: $NH_3 + hv \rightarrow NH_2^+ + H$ at different photon energies where we could verify the existence of the UFD in NH_3, correlate Auger final states to different fragmentation patterns and confirm the Auger states (381-383 eV) are related to NH_2^+ fragments which were first observed in a previous study [4] by resonant Auger spectroscopy.

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Quantifying Water Ionization by Soft X-rays

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ABSTRACT

The description of the biological effects of ionizing radiation requires a good knowledge of the dose deposition processes at both the cellular and molecular scales. However, the specific behavior of the subkeV electrons appearing at the end of ionization cascades to deposit their energy in nanometric volumes, remains poorly described. Soft X-rays (100-1000 eV) are here used to probe the physical and physicochemical events occurring upon exposure of liquid water to subkeV electrons. Liquid water samples were irradiated with a monochromatic photon beam at the SOLEIL synchrotron. Hydroxyl radical quantification was conducted through HO scavenging by benzoate to form fluorescent hydroxybenzoate. Yields of OH radicals exhibit a minimum around 1.5 keV, in good agreement with the literature. Moreover, they are relatively independent of the benzoate concentration in the range investigated, which corresponds to scavenging times of 170 ns to 170 ps. Implementation of a microfluidic cell in the setup is developped to increase the signal/noise ratio, since the small volume used negates the need to start with a diluted solution with the scavenger.

Keywords— SOFT-XRAYS, HYDROXYL RADICAL SCAVENGING, WATER RADIOLYSIS

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Preliminary Analysis of the Interacting Pentad Bands (ν_2+2ν_4, ν_2+ν_3, 4ν_2, ν_1+2ν_2, 2ν_1) of CF_4 in the [1600-1800] cm^{-1} Region

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ABSTRACT

Tetrafluoromethane CF_4 is very powerful and long living greenhouse gas. Because of its chemical stability the lifetime of CF_4 in the atmosphere is estimated as more than 50000 years[1]. This molecule has both natural and anthropogenic origin. It is released predominantly during aluminum refining and semi-conductor manufacturing[2] into the atmosphere in significant quantities. Consequently, the knowledge of the infrared spectrum of this molecule is essential for atmospheric measurements.

Experimental CF_4 spectra in the region [1600-1800] cm^{-1} have been recorded in Reims using a Fourier transform Spectrometer of Connes type coupled to a multi-pass cell at 294° K with a spectral resolution of 0.003 cm^{-1}.

All spectrum analyses and fits have been realized using the MIRS software[3] based on tetrahedral tensorial formalism. In addition, direct predictions have been made possible using full *ab initio* ro-vibrational normal mode predictions[4] and non-empirical contact transformation Hamiltonian[5]. The root mean square deviation for 1831 line positions of the cold bands (ν_2+2ν_4, ν_2+ν_3, 4ν_2, ν_1+2ν_2, 2ν_1) is of 1.590×10^{-3} cm^{-1} up to J= 70, while for line intensities, some effective dipole moment parameters have been adjusted directly on those predicted by the *ab initio* variational calculations[6]. In this work, the standard deviation for line intensities for the cold bands (ν_2+2ν_4, ν_2+ν_3, 4ν_2, ν_1+2ν_2, 2ν_1) is of 1.1%, while, for the hot bands (2ν_2+2ν_4-ν_2, 2ν_2+ν_3-ν_2) and (ν_2+3ν_4-ν_4, ν_2+ν_3+ν_4-ν_4), the standard deviation is of 8% and 5% respectively.

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Structure of a Multiprotein Assembly of the DNA Double-strand Breaks Repair Pathway

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ABSTRACT

Many anti-cancer treatments, like chemotherapy or radiotherapy, aim at generating DNA double-strand breaks. Tumor cells are indeed more sensitive to double-strand breaks than healthy cells due to their phenotype and genotype [1]. One important axis in radiobiology is nowadays to combine radiation therapy with inhibitors of DNA repair pathway to increase radio-sensitivity and overcome radiation resistance of cancer cells [2]. A major challenge is to find powerful inhibitors of the main human double-strand break repair pathway called NHEJ (Non Homologous End Joining). Our team studies the molecular mechanisms of the proteins involved in this repair pathway and different strategies to inhibit them.

Mechanistic studies of this pathway clearly highlighted these last years, the central role of Ku70-Ku80 heterodimer. It interacts with the ends of double-strand breaks, allowing the initiation of NHEJ pathway and it allows the recruitment of the enzymes of this pathway by direct interactions. Many interactions involve peptide motifs KBM (Ku Binding Motif) of similar sequences.

We have determined crystallographic structures of protein complexes of the NHEJ pathway, such as the structure of a DNA ligation complex [3] and, more recently, the Ku70-Ku80 with two of its partners, XLF and APLF [4]. More recently, we characterized the mode interaction of Ku with two other partners, WRN and PAXX. The protein WRN presents the same KBMs as XLF and APLF and the protein PAXX present a new KBM. We present our first data obtained by microcalorimetry, SAXS and TEM on these interactions.

The challenge now is to characterize a larger protein assembly, the "NHEJosome", which in itself is a molecular machinery capable of recognizing and repairing double-strand breaks, and studying the influence of the nature of the double-strand break on the structure of this assembly. It is the assembly of the Ku70-Ku80 dimer and the ligation complex ligase4-XRCC4-XLF. This assembly, with a size of about 380 kDa, has not yet been crystallized.

This project is carried out in collaboration with recognized NHEJ biologists (JP de Villartay, Imagine Institute, Paris, P. Calsou, IPBS, Toulouse).

