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|  | Journée Scientifiques Grands Instruments  Lundi 2 décembre 2024  Salle D420 |

**Programme**

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| 09h00 – 09h25 | Accueil des participant.e.s |
| 09h25 – 09h30 | Introduction |
| 09h30 – 10h10 | **Andrea Perruchi** (Fermi, Elettra-Sincrotrone Trieste, Italy)  *“Terahertz nonlinear and ultrafast studies at TeraFERMI”* |
| 10h10 – 10h35 | **Hester Blommaert** (Institut Néel)  *“Gold complexes as chemotherapeutic agents: HERFD-XAS as a tool to study their biotransformation in human cancer cells”* |
| 10h35 – 11h00 | **Arthur Thalarmin** (Institut Néel)  *“Searching for axions from the galactic dark matter halo with haloscopes”* |
| 11h00 – 11h25 | Pause |
| 11h25 – 12h05 | **Xavier Fabrèges** (Laboratoire Léon Brillouin, UMR12, CEA Saclay)  *“ICONE: the French HiCANS Neutron Source”* |
| 12h05 – 12h30 | **Georg Knebel** (CEA)  *“Multiple superconducting phases in the heavy fermion superconductor UTe”* |
| 12h30 – 14h00 | Déjeuner / Buffet |
| 14h00 – 14h40 | **Victor Porée** (Synchrotron SOLEIL, Gif-sur-Yvette, France)  *“Advancing RIXS: New Instrumental Capabilities for Operando and Field-Dependent Studies at the SEXTANTS Beamline”* |
| 14h40 – 15h05 | **Jean-Sébastien Micha** (SyMMES – CRG-IF)  "*LaueMAX: a high-flux Laue diffraction X-ray microscope for materials science and nanoscience*" |
| 15h05 – 15h30 | **Coline Theron** (Institut Néel)  *“The complementarity of in-situ and synchrotron-based techniques to study the schematic Holocene rock art”* |
| 15h30 – 15h55 | **Igor Vinograd** (LNCMI)  *“Nuclear Magnetic Resonance in extreme conditions at LNCMI”* |
| 15h55 – 16h15 | Pause |
| 16h15 – 17h00 | **Echanges sur l’activité de l'axe** |

**Résumés (pages suivantes)**

Andrea Perucchi

**Terahertz nonlinear and ultrafast studies at TeraFERMI**

**Andrea Perucchi**

Fermi, Elettra-Sincrotrone Trieste S.C.p.A., Trieste, Italy

TeraFERMI is the THz beamline of the FERMI Free-Electron-Laser facility. TeraFERMI provides broadband ultrashort intense pulses with peak fields exceeding 5 MV/cm and Tesla magnetic fields. Thanks to these extremely large THz fields, TeraFERMI allows for nonlinear spectroscopy and pump-probe studies. We review here the characteristics of the beamline, the available experimental set-ups, as well as some selected experimental results. We will particularly focus on the study of Dirac materials which are of special interest due to their peculiar band dispersion. The absence of parabolicity at the bottom of the conduction band is at the origin of intrinsic nonlinearities in the terahertz range and gives rise to a wealth of fascinating and technologically relevant phenomena, from saturable absorption to plasmon softening and terahertz harmonics generation.

H. Blommaert

**Gold complexes as chemotherapeutic agents: HERFD-XAS as a tool to study their biotransformation in human cancer cells**

**H. Blommaert1**, O. Proux2, I. Kieffer2, M. Rovezzi2, Y. Joly1, E. Lahera1, C. Soep3, B. Bertrand3, M. Salmain3, S. Bohic4, J-L. Hazemann1

1 Institut Néel, Univ. Grenoble Alpes, CNRS, Grenoble INP, 38000 Grenoble, France

2 OSUG, UMS 832 CNRS - Université Grenoble Alpes, F-38041 Grenoble, France

3 Sorbonne Université, CNRS, Institut Parisien de Chimie Moléculaire (IPCM UMR 8232), F-75005 Paris, France.

4 Université Grenoble Alpes, INSERM, UA7 STROBE, Synchrotron Radiation for Biomedicine, F-38400 Saint Martin d’Hères, France

Organogold(III) complexes have recently attracted attention due to their promising anticancer properties, highlighting their potential as chemotherapeutic agents. However, detailed knowledge of the chemical transformations these Au(III) complexes undergo in biological environments, such as ligand exchange or reduction to Au(I)/Au(0), remains scarce. This gap limits our understanding of their molecular mechanisms of action. To address this, we employed High Energy Resolution Fluorescence Detected X-ray Absorption Near Edge Structure (HERFD-XANES) at the BM16-beamline to investigate the intracellular speciation of a series of organogold(III) complexes incubated in human cancer cells.

In this presentation, I will detail the sample preparation steps, comment on the (dis)advantages of HERFD-XANES for biological samples, and compare the experimental spectra with modelled spectra obtained with the FDMNES code. Finally, I will relate the observed intracellular speciation with the anticancer activity of these complexes.

Arthur Thalarmin

**Searching for axions from the galactic dark matter halo with haloscopes**

**Arthur Thalarmin**

The axion, a hypothetical fundamental particle, is a promising candidate to dark matter. This mysterious form of matter, first speculated in the early 1930s, would notably explain the stability of galaxies and other structures, and is thought to represent about 85% of the mass of the Universe.

It was shown that dark matter axions might be detected in a terrestrial laboratory through their conversion, thanks to a strong static magnetic field, into quasi-monochromatic microwave photons that excite a resonant cavity: the idea of the haloscope was born.

Today, important efforts are made to search for galactic axions all around the world. However, probing upper mass bounds of axion dark matter remains a challenge, because increasing the resonance frequency implies to reduce cavity radius, thus, detection volume.

In this talk, I will first expose generalities about haloscopes, then focus on the work done during my first year of PhD with GrAHal in Grenoble to develop a new frequency tuning method to be implemented in complex cavities reaching high frequencies while keeping a large volume. This technique, based on slow liquid helium filling of the cavity, could be applied to future haloscopes operating in the superconducting outsert of LNCMI hybrid magnet.

Xavier Fabrèges

**ICONE: the French HiCANS Neutron Source**

**Xavier Fabrèges**

Since the shutdown of the Orphée reactor, France is missing a national neutron facility to support its scientific community. Neutron sources worldwide are progressively transitioning from traditional reactor-based sources (such as ILL, Orphée, and FRM II) to pulsed sources (ESS, SNS, J-PARC). In parallel, the development of High Current Accelerator-driven Neutron Sources (HiCANS) offers a cost-effective route for building high-performance pulsed neutron sources on a smaller scale.

In this context, CEA and CNRS are working on the ICONE project, which aims to establish a French HiCANS facility designed to serve the national scientific community, prepare for optimal use of the ESS and train the younger generation. The project is in the “Avant Projet Détaillé” phase, during which the complete design of the facility is being developed.

A key aspect of this effort is the development of an instrument suite in collaboration with the community. This is done by collecting needs, collaborating on specific aspects through the APICONE call for proposals held in 2024 and the input of the Scientific Council. The planned suite consists of 10-12 instruments, installed on two targets optimized for flux (SANS, reflectometry, …) or resolution (diffraction, inelastic neutron scattering, …).

This presentation will provide an overview of the ICONE project and discuss the details of the instrument suite, with a focus on the specificities and opportunities arising from the pulsed nature of the source.

Georg Knebel

**Multiple superconducting phases in the heavy fermion superconductor UTe**

**Georg Knebel**

The unconventional superconductor UTe­2 has attracted much attention due to the possible spin triplet pairing in the superconducting state. Hallmarks for this are the extremely high superconducting critical fields along the different crystallographic directions and the appearance of multiple superconducting phases as a function of magnetic field and high pressure. In particular, when the field is applied along the b axis of the magnetic hard direction a spectacular re-enhancement of superconductivity is observed. While initially the proximity to a ferromagnetic quantum phase transition had been proposed as driving mechanism for superconductivity, inelastic neutron scattering clearly show the appearance of incommensurate antiferromagnetic magnetic fluctuations. Furthermore, under the application of high-pressure antiferromagnetic order occurs. In this presentation, we will give an overview on recent experiments obtained at the LNCMI Grenoble and by neutron scattering under extreme conditions emphasizing the rich physics in UTe2.

Victor Porée

**Advancing RIXS: New Instrumental Capabilities for Operando and Field-Dependent Studies at the SEXTANTS Beamline**

**Victor Porée**

Over the past decade, Resonant Inelastic X-ray Scattering (RIXS) has emerged as a powerful experimental tool for probing key electronic, magnetic, and lattice excitations in condensed matter systems. Recent advancements, particularly in spectral resolution and theoretical understanding, have enabled RIXS to capture these excitations with unprecedented precision, establishing it as essential for exploring complex material properties. With this evolution, interest in applying RIXS to study materials under specific conditions—such as operando and under external fields—is rapidly growing, motivating new experimental developments.

To address this growing demand for studying materials under specific conditions, a unique sample environment was designed on the RIXS spectrometer at the SEXTANTS beamline (SOLEIL). This setup, called MAGELEC, enables RIXS measurements under controlled electric and a vectorial magnetic field up to 0.5 T, allowing for operando RIXS(-MCD/MLD) studies. Additionally, we have integrated a new spectrometer dedicated to X-ray Excited Optical Luminescence (XEOL) measurements, enabling the measurement of photoluminescence phenomena and to correlate them with the electronic structure measured by RIXS. Finally, a newly commissioned CMOS detector drastically improves data acquisition and preprocessing for RIXS. All together, these advancements provide enhanced experimental versatility, enabling more comprehensive investigations of material properties in controlled settings.

In this presentation, I will provide an overview of these recent improvements, including the MAGELEC sample environment, the integration of the XEOL spectrometer, and the enhanced capabilities offered by our new detector. In addition to experimental illustrations of the instrument’s new capabilities, I will present how these features can be combined to study systems of currentinterest, exemplified by the topical van der Waals magnet CrSBr.

Jean-Sébastien Micha

**LaueMAX: a high-flux Laue diffraction X-ray microscope for materials science and nanoscience**

**Jean-Sébastien Micha**

The Laue microdiffraction end-station on the French CRG-IF BM32 beamline at ESRF was upgraded in early 2024 thanks to the Equipex+ MAGNIFIX project. Compared to the previous setup, the intensity of the beam incident on the sample has been multiplied by at least a factor of 10, with a size of the X-ray beam of 300x300 nm².

Laue microdiffraction is a well-established technique for microstructural characterisation in polycrystalline materials on a scale of a few hundred nanometres, with high angular resolution for determining orientation, strain levels and lattice parameters within a resolution of 0.01%. Non-destructive, it is suitable for all types of crystallized materials (oxides, metals, semiconductors), whether isolated or assembled. In addition to standard measurements, the precise energy of peaks can be determined to assess the local stress tensor, and the depth resolution obtained by displacing a mask between the sample and the detector (DAXM - Differential Aperture X-ray Microscopy). Finally, *operando* or *in situ* studies can be carried out (temperature, mechanical load, light emission, etc.).

In conjunction with these instrumental advances, the analysis of massive data (from mapping, screening...) is being accelerated (as part of the PEPR DIADEM/‘ESRF’ project) thanks to the design of processing chains using intensive computing on several tens of thousands of Laue diagram images that may contain several thousand diffraction spots. Automatic and rapid indexing using artificial intelligence enables the analysis of complex Laue diagrams from a dozen probed crystals or crystallographic lattices with low symmetry.

Thanks to these developments, on the one hand, rapid knowledge of the structural data during the collection time will make it possible to better guide the collection and, on the other hand, the reliability and representativeness of the results will be increased.

We will illustrate this work with examples taken from recent measurements.

Coline Theron

**The complementarity of *in situ* and synchrotron-based techniques to study the schematic Holocene rock art.**

**Coline Théron**, Pierre Bordet, Emilie Chalmin, Claudia Defrasne, Pauline Martinetto

Writing and drawing on walls is a human behavior know since prehistory. A specific schematic expression attributed to Neolithic societies, is present over a vast geographical area, from the Iberian Peninsula to Italy, still misunderstood . Pictorial matter is used here to highlight graphic syntax and social practices. This presentation will discuss the physical and chemical characterization of the pigments of the main schematic rock art site of southern France, the Otello rock shelter (Saint-Rémy-de-Provence, Bouches-du-Rhône).

This important site represents many challenging for scientists: localization of the sites (30-minutes hike) and the paintings (disposition of the figures on the rock panel) , alterations (open shelter), and sampling difficulties (representativity, cultural heritage protection). The cross-utilization of non-invasive analytical techniques in situ and large instruments on micro-samples is required to investigate matter despite these difficulties.

X-Ray fluorescence (XRF), performed in situ with the portable MobiFlu instrument, is one of the first analytical steps, allowing us to read the rock panel and work on the elemental composition of sampling area or equivalent. We also perform powder X-Ray diffraction (XRD) on micro-samples on two ESRF beamlines to contuct high-resolution (ESRF-ID22) and high-spatial-resolution (ESRF-ID13) acquisitions. Our experiments took place as part of beam time dedicated to historical material Block Allocation Group (BAG) for cultural heritage.

We will present our results on the composition of the coloring matter, alteration, and substrate: understanding of the stratigraphy, precise analyses of the coloring matter composition, quantification by Rietveld refinement, localization of the phases on the rock panel, link with the color geological material.

Igor Vinograd

**Nuclear Magnetic Resonance in extreme conditions at LNCMI**

**Igor Vinograd**

The periodic table of elements provides the building blocks for a vast array of compounds with exciting electronic properties related to magnetism, ferroelectricity, superconductivity or topology. To optimise these properties, external tuning parameters such as high magnetic fields or pressure can be used. In this talk I will discuss how these tuning parameters are applied at Laboratoire National des Champs Magnétiques Intenses (LNCMI). LNCMI is an institute specialised in high magnetic fields and I will discuss how we investigate electronic properties by nuclear magnetic resonance - a method whose basic principle is also used for magnetic resonance imaging (MRI).