X AUSE Conference & V ALBA User's meeting

Monday, 5 September 2022 - Thursday, 8 September 2022

ALBA Synchrotron

Book of Abstracts

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Opening

AUSE Plenary I / 25

EBS: A New Light for Science - first scientific highlights

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The ESRF is the first high-energy, fourth-generation synchrotron, which constitutes a landmark for fundamental and innovation-driven research. With the support of the ESRF's international partner countries, a brand-new generation of high-energy synchrotron, the ESRF's Extremely Brilliant Source (EBS) was launched in 2020 with superior X-ray performances (up to a factor 100) in terms of brilliance, coherence and emittance. In the quest to push the boundaries of knowledge and technology for the benefit of society, EBS produces the most brilliant X-rays to unveil the structure of matter. Thus, EBS provides scientists from all over the world with new opportunities to pioneer new fields of investigation for fundamental research, also permitting unprecedented analysis and understanding of materials down to atomic resolution. Based on scientific excellence, research carried out with the EBS contributes to addressing the complex global challenges that our society faces, such as health, energy and the environment. Pushing the frontiers of science, ESB makes the invisible visible, unveiling the secrets of matter to advance fundamental knowledge and new applications, covering biomedical science, novel materials for energy, extreme conditions (planetary research and geoscience, cutting-edge materials), nanomaterials, etc. It also contributes to the development of new and clean technologies for industry and to preserving humanity's cultural heritage, lighting the way to a brighter, sustainable and peaceful future.

This talk will present the EBS benefits, its exploitation and the new experimental capabilities available to academic and industrial users in Physical and Life Sciences. The first scientific highlights from the main flagship and refurbished beamlines will be briefly described. Like a super-microscope, the presentation will illustrate how the enhanced performance of the X-rays, combined with new stations and state-of-the-art instruments, will revolutionize biomedical phase-contrast imaging, and will make the study the structure of condensed matter possible at the nanometre scale under operando or extreme thermodynamical conditions with higher resolution, greater image quality and faster framerate. Finally, this presentation will give a summary of the status of the beamlines under construction, their design choices and strategic research, a snapshot of its present status and some considerations of their future perspectives.

Would you like to participate in the Poster Prize competition?:

No

AUSE B - 5/09/22 / 56

New possibilities of hard X-rays photon-in/photon-out spectroscopies

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Photon-in/photon-out (PIPO) spectroscopies are increasingly applied in the study of physical and chemical properties of materials to investigate the local electronic and geometrical structure with element selectivity. Herein, PIPO spectroscopies refer to the techniques derived from the combination of X-ray absorption and emission spectroscopies (XAS-XES), such as resonant inelastic X-ray scattering (RIXS). The rapidly growing use of these techniques comes in parallel with the recent boom in the development of wavelength dispersive emission spectrometers with energy bandwidth around 1 eV at synchrotron experimental stations and also at X-ray free electron lasers and home laboratories. This contribution will focus on new possibilities of PIPO spectroscopies using hard X-rays, which entails interesting experimental advantages like bulk sensitivity and compatibility with complex sample environments (e.g. liquid phase) [1]. The first part of the contribution will be dedicated to a novel approach for retrieving range-extended XAS in materials with elements causing edge interference. The method of extending the XAS signal beyond unwanted edges using a XES instrument in combination with the standard total fluorescence yield detection will be introduced, discussing experimental aspects and illustrative examples of applications in RE-doped (RE= rare earth) Mn-based perovskites [2,3]. The second part of the contribution will focus on the combination of RIXS with X-ray magnetic circular dichroism (RIXS-MCD) [4] and a recent experimental development at ID26 beamline of the ESRF synchrotron for the investigation of magnetic systems in liquid phase, based on a continuous liquid jet setup coupled with a compact electromagnet. The first results of RIXS-MCD collected in the liquid jet setup on a set of commercial Fe3O4 nanoparticles in solution, show the feasibility of the experimental approach and open up the door for advanced, bulk-sensitive magneto-spectroscopic characterization of magnetic liquids at room temperature (no freezing required) and free of radiation damage [1].