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List of Other Posters

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PO-02	Advanced non-destructive in-situ characterization on the French CRG D2AM/BM02 beamline ***N. Boudet***
PO-03	Fermi surface anisotropy of the metallic boron doped diamond ***H. Guyot***
PO-04	Mesure de la section efficace de photoionisation du radical hydroxyle ***O. Harper***
PO-05	Uranyl covalency change in borate glasses probed by XAS ***M.O.J.Y. Hunault***
PO-06	Cadmium phytoremediation by the hyperaccumulating plant Conyza Sumatrensis ***M. Ikogou***
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PO-11	A new high temperature reactor for operando XAS characterization of catalysts ***O. Proux***
PO-12	Localization of minerals and phenolic compounds in apple fruit ***C. Rivard***
PO-13	Spectroscopic parameters of CH_3Cl in the $^{Q}P(J,K)$ and $^{Q}Q(J,K)$ of the v_3 fundamental band ***M. Rotger***
PO-14	FAME-UHD: French X-ray absorption beamline dedicated to high energy resolution fluorescence detection at ultra-high dilution level ***M. Rovezzi***
PO-15	Nanotomography at the ANATOMIX beamline ***M. Scheel***

Transition Metal K-edge XMCD for the Study of the Structure-property Relationship in PBA

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ABSTRACT

Prussian Blue Analogues (PBA) of general formula $Y_xA_4[B(CN)_6]_{(8+x)/3}$ (Y = alkali cation ; A, B = transition metal ; x = 0-4) present, for some stoichiometries, relevant photomagnetic properties for data storage devices. Nevertheless, such property is observed at too low temperature for a real application and a deep understanding of the structure-photomagnetic property relationship in PBA is needed. The key-parameter to understand, control and adjust this photomagnetic property of PBA seems to be the slight structural distortions of the A—NC—B linkage. But the classical tools for structural characterization are not sensitive enough and so our current research focuses on using transition metal (TM) K-edge X-ray Magnetic Circular Dichroism (XMCD) to probe and quantify these very small structural distortions.

In collaboration with the ODE beamline, we are thus involved in a long-term project aiming at quantifying small structural distortions from TM K-edge XMCD. To do so, we use non-photomagnetic PBA as model-compounds to (i) develop a methodology that enables to extract quantitative structural information from the TM K-edge XMCD signal and (ii) disentangle the physical parameters originating TM K-edge XMCD. The ultimate goal is to (i) apply this methodology to transfer at room temperature the working temperature of photomagnetic PBA, and (ii) extend it for any materials whose properties are controlled by such small structural distortions. All the fundamental spectroscopic knowledge obtained through the development of the methodology will also bring new information on the role of the p orbitals in magnetism.

We will present our first results of this long-term project on two aspects of TM K-edge XMCD. First, we studied the effect of an external parameter (temperature, magnetic field) on the signal (shape, intensity); we observed that varying either the temperature or the magnetic field has no effect on the signal shape but can have a significant one on the intensity. We used the results to determine the experimental conditions for the whole series of measurements planned to establish the methodology. This also ensures that in the next measurements, we can unambiguously attribute the changes in the XMCD signal to variations of a physical/chemical internal parameter. Second, following this first experiment, we initiated the systematic investigation of the model AFe PBAs (A = Mn, Co, Ni, Cu) by looking at the effect of the nature of the A^{2+} cation on the signal. All the presented results were obtained on the ODE beamline at the two edges of each model PBAs (A and Fe), which is crucial to understand what happens on each side of the A—NC—B linkage.

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Advanced Non-destructive *in-siCu* Characterization on the French CRG D2AM/BM02 Beamline

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ABSTRACT

The new possibilities of accessing non-destructively the structural properties of devices, using intense X-ray synchrotron source, combined with specific equipment, enabled the possibility of conducting *in-situ* and *operando* structural characterizations. This tool attracted researchers, in particular, metallurgists for conducting more complex and ambitious experiments aiming to answer questions yet unresolved regarding formation mechanisms, phase transitions, magnetism or characterizing more complex alloys for industrial application. In this paper, we introduce the D2AM beamline (Diffraction Diffusion Anomale Multi-longueur d'onde), a French CRG (collaborative Research Group) beamline at the European Synchrotron ESRF, dedicated to *in-situ* X-ray scattering techniques. The design of the beamline, together with the combination of the available equipment (two-dimensional fast photon counting detectors, sophisticated high precision kappa diffractometer, a variety of sample environments, continuous scanning for X-ray imaging and specific software for data analysis) made the D2AM beamline a highly efficient tool for advanced *in-situ* synchrotron characterization in materials science, i.e. crystals, powders, liquids, polycrystalline materials, thin films and micro/nano-structures. Aiming to provide a complete database for planning future projects and beamtimes, this poster gathers the main elements and equipment available at the beamline and shows its potential and flexibility for performing a wide variety of *in-situ* time and space resolved X-ray synchrotron measurements.

Fermi Surface Anisotropy of the Metallic Boron Doped Diamond

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ABSTRACT

Doping pure diamond thin films with boron atoms induces a phase transition towards a metallic state. The boron doping lifts the top of the diamond valence band above the Fermi level, and makes this metallic phase easily measurable by photoemission spectroscopy [1]. High resolution ARPES has evidenced a small Fermi surface centered at the center of the Brillouin zone, and the polarization of the SR light oriented in several directions has allowed to separate the three different hole sheets of the Fermi surface. The experimental data are compared with the theoretical Fermi surface obtained using the k.p model.

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Mesure de la Section Efficace de Photoionisation du Radical Hydroxyle

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ABSTRACT

Surnommé parfois le « détergent » oxydant de l'atmosphère terrestre [1] mais aussi présent dans différents milieux astrophysiques (comètes [2], nuages interstellaires [3], etc.), le radical hydroxyle, de formule OH, joue un rôle clé dans un grand nombre de processus photophysiques complexes dans ces différents milieux. Produit lors de la photolyse de H_2O en particulier, OH peut être photoionisé par un rayonnement dans l'ultra-violet du vide (VUV) et sa forme cationique peut ainsi participer à la régénération de H_2O (voir Figure 1) [4]. La photoionisation du radical OH constitue donc une étape fondamentale dans le cycle photochimique de l'eau. Il est donc crucial de quantifier la section efficace de photoionisation de OH dans le VUV pour pouvoir modéliser correctement ce cycle.

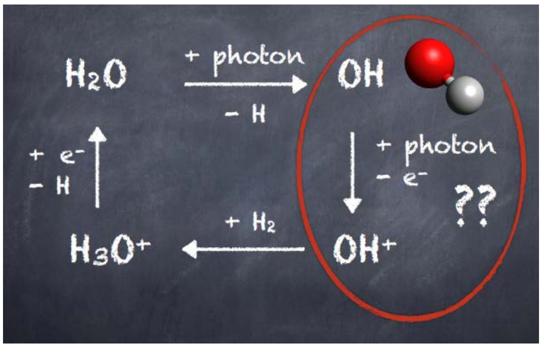

Figure 1 : Cycle photochimique de H_2O présent dans divers milieux astrophysiques et atmosphériques

En utilisant le rayonnement VUV de la ligne DESIRS du synchrotron SOLEIL couplé au spectromètre de photoions et photoélectrons en coïncidence DELICIOUS III, nous avons étudié la photoionisation du radical OH entre 13 et 15 eV. Le radical est produit dans un réacteur à écoulement par réaction entre H_2O et du fluor atomique généré à partir de F_2 dans une décharge micro-onde. Nous avons calibré le rendement d'ions OH^+ en section efficace absolue grâce à un point de mesure à énergie fixe en comparant, dans les spectres de masses obtenus, la consommation du parent (H_2O) et la production du radical (OH) correspondant à l'abstraction d'un atome d'hydrogène. L'originalité de la méthode utilisée est qu'elle ne nécessite pas de connaître la quantité absolue de radicaux OH ni de calibrer le spectromètre de masse au préalable.

La section efficace de photoionisation de OH ainsi obtenue [5] remet en question la valeur utilisée dans les modèles jusqu'à présent, ainsi que celle obtenue récemment par une méthode très indirecte [6].

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Uranyl Covalency Change in Borate Glasses Probed by XAS

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ABSTRACT

Determining the uranyl (VI) reactivity in oxides is necessary to control its mobility.[1] The intrinsic versatility of borate structural units containing both triangular BO_3 and tetrahedral BO_4 makes them original and rich hosts for uranyl.[2] As part of the effort to determine the uranium stability in oxide glasses, we have determined the speciation of uranium(VI) in two lithium borate glasses containing respectively 10 mol% and 30 mol% Li_2O using X-ray absorption spectroscopy (XAS).

M_4-edge high-resolution XAS is a unique tool to probe uranium 5f orbitals and determine oxidation state and covalency.[3] We have recently implemented the technique on the MARS beamline taking advantage of the lower bound of the beamline energy range. It allows us to demonstrate the speciation of U(VI) as uranyl in both glasses.

Comparison of uranyl bond distances obtained by L_3-edge EXAFS with distances found in borate crystals reveal that in the low alkali borate glass uranyl is present as UO_8 hexagonal bipyramids. This local environment was never observed in any other oxide glass. We show that the increase of the lithium content decreases the equatorial coordination shell to partially convert the UO_8 species into UO_7. The associated decrease of the covalency of the uranyl trans-dioxo bonds in parallel to uranyl bond elongation suggests the influence of the equatorial ligands.

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Cadmium Phytoremediation by the Hyperaccumulating Plant *Conyza Sumatrensis*

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ABSTRACT

Phytoremediation represents an ecological, low-cost, and efficient technique to remove heavy metals from contaminated soils. To develop methods that can optimize the cadmium (Cd)-hyperaccumulating capacity of plants employed to decontaminate Cd-polluted soils, it is essential to understand the sequestration mechanisms and Cd chemical forms in the plants. Previous studies have used X-ray absorption spectroscopy (XAS) techniques despite their inherent limitation when studying Cd speciation in plants [1-3]. One of the limitations is the low concentration of cadmium in plants that make the study of its chemical forms using XAS technique highly challenging.

Previous study has evidenced the Cd-hyperaccumulating capacity of *Conyza sumatrensis*, a cosmopolitan annual herb, in field conditions [4]. In this context, we first of all cultivated *C. sumatrensis* in pots containing increasing concentrations of cadmium and under controlled greenhouse conditions in order to determine the Cd-limiting concentration for plant growth and XAS analyses.

In the pot experiments containing 280 mg/kg of cadmium in soil, the plant growth was negatively affected, biomass decreased and no stem was produced in comparison to plant grown in pot experiments below 120 mg/kg of cadmium in soil. Results from ICP-OES analyses indicated that mean Cd levels in this plant could be similar to those measured in the same type of plant tested in field conditions (i.e. about 25 mg/kg dry weight), however Cd was mainly translocated into plant knots (up to 90 mg/kg of cadmium in dry sample). Bulk Cd K-edge X-ray absorption near edge spectroscopy (XANES) analyses indicated that Cd speciation was similar in the different part of the shoots (i.e. stem, knots and leaves). These results might help performing further experiments including Cd-resistant endophyte bacteria in order to enhanced Cd phytoremediation by *C. sumatrensis* and determine Cd speciation in plant system.

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Using FASTOSH to Determine Lead Speciation in Contaminated Soils

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ABSTRACT

FASTOSH is a new standalone program to process X-ray Absorption Fine Structure (XAFS) spectroscopy data [1]. It should be particularly useful for geochemical and environmental applications where the XAFS technique is employed. The main graphical interface is user-friendly and inspired from Athena featured in Demeter & Ifeffit Software Package [2]. Imported functions from Larch [3] allow normalizing XAFS spectra and conveniently background subtracting EXAFS scans collected with a step-by-step or rapid continuous acquisition mode. To fit the pre-edge region of an unormalized spectrum, a linear (Larch built-in) or quadratic (FASTOSH) function can be employed. The latter may be useful to correctly normalize the spectrum, collected in fluorescence mode, corresponding to an element present at a low concentration in a sample such as a soil or sediment containing a contaminant. The code enables beam line users to follow in real-time the progress of their acquisition by automatically displaying the XANES or EXAFS spectra collected including the merge and progressive improvement of its signal-to-noise ratio. It also proposes an interactive background-subtraction tool for Multi-Channel Analyzer (MCA) patterns collected by multi-pixel fluorescence detectors. This can help minimize, in the XAFS spectrum extracted from MCA patterns, distortions due to acquisition artefacts such as diffraction phenomenon arising from well-crystalline solid or frozen liquid samples. Additionally, the code features auto-deglitching options, and a PCA/Target Transformation module that can instantaneously process a large library of XAFS spectra. It also proposes a tool to post-treat data processed by the MCR-ALS Matlab Toolbox of Jaumot et al [4]. This enables to calculate an amplitude correction factor that allows comparing the EXAFS spectra of the extracted pure phases with those corresponding to references [5]. This study showcases the functionalities of FASTOSH. It also demonstrates how a combination of Target Transformation and MCR-ALS approaches can be helpful in identifying the chemical forms of lead (Pb) present in polluted soils [5].

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Ligne Française CRG-IF BM32: Activités et Perspectives Post-upgrade de l'ESRF

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ABSTRACT

La ligne de lumière InterFaces (IF) localisée au synchrotron européen de troisième génération à Grenoble (ESRF) possède trois instruments et une panoplie de techniques de diffraction et diffusion des rayons intenses de 5 à 30keV. Les surfaces, interfaces et microstructures sont étudiées à l'aide d'une part d'un faisceau monochromatique de plusieurs centaines de microns en taille et d'autre part d'un faisceau polychromatique de quelques centaines de nanomètre pour les expériences de microdiffraction Laue. Les techniques de mesures et les logiciels de traitement de données sont adaptées à l'exploration et la mesure des propriétés structurales des matériaux et dispositifs dans les domaines de recherches fondamentaux et amont. Grâce à des mesures *in situ* et *operando* [1], notamment sous ultra-vide [2], la ligne IF dispose de moyens capables de comprendre et contrôler les mécanismes fondamentaux dans des systèmes modèles, complexes ou dans ceux impliqués dans les procédés technologiques (matériaux microélectronique, photoniques, pour l'énergie). La ligne IF est particulièrement performante pour mener des recherches en nanoscience, comprendre les relations structure-propriétés dans les matériaux innovants et fonctionnels [3].

En septembre 2020, les trois instruments de la ligne de lumière reprendront le service aux utilisateurs après les 18 mois nécessaires à l'installation de leur nouvelle source de rayons X plus brillante (programme d'upgrade de l'ESRF). Cette période d'arrêt sera mise à profit pour poursuivre les développements logiciels pour l'assistance aux utilisateurs pendant l'acquisition des données ainsi que la visualisation et la manipulation des données toujours plus massives et complexes. Ces systèmes s'appuieront sur l'efficacité du nouveau système contrôle-commande déployé à l'ESRF (BLISS). Seront aussi poursuivis l'optimisation et le développement des outils d'analyse de données reposant sur l'emploi de détecteurs 2D grand champ et rapides. Les possibilités de modernisation d'envergure des équipements et des infrastructures de la ligne adaptées à la nouvelle source sont multiples. Elles permettront d'accroître les capacités de mesures en termes de volume et de précision avec de meilleures résolutions spatiale et temporelle (projet d'EQUIPEX MAGNIFIX).

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Microtomography at the ANATOMIX Beamline

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ABSTRACT

ANATOMIX is a long undulator beamline for full-field radiography and tomography with X rays (monochromatic or white beam) in the energy range from 5 keV upward [1,2], offering absorption and phase-contrast microtomography in parallel-beam projection geometry (Figs. 1, 2) and nanotomography with a transmission X-ray microscope (TXM) [3,4]. The beam size at sample without any optics in the beam is approximately 20 mm × 15 mm (h×v). It can be increased horizontally to more than 40 mm by a meridionally-focusing double mirror with horizontal deflection. Since summer 2017, the beamline has been taking microtomography data. The TXM has been opened for proposals in the current call.

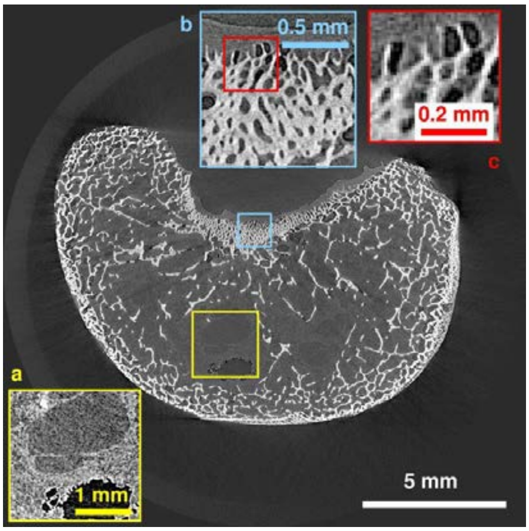

Figure 1. White-beam tomogram of a chicken tibia. Peak energy 20 keV, pixel size 9.3 µm. Details: (a) soft tissue; (b,c) trabecular bone. 1000 projections, exposure time per projection 0.06 s.

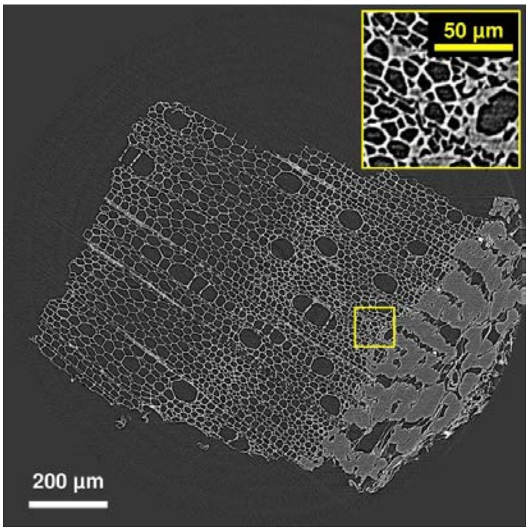

Figure 2. White-beam phase-contrast tomogram of a piece of stem from a hemp plant. Peak energy 10 keV, pixel size 0.65 µm, detector–sample distance 12 mm. 1500 projections, scan duration 5 minutes. (Sample: J. Beaugrand, INRA, Nantes.)

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The LOREA ARPES Beamline at the ALBA Synchrotron

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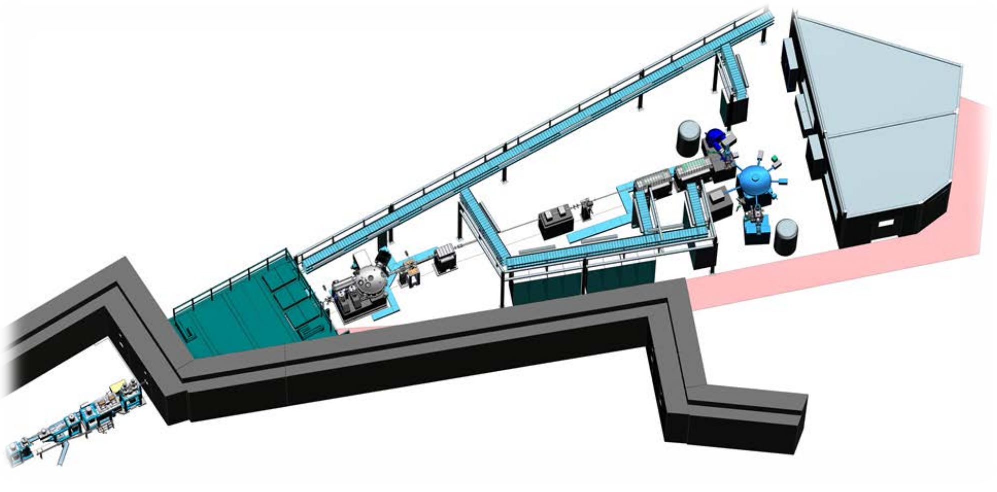
ABSTRACT

In the present work, we report the design and construction status of LOREA, the ALBA synchrotron beamline devoted to electronic structure investigation by means of Angle Resolved Photo-Emission Spectroscopy (**ARPES**).

LOREA is the ninth beamline of the **ALBA synchrotron radiation source**, it is under construction and will be in operation in 2020.

The beamline is designed to cover **the photon energy range of 10-1000 eV**, with continuously variable polarization, resolving power of more than 10^4 in the whole range, and spot size of about 10x10 μm^2. The photon flux is expected to be of the order of 10^{13} (ph/s/0.1%BW) for photon energies up to 350 eV, and above 10^{12} (ph/s/0.1%BW) in the 350-1000 eV. Thanks to the wide energy range and high photon flux, LOREA will be suitable for high resolution **VUV ARPES** investigation in the range of 10-200 eV, with the possibility to extend the ARPES measurements in the 200-600 eV energy range (**Soft X-ray ARPES**). In addition, core level spectroscopy, resonant photoemission and X-ray absorption spectroscopy will be accessible in the whole energy range.

The end station of LOREA will be composed by a central radial distribution chamber to which all other vessels are connected, including chambers for ARPES investigation, **in situ UHV deposition** and **characterization**, high pressure deposition (**Chemical Vapor Deposition**, CVD, and **Atomic Layer Deposition**, ALD), **organic molecule** deposition; sample storage, docking of **vacuum suitcases**, docking of **STM**, and fast entry load lock.



A New High Temperature Reactor for *operando* XAS Characterization of Catalysts

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ABSTRACT

Heterogeneous catalysts commonly exhibit a variety of different surface sites that are difficult to identify. Identification of the active sites is critical for the design and development of improved catalytic materials. Ideally, characterization of a catalyst involves the measurement of its corresponding properties during the catalytic reaction, *i.e.*, *operando* conditions. Currently, X-ray absorption spectroscopy (XAS) is one of the most widely used techniques for analysis of catalysts under reaction conditions due to the penetration depth of the high-energy X-rays, enabling adequate analysis of the electronic and structural properties of heterogeneous catalysts. We developed a new high temperature reactor for *operando* XAS[1], which offers the capability of using fluorescence and transmission detection modes. The reaction cell includes a plug-flow reactor made from glassy carbon which allows almost all of the X-rays to be transmitted to the sample. The oven of the reaction cells is able to heat up to 1000 °C and ensures a homogeneous temperature profile along the catalytic bed which is important to the study of catalysts under *operando* conditions. To validate our final design, the reaction cell was used for the characterization of a low metal loading Ni/ZrO_2 powder catalyst in the DRM reaction under realistic conditions (750 °C). The reaction system includes a fully remote-controlled gas distribution system. The combination with mass spectrometry for monitoring the gas composition in real time offers a powerful tool for simultaneous characterization of a catalyst and the measurement of its catalytic activity. The performance of the reaction cell was validated by comparing it with the catalytic results obtained in a conventional dynamic microreactor (PID Eng & Tech) using the same conditions.

The complete setup dedicated to the study of catalysts has been used successfully in different studies[2,3] and is permanently installed on the CRG-FAME and FAME-UHD beamlines (BM30B and BM16) at the European Synchrotron Radiation Facility (ESRF) in Grenoble, France.

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Localization of Minerals and Phenolic Compounds in Apple Fruit

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ABSTRACT

Metallic ions and phenolic compounds are both linked to fleshy fruit organoleptic characteristics, such as texture, color and taste of fresh and processed products. Potassium and calcium participate to tissue turgor pressure and cell wall polysaccharides cross-links associated to texture, while transition metal cations (iron, manganese, zinc or copper), free and/or complexed in metallo-proteins, are involved in oxidation reactions, which disassemble the cell wall during fruit ripening or modify phenolics impacting color and taste. To better understand the relationships between metallic cations and phenolics on fleshy fruit quality, the distribution of these compounds was investigated in apple. To circumvent low metal and phenolic concentrations and high diffusible behavior, an original cryo-processing approach was developed. The resulting cryo-processing methods were implemented for synchrotron cryo-X-ray and cryo-deep-UV fluorescence imaging of two texture and phenolic-contrasted apples varieties. An adapted qualitative analysis treatment was developed.

Results showed gradient distribution and content of metallic ions and phenolic. Cations were observed mainly in the cell walls and cuticle. Calcium and iron presented a gradient distribution from the cuticle to the inner cortex, while potassium was distributed homogeneously in the fruit tissue cell walls. Phenolic compounds were localized within cell but also in cell walls as hydroxycinnamic acid. Their distribution differed mainly within the cuticle and epidermal cell layers. The distribution of these compounds will be discussed with regards to fruit metabolism and possible consequences on fruit texture, color and flavor elaboration. This approach will be transferred to other varieties of fleshy fruits such as grapes.

Spectroscopic Parameters of CH_3Cl in the $^{Q}P(J,K)$ and $^{Q}Q(J,K)$ of the ν_3 Fundamental Band

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ABSTRACT

Methyl chloride is the only chlorinated compound present in the atmosphere with a very predominantly natural origin [1]. This molecule is emitted by the oceans where it is produced by algae [2], forest fires [3] and certain tropical plants [4]. It is a weakly reactive molecule that can cross the troposphere and reach the stratosphere. Its lifespan in the atmosphere is 1 to 3 years [5]. The release of radical Cl can then participate in the destruction of ozone through the catalytic cycle ClO_x .The Montreal Protocol (October 1999) and its subsequent amendments recommended a sharp reduction in the production and use of CFCs. Of these CFCs, CH_3Cl is the most abundant halocarbon present in the atmosphere (530 and 560 ppt). This molecule represents 30% of atmospheric chlorine and is one of the main factors for the destruction of stratospheric ozone.

Modeling the infrared spectra of the CH_3Cl molecule requires knowledge of the parameters characterizing the individual absorption lines (intensity, broadening coefficients ...).These parameters have been investigated at room temperature in the region between 600 and 1200 cm^{-1} for the vibrational fundamental band ν_3 of CH_3Cl self-perturbed. The spectra of the CH_3Cl molecule were recorded at the AILES line of the SOLEIL Synchrotron in Saint-Aubin Paris at a resolution of 0.003 cm^{-1} for pressures between 1.02 and 10.24 mbar. In this work, we present the results obtained for the $^{Q}P(J,K)$ and $^{Q}Q(J,K)$ sub branches of this band. These spectra were analyzed using a multi-spectrum fitting method with a Voigt profile.

All the previous works in this band have been performed using tunable diode-laser spectrometer for a small spectral region and limited number of lines [6-8]. In summery this work enables us to achieve a large line list of measurements of line intensities and broadening coefficients to update spectroscopic database and to validate theoretical models.

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FAME-UHD: French X-ray Absorption Beamline Dedicated to High Energy Resolution Fluorescence Detection at Ultra-high Dilution Level

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ABSTRACT

The study of highly diluted elements by X-ray Absorption Spectroscopy (XANES and EXAFS) is challenging, especially in the environmental bio-/geo-chemistry sciences. This large and diverse research field aims at understanding the interaction between a pollutant and a biotope at natural concentrations, that is, below 10 ppm (parts-per-million, mg/kg). The French x-ray Absorption spectroscopy beamline for Material and Environmental sciences at Ultra-High Dilution (FAME-UHD), located on the port BM16 of the European Synchrotron Radiation Facility (ESRF), was built to routinely work at this dilution level.

FAME-UHD is a bending magnet beamline optimized for photon flux and energy resolution in the hard X-ray energy range, from 4.8 to 20 keV. The primary optics consists of two Rh-coated mirrors. The first mirror acts as a vertical collimator and harmonics rejector, while the second one focuses the beam vertically on the sample. The monochromator is composed of two Si(220) crystals with large horizontal acceptance, up to 110 mm, covering 2 mrad divergence of the source. The first crystal is flat and liquid nitrogen cooled. The second crystal is dynamically sagittally bent, permitting horizontal focusing at the sample position. The beam size on the sample is 100×200 µm2 (full-width-at-half-maximum, vertical × horizontal) with a flux of 9×10^{11} ph/s at 12 keV.

The experimental station is based on a heavy duty large hexapode table hosting a versatile sample environment, four sequential beam monitors with slits, two silicon-drift fluorescence detectors, and a crystal analyzer spectrometer. The wavelength dispersive spectrometer is composed of fourteen spherically bent crystal analyzers of 1 m radius, arranged in two rows of seven crystals each, describing a two-circles Rowland geometry. Selected fluorescence photons are collected by a hybrid pixel two-dimensional detector. The spectrometer operates in the Bragg angular range from 89° to 65°, with an energy resolution, $\Delta E/E$, in the order of 10^{-4}. Full sets of silicon and germanium crystal analyzers are available in standard cutting directions.

Currently, three sample environment configurations are available: 1) liquid helium cryostat; 2) high-pressure/temperature autoclave; 3) catalytic reactor with gas lines. Furthermore, specific sample environments may be provided directly by the users.

The beamline is open to users' operation since January 2017 and has demonstrated its performances in key experiments: 1) the speciation of Ce at 1 ppm dilution in natural organic matter; 2) 1% of Ba in confined UO2 samples, heated in a controlled gas up to 700 °C.

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Nanotomography at the ANATOMIX Beamline

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ABSTRACT

The transmission X-ray microscope (TXM) [1] on SOLEIL's ANATOMIX beamline [2,3], based on diffractive optics, enables full-field nanotomography at photon energies around 6, 10 and 17 keV, at resolutions down to 100 nm or less and pixel sizes down to 30 nm. The diffractive optics for the TXM —beam shapers [4], iridium zone plates [5,6] and phase masks— are manufactured at the Paul Scherrer Institut.

Several test and commissioning campaigns on the optics and mechanics of the instrument were recently conducted (Fig. 1), including acquisition of tomography data (Fig. 2).

The instrument will go operational in the second half of 2019 and is open for proposals in the current SOLEIL call for projects (working energy currently limited to 10 keV).

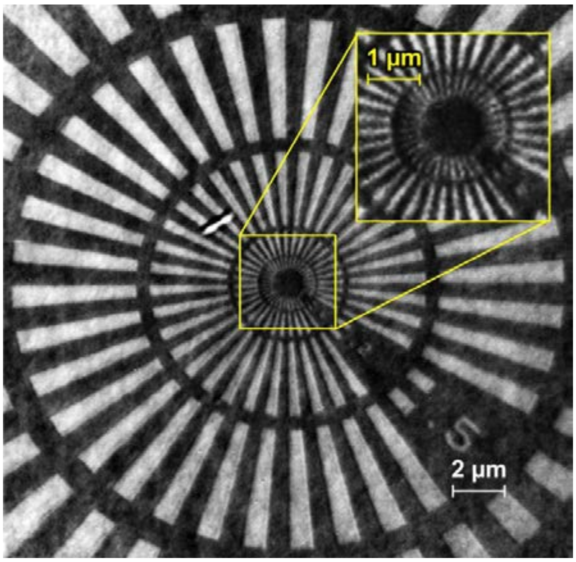

Figure 1. Detail of a TXM micrograph at 10 keV showing a reference chart with smallest widths of lines and spaces of 50 nm (center of inset).

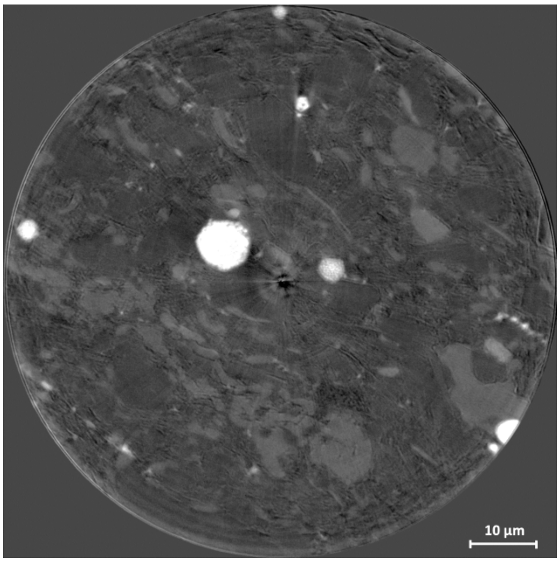

Figure 2. Sagittal TXM tomography slice of a shale sample with pyrite inclusions (light gray).

REFERENCES

[1] M Scheel et al, Microsc. Microanal. 24(S2) (2018) 246.
[2] T Weitkamp et al, J. Phys. Conf. Series 849 (2017) 012037.
[3] T Weitkamp et al, Microsc. Microanal. (2018), 24(S2) (2018) 244.
[4] I Vartiainen et al, Opt. Lett. 39 (2014) 1601.
[5] J Vila-Comamala et al, Opt. Express 19 (2011) 175.
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TUTORIALS

TUTORIALS

Friday, January 18th

Photoemission

Synchrotron SOLEIL - Salle Formation – Bât. T5

TU-01

X-Ray Photoemission Spectroscopy: Processing, fitting and analyzing data acquired with synchrotron light

J. Rault** & **M. Silly

Coherence

Synchrotron SOLEIL - Salle Libra – Bât. Central

TU-02

Introduction générale à la cohérence et les techniques associées

F. Berenguer

TU-03

Challenges of bio-inspired material science and perspectives in the - coherent - light of 4th generation Synchrotron sources

V. Chamard

TU-04

Bragg Coherent Diffraction Imaging benefits for materials science

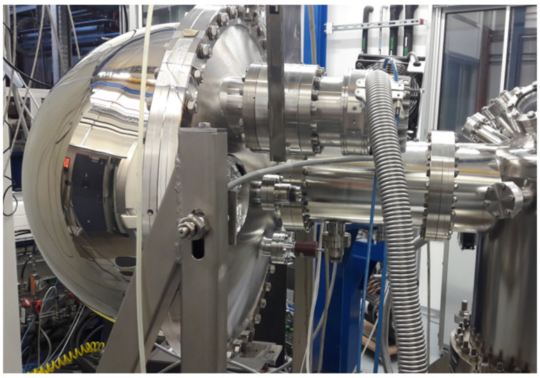
S. Labat

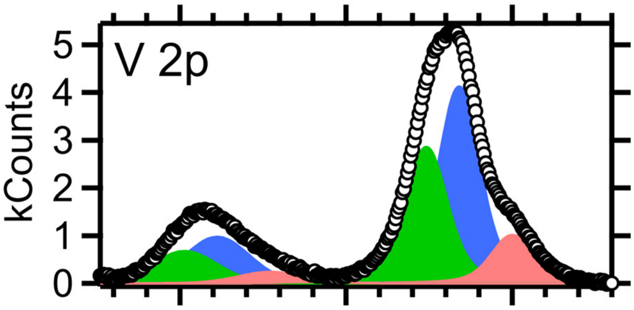
TU-05

Benefits of coherence for imaging of complex natural and manufactured materials

L.J. Michot

X-Ray Photoemission Spectroscopy: Processing, fitting and analyzing data acquired with synchrotron light



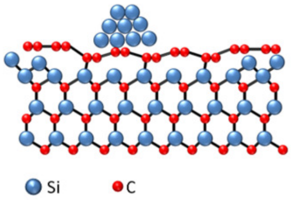


Instructors: Julien Rault (Cassiopee) and Mathieu Silly (Tempo)

Schedule : Friday, January 19, 3pm to 6pm

Location: SOLEIL, Building T5

The aim of this tutorial is to give first-hand experience on X-ray Photoelectron Spectroscopy (XPS) data processing and analysis, focusing on the specificities offered by synchrotron light. A brief introduction will present the data acquisition and the very first data treatments, followed by two practical case studies on Soleil computers:



- Low energy XPS – Surfaces and 2D materials
  Identification of surface / interface components using variable energies.
- High energy XPS (HAXPES) – Buried interfaces
  Potential / charge profile via angle-dependent experiments.
  Chemical depth profile using standing-wave methods.

This tutorial should help users be more autonomous to analyze their XPS data but also in submitting proposals to XPS/HAXPES beamlines in synchrotron facilities.

The number of participants is limited to 20 people.

Tutorial : COHERENCE

L'objectif de ce tutorial est de faire une présentation générale de l'apport de la cohérence sur synchrotron pour les différentes communautés d'utilisateurs. Elle s'adresse à un public non averti, désireux de connaître les potentiels de ces techniques émergentes.

Les différentes techniques basées sur la cohérence seront présentées dans un premier temps (imagerie par diffraction cohérente, ptychographie, tomographie avec contraste de phase, holographie), et illustrées par des exemples provenant de différentes communautés scientifiques.

Dans une deuxième partie, différentes présentations illustreront les apports de l'évolution vers des synchrotrons de 4$^{\text{ème}}$ génération pour ces techniques.

The objective of this tutorial is to make a general presentation of the interest of coherence of synchrotron radiation for the different communities of users. It is conceived for non-specialist public, eager to know the potential of these emerging techniques.

The different coherence-based techniques will be presented (coherence diffraction imaging, pychography, phase contrast tomography, holography) and illustrated with examples from different scientific domains.

In a second part, different presentations will illustrate the contribution of evolution to 4th generation synchrotrons for these techniques.

Challenges of Bio-inspired Material Science and Perspectives in the - *Coherent* – Light of 4th Generation Synchrotron Sources

V. Chamard

Aix-Marseille Univ, CNRS, Centrale Marseille, Institut Fresnel, Marseille

ABSTRACT

Biominerals and bio-inspired materials are subject to intense studies [1] owing to their major roles in *e. g.*, ecology [2], paleoclimatology [3] and material design [4], to cite only a few. On the contrary to their geological counterparts, those materials are characterized by a hierarchical 3D structure arising from non-classical organic-mediated crystallization pathways. Consequently, biominerals and bio-inspired crystals present strong chemical (trace elements, amorphous phases) and physical (granular morphology) structural distributions, covering several length scales.

These specificities challenge the experimentalists. In particular mimicking the relationship between the mechanical properties and the structure, deciphering the pathways underlying crystallisation and dissolution processes and understanding the role of the trace elements illustrate the most acute questions in the field. In this context, the advent of fourth generation synchrotron sources delivering highly intense coherent beams will open major perspectives, for developing fast, multi-length scale, physical and chemical sensitive, coherent diffraction imaging approaches [5, 6]. They will be reviewed in this presentation.

REFERENCES

1. DeYoreo *et al*., Science (2015).
2. A. Ridgwell and R. Zeebe., Earth and Planetary Science Letters 234 (2005).
3. D. Lea *et al*., Science **289** (2000).
4. L. Li and C. Ortiz, Adv. Funct. Mater **25** (2015)
5. S. O. Hruszkewycz *et al.*, Nature Materials (2017).
6. F. Mastropietro *et al.*, Nature Materials (2017).

Bragg Coherent Diffraction Imaging Benefits for Materials Science

S. Labat

Aix-Marseille Univ, IM2NP, Marseille

ABSTRACT

Coherent Diffraction Imaging in Bragg condition (BCDI) is a non-destructive method allowing studies of crystalline materials thanks to its high sensitivity to displacement field and electronic density. The use of focusing optics and 3rd generation synchrotron radiation sources has increased the capability of imaging sub-micron crystals with a spatial resolution of few nms and a displacement accuracy of 1 pm. The following examples of studies using BCDI will be presented: inversion domain boundaries in GaN nanowires, dislocations in tetrahexaxedral Pt nanoparticles, interdiffusion in Ge-Si Core-Shell nanowires and mechanical behavior of individual grain in polycrystalline Au thin film.

Benefits of Coherence for Imaging of Complex Natural and Manufactured Materials

L. J. Michot

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ABSTRACT

Most environmental materials as well as numerous building materials are multi-scale objects that are highly variable and heterogeneous. Understanding and predicting reactivity, transport, mechanical properties, etc… of such systems therefore requires the use of a combination of various simulation methods and characterization tools. Among those, X-ray imaging techniques in both the hard and soft X-ray range are particularly valuable. Furthermore, the increase in coherence provided by the new sources under development could open new and unique opportunities in the field. Based on a few selected examples, we will try to assess the potential of the use of highly coherent X-rays in the study of complex multiscale natural and manufactured materials.

LIST OF COMMERCIAL EXHIBITORS

SUM19 - List of Commercial Exhibitors

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Added Value Solutions	Pedro NOGUERA CRESPO Miguel Angel CARRERA ASTIGARRAGA	34 661 325 019 34 676 23 87 33	pnoguera@a-v-s.es macarrera@a-v-s.es
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