[1] S. Lafuerza et al., "New reflections on hard X-ray photon-in/photon-out spectroscopy"Nanoscale 12, 16270 (2020)
[2] S. Lafuerza et al., "High-resolution Mn K-edge x-ray emission and absorption spectroscopy study of the electronic and local structure of the three different phases in Nd0.5Sr0.5MnO3"Phys. Rev. B 93, 205108 (2016)
[3] G. Subías et al., "Effects of A-site ordering on the Mn local structure and polar phases of REBaMn2O6 (RE: La, Nd, Sm and Y)"(submitted)
[4] M. Sikora et al., "Strong K-edge Magnetic Circular Dichroism Observed in Photon-in–Photon-out Spectroscopy"Phys. Rev. Lett. 105, 037202 (2010)

Would you like to participate in the Poster Prize competition?:

No

AUSE A - 5/09/22 / 31

The W's of Cultural Heritage (Why is worth to study Cultural Heritage? Why Synchrotron Light Sources? Who is interested? Since When? What do we do? How?)

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The study of Cultural Heritage involves the investigation of what is left of our past (**materials**) to learn about the immaterial (**knowledge**).
The subject by definition involves many disciplines such as History, Archaeology, Conservation, Museology, Materials Science, Technology, Anthropology among other, which have their own methodology designed to obtain information relevant to them. The interdisciplinarity of the subject adds

interest and difficulty to the collaboration.
Our group is formed by scientist of various disciplines (Physics, Chemistry, Mineralogy and Crystallography, Microbiology, Material Science). As Scientists our main interest is to learn about the materials and methods of production used in the Past: to unveil the **Lost Technologies**, identifying the changes happened through time in both, materials and processes, and, finding the technological breakthroughs of the past. Our approach: a **Reverse Engineering** methodology, which includes the analysis of the objects and replication of the procedures.
The analysis of Historical materials has some particularities: limited sampling, reactivity, aging and corrosion to which we have to add the complexity specific of the material under study (organic-inorganic materials, crystalline-amorphous compounds, micrometric and sub-micrometric layers and particles, presence of impurities) and the lack of information about materials processing and production processes.
We will try to answer the **W's** questions presenting a selection of studies including paintings, ceramic glazes, stained glass, waterlogged wood addressing conservation issues and unveiling the science behind the object.

Would you like to participate in the Poster Prize competition?:

No

AUSE B - 5/09/22 / 60

On-surface design of an 1D semiconductor by metal-organic coordination

Author: Shanmugasibi Mathialagan[1]

Co-author: Sofia Parreiras [1]

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Investigation of the magnetic properties of a metal-organic network consisting DCAAQ (N,N'-(anthracene-9,10-diylidene) dicyanamide) molecules coordinated with Co atoms on Au(111).

Would you like to participate in the Poster Prize competition?:

No

AUSE A - 5/09/22 / 12

Early age cement hydration acceleration followed by in situ synchrotron X-ray powder diffraction

Author: Miguel Ángel García Aranda[1]

Co-authors: Alejandro Morales-Cantero [1]; Cuesta Ana [1]; De la Torre Angeles G. [1]; Santacruz Isabel [1]; Borralleras Pere [2]

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Portland cement (PC), is one of the most manufactured commodity in the world. Moreover, cement industry is one of the major contributors for greenhouse gases emissions. In the fabrication of one tone of PC clinker, about 0.87 tons CO2 are emitted to our atmosphere. There are two main approaches to decrease the carbon footprint of cements. On the one hand, PC can be party replaced by Supplementary Cementitious Materials (SCMs) with lower CO2 footprint. On the other hand, instead of PC, belite cements (BC) could be used. BCs are similar to Portland cements but the amounts of the two main phases, alite (or C3S, an impure form of Ca3SiO5) and belite (or C2S, an impure form of Ca2SiO4), are reversed. In any case, the main disadvantage of both type of binders is their low mechanical strengths at early ages. They have very good mechanical strength values and durability performances at late ages, after a few weeks.
Therefore, a key research avenue in cement science is to increase the mechanical properties at early ages of low carbon cements. Our research frames within this societal challenge by using accelerator admixtures (chemical products) which activate the hydration of cements at early ages, i.e. during the first 1-3 days.
To do this, an in-situ synchrotron X-ray powder diffraction (SXRPD) set of studies was performed up to 48 hours of hydration using three different PCs with selected accelerating admixtures. For instance, the role of C-S-H gel based admixtures (Master X-Seed 100, Master X-Seed 130 and Master X-Seed STE53) have been studied. Data were collected at the BL04-MSPD beamline at ALBA synchrotron (Barcelona, Spain). It is important to understand the acceleration mechanism of these admixtures to implement them for low carbon cements and to improve their performances. This work is part of our wider investigations dealing with early age hydration acceleration of belite cements and limestone calcined clay cements.
Fig. 1 shows, as an example, the SXRPD patterns for the three studied Portland cements during the key first 13 hours. The evolution (dissolution/disappearance for the anhydrous phases and crystallization/appearance for the hydrated phases) of the key components is highlighted by labelling their most important non-overlapped diffraction peaks. Those phases are named following the cement notation: C3S, C3A (for tricalcium aluminate or Ca3Al2O6), C4AF (for tetracalcium ferro-aluminate Ca4Al2Fe2O10), CH (for portlandite or Ca(OH)2) and AFt (for ettringite or Ca6Al2(SO4)3(OH)12·26H2O). In addition to the reference pastes, i.e. the pastes without accelerating admixtures, the SXRPD patterns for accelerated samples are also displayed. The patterns are being analysed by the Rietveld methodology to determine the phase content evolutions with time and with the added activators.
In this study, we have obtained three main preliminary conclusions. Firstly, the acceleration mechanism seems to strongly depend upon initial sulfate contents and availabilities. Secondly, C-S-H seeding accelerates the hydration of the three cements at early ages, mainly by enhancing calcium sulfate and calcium aluminate dissolutions. It has also been observed that admixtures do very moderately accelerate the hydration of crystalline C3S. Thirdly and quite interestingly, it has been observed a synergistic effect between C-S-H seeding and alkanolamines, when compare to single alkanolamine dosage. Further details will be given in this communication. A fraction of this work has been already submitted for possible publication [1].
[1] Morales-Cantero, A.; Cuesta, A.; De la Torre, A.G.; Santacruz, I.; Mazanec, O.; Borralleras, P.; Weldert, K.S.; Gastaldi, D.; Canonico, F.; Aranda, M.A.G. C-S-H seeding activation of Portland and Belite Cements: an enlightening in situ synchrotron powder diffraction study. (2022) submitted.

Would you like to participate in the Poster Prize competition?:

No

AUSE B - 5/09/22 / 59

Arsenic speciation and intracellular localization in Sargassum algae

Authors: Maria Angels Subirana[1]; Véronique Vacchina[2]; Etienne Gontier[3]; Fabienne Seby[2]; Patrick Ollivier[4]; Dirk Schaumlöffel[1]

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In recent years, unprecedented amounts of algae from the Sargassum genus have washed ashore on the beaches of the Caribbean1. During their life cycle, these seaweeds accumulate a high concentration of pollutants, especially arsenic (As). They are disposed of by collecting them and then spreading them along shorelines or inland. Their degradation, as well as rainfall, generate leachates that also contain several mg/L of As, causing environmental issues.
In this context, an in-depth characterization of As speciation and distribution in Sargassum algae (before and during its degradation) is essential to understand the mechanisms of As uptake and leaching, and to assess the risk for the environment.
The distribution of As in the leaves, stems and floats of sargassum algae was determined using both nano-XRF and Nano secondary ion mass spectrometry (NanoSIMS). Both techniques are able to achieve a high lateral resolution, of around 50-100 nm, which allows the mapping at the sub-cellular scale. The same samples were also studied by Transmission Electron Microscopy (TEM). A sample preparation adequate for the three techniques enabled the obtention of correlative imaging of the same cell.
Thus, it was shown that arsenic was mainly accumulated in the cell walls, in agreement with previous studies2, with a small amount of arsenic also visible in the cell internal organelles.
In the same manner, in order to determine the forms in which As is bound into the cell walls, speciation was studied by XAS and HPLC-ICP-MS. The characterization with HPLC-ICP-MS showed that inorganic species of As are the main components in the algae, but that organic species, especially DMA, but also AsB and TMAO, are also present. It also revealed that the fraction of organic As increases with the degradation of the algae.
In addition, X-Ray Absorption Spectroscopy (XAS) permits the investigation of frozen samples, removing the need for pre-treatment and extraction steps, and enables the determination of labile species such as As bound to sulfur and As bound to carbon. XAS demonstrated that fresh algae collected in the open sea contains mainly inorganic As(III) and As bound to sulfur, with some As bound to carbon present in a lower amount. However, during the decomposition of algae at the beach, As speciation evolves to more organic forms, where As is bound to carbon, and to As (V), possibly due to microbiological processes and oxidation involved in the fouling process.
The obtained arsenic distribution and speciation knowledge can contribute to understand better the toxicity and environmental impact of the sargassum and their As-rich leachates. It can enable the development of adequate remediation technologies in order to handle the stranded Sargassum.

1. Milledge, J. and Harvey, P. (2016), Golden Tides: Problem or Golden Opportunity? The Valorisation of Sargassum from Beach Inundations, J. Mar. Sci. Eng., 4, 60

2. Ender, E. et. al. (2019), Why is NanoSIMS elemental imaging of arsenic in seaweed (Laminaria digitata) important for understanding of arsenic biochemistry in addition to speciation information?, J. Anal. At. Spectrom., 34, 2295

Would you like to participate in the Poster Prize competition?:

No

AUSE A - 5/09/22 / 4

Metal iodates under pressure

Author: Daniel Errandonea[1]

Co-authors: Akun Liang [2]; Robin Turnbull [2]; Javier Manjon [3]; Placida Rodriguez-Hernandez [4]; Alfonso Muñoz [4]; Catalin Popescu [5]; Ybraheem Yousef [5]

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Metal iodates form a diverse range of non-centrosymmetric structured materials, which exhibit useful and interesting properties such as non-linear optics; visible to far-IR transparency; large second-harmonic generation coefficients; a high optical damage threshold; and good thermal stability. They have been intensely studied under ambient conditions. In contrast, there remains a large deficit of studies of metal iodates under high-pressure (HP) conditions despite the clear possibility for new insights into pressure-induced effects, in particular changes regarding the stereochemically active lone electron pair (LEP) of the iodate ion.

During the last two years we have systematically studied different iodates using synchrotron radiation at the MSPD and MIRAS beamlines of ALBA [1-3]. Our studies have been focused in Mg(IO3)3, Zn(IO3)2, and Co(IO3)2. High-pressure synchrotron powder X-ray diffraction studies on these compounds have provided evidence of the existence of several phase transitions at relative low pressures. They have also revealed a highly anisotropic behavior. A structural analysis from experiments have shown the existence of an extremely compressible direction which coexist with a counterintuitive pressure-induced expansion along other crystallographic directions. High-pressure infrared and Raman spectroscopy have shown that there are internal modes of the iodate molecule which soften under compression. This has been related to a pressure-driven increase of the length of I–O bonds. This phenomenon is induced by the high-pressure behavior of the lone electron pairs of iodine atoms. The discovered structural changes are characterized by the increase of the oxygen coordination of the iodine atoms and the formation of up to three additional I-O bonds. Pressure–volume equations of state are presented, as well as a detailed discussion of the pressure dependences of the observed vibrational modes. With the help of DFT calculations, the results of structural studies have been used to explain changes under compression of the band-gap energy of Mg(IO3)3, Zn(IO3)2, and Co(IO3)2 which have been determined from optical-absorption measurements.

[1] A. Liang et al. Phys. Rev. B 103, 054102 (2021).
[2] A. Liang et al. J. Phys. Chem. C 125, 17448 (2021).
[3] A. Liang et al. Phys. Rev. B 105, 054105 (2022).

Would you like to participate in the Poster Prize competition?:

No

AUSE B - 5/09/22 / 47

Application of synchrotron-based techniques for the study of calcium oxalate hydrates transformation

Authors: Iris H.Valido[1]; Roberto Boada Romero[1]; Montserrat Resina-Gallego[1]; Victor Fuentes-Cebrián[1]; Ibraheem Yousef[2]; Oriol Vallcorba Valls[2]; Manuel Valiente[3]; Montserrat López-Mesas[4]

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Renal Nephrolithiasis is a clinical condition that implies the formation of microcrystals aggregates on the kidney. This disease affects up to 12% of the population with a recurrence rate around 50% [1]. Among the eleven types of kidney stones, 66% of the incidence is represented by calcium oxalate hydrates species: the dihydrate (weddellite, COD) and the monohydrate (whewellite, COM) [2]. The process which accounts for the transformation of COD into COM has been studied in mineral systems and in vitro. The formed stone after a total transformation (called TRA) is, chemically, COM, since it only contains one water molecule in its crystalline structure. TRA is difficult to differentiate from the stones nucleated as COM due to their high appearance, differentiation that is of great importance since both species are caused by different pathologies, so different treatment is needed to prevent recurrence. Therefore, the studies of this transformation process, as well as the stabilization of the dihydrated species, are important to understand the physiopathology, to propose an adequate treatment and, above all, to prevent recurrence.

The main objective is to fill in the knowledge gap regarding the crystalline conversion of calcium oxalate dihydrate, as well as the appropriate identification of the calcium oxalate monohydrate formation origin, in kidney stones. To accomplish this, different synchrotron radiation techniques have been applied (XAS, μFTIR and μXRD), since they allow to measure with a small spot size (microns) with a high spectral brightness (allowing a better signal to noise ratio): XAS measurements were performed to study the differences in the local coordination environment of calcium in both species [3]; SR- μFTIR was used to analyze the organic matter distribution, determining their role as promotors/inhibitors of COM and in the stabilization of COD crystals [4]; SR-μXRD was performed to evaluate the crystallographic textures differences between COM and TRA, correlating the results with the morpho-constitutional analysis applied for their classification [5].

In brief, these techniques have allowed us to differentiate between the calcium oxalate monohydrate species and to better understand the role of the organic matter on the transformation process.

[1] T. Alelign, et. al., Adv. Urol. 2018, 2018, 12
[2] M. Daudon, et. al, Comptes Rendus Chimie 2016, 19, 1470-1491
[3] I. H.Valido, et. al. ChemPhysChem. 2020, 21(22)
[4] I. H.Valido, et. al. J Biophotonics. 2020, 12(12)
[5] I. H.Valido, et. al. Analyst. 2021, 147(6)

Would you like to participate in the Poster Prize competition?:

No

AUSE A - 5/09/22 / 67

High pressure structural and vibrational studies of β- and α-In2Se3-like Ga2S3

Author: Samuel Gallego Parra[1]

Co-authors: Rosario Vilaplana ; Óscar Gomis ; Plácida Rodríguez Hernández ; Alfonso Muñoz ; Jesús Antonio González ; Juan Angel Sans ; Catalin Popescu ; Francisco Javier Manjon

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Tetradymite α-Bi2Te3 (space group (S.G.) R-3m, centrosymmetric) is well known to be found in a few group-V A2X3 compounds (A=As, Sb, Bi) at room conditions (RC). Under high temperature (HT), this R-3m can be obtained in the In2Se3, the β phase [1], which belongs to the group-III A2X3 compounds (A=Al, In, Ga). A few theoretical works have shown that this β- In2Se3-like structure is stable above the theoretical Tc calculated, following a tendency of Al2X3 > Ga2X3 > In2X3 [2], starting from the α-In2Se3-type structure (s.g. R3m, non-centrosymmetric), which is stable at RC. Such structure is dynamically stable for all this family at RC [2], unlike the β-In2Se3-like structure [3]. The seeking of centrosymmetric and non-centrosymmetric structures, together with the easiest way to switch

between them, are being studied for ferroelectric, pyroelectric, and piezoelectric applications, among others.
Multiple high-pressure works on such A2X3 compounds, both from V and III groups have been released for years, where in situ high-pressure x-ray diffraction (HP-XRD) measurements have been deployed to characterize the phase transitions (PTs) observed and the related structural changes. In addition, other experimental techniques are employed, supported by DFT calculations, to fully understand these PTs. In this sense, α-In2Se3 undergoes a PT to β-In2Se3 at above 10-12 GPa, after transforming into β'-In2Se3 at 1 GPa [4]. Very recently, Ga2S3 transforms into this β-In2Se3-like structure was observed at about 16 GPa [7]. Evidence of such PT has been stressed in subsequent works [8, 9]. What is more unexpected, after this α'-β'PT on Ga2S3, two other polymorphs have been synthesized upon decreasing pressure, at 9.0 and 3.0 GPa, respectively [8]. However, further information about the nature of both polymorphs was not given.
In this work, we have confirmed this β'-Ga2S3 under HP via XRD and Raman measurements, joint theoretical simulations. Upon decreasing pressure, α-In2Se3-like structure matches quite well with the 1st polymorph observed at 9.0 GPa (φ-Ga2S3). Raman signatures and pressure dependence of structural parameters have allowed us to discern such β'- φ PT. The 2nd polymorph below 1.0 GPa has been identified with a disordered zincblende (γ-Ga2S3). To complement our results, we discuss the relation between the PTs of both Ga2X3 and AGa2X4 compounds.
[1] G. Han et al., Small 2014, 10, 2747-2765.
[2] J. Liu et al., 2D Mat. 2019, 6, 025001.
[3] Y.-T. Huang et al., Appl. Phys. Rev. 2021, 8, 031413
[4] R. Vilaplana et al., Inorg. Chem. 2018, 57, 8241-8252.
[7] X. Lai et al., J. Appl. Phys. 2014, 116, 193507.
[8] L. Yang et al., J. Mater. Chem. C 2021, 9, 2912-2918.
[9] S. Gallego-Parra et al., Phys. Chem. Chem. Phys. 2021, 23, 6841-6862.

Would you like to participate in the Poster Prize competition?:

No

LEAPS and ESUO / 125

The European Synchrotron and FEL user organization (ESUO): a brief introduction

Author: Olga Lopez[1]

[1] *IQAC-CSIC*

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ESUO, the European Synchrotron and FEL user organization, was founded in 2010 as a body to represent all European photon science users. Today, ESUO is a legal entity that represents about 30 000 users from 31 European member states and European associated countries. The mission of the organization is supporting a thriving European synchrotron and FEL user community with equal opportunities of access and participation for all scientists based solely on the scientific merit of their ideas. Different activities to support needs of users, to increase collaboration, cooperation and lobbying, and to stablish an ESUO advocate network through national user delegates are being addressed.

Would you like to participate in the Poster Prize competition?:

No

LEAPS and ESUO / 111

LEAPS and ESAPS2022

Author: Caterina Biscari[1]

[1] *ALBA Synchrotron*

Corresponding Author: cbiscari@cells.es

LEAPS –the League of European Accelerator-based Photon Sources –is a strategic consortium of the Synchrotron Radiation and Free Electron Laser user facilities in Europe. Its primary goal is to actively and constructively ensure and promote the quality and impact of fundamental, applied and industrial research carried out at each facility to the greater benefit of European science and society. The talk will describe the recently published European Strategy for Accelerator-based Photon Sources, ESAPS 2022, a coherent plan addressing the future challenges and needs of the new era in research and innovation. It encompasses the expansion of service provision to speed-up emerging research for societal challenges, the coordinated upgrade of synchrotrons and FELs facilities, joining forces to enhance facility operation by implementing new digital technologies. The ESUO partnership provides a seamless interaction between the facilities and their users.

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No

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AUSE Assembly

AUSE Plenary II / 104

Looking at catalysts under pressure

Author: Jeroen A. van Bokhoven[1]

[1] *ETHZurich and Paul Scherrer Institute*

The continued quest for novel and better catalysts is helped by providing an understanding of the relationship between structure and property. The obvious difficulties to obtain such relationships are on the one hand the complexity of the heterogeneous catalyst and on the other, the demanding conditions under which catalytic reactions are performed. One understandable approach is to make use of model systems and to employ milder reaction conditions. Oppositely, doing so may lead to erroneous conclusions when extrapolation results to actual catalysts and conditions.
I will show our efforts to identify the structure of heterogenous catalysts, notably archetype $Cu/ZnO/Al_2O_3$ for the synthesis of methanol from carbon dioxide. This reaction is of high interest to generate fuels and chemicals from waste carbon dioxide and sustainable hydrogen. Through systematically varying the pressure of hydrogen on the one hand and of CO_2/H_2 mixtures on the other, the association between structure and pressure becomes evident. Pressure is an essential ingredient to form the active catalyst. The combination of high-pressure isotope exchange experiments, joint by simultaneous infrared spectroscopy, and operando XAS at the Cu and Zn K edges, the reaction mechanism and its relation to catalyst structure emerge. Based on the conclusions from such studies, catalysts can be synthesized that further help interpret the relationship between zinc alloy-formation and the role of zinc oxide in generating selective methanol synthesis catalysts.

Would you like to participate in the Poster Prize competition?:

No

AUSE B - 6/09/22 I / 3

Few atoms metal clusters with high catalytic and cytotoxic activity characterized by X-Ray Absorption Spectroscopy.

Authors: Judit Oliver-Meseguer[1]; Francisco Garnes Portolés[2]; Rossella Greco[2]; Antonio Leyva Pérez[2]

[1] *Instituto de Tecnología Química ITQ (UPV-CSIC)*

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Here, we show three examples of how XAS techniques are very useful to provide an exhaustive information about the oxidation state and coordination environment of MCs and SACs::
- Pd SACs spontaneously formed after dissolving in neat benzyl alcohols. The gram-scale preparation and stabilization of Pd SACs within the functional channels of a novel methyl-cysteine-based metal–organic framework (MOF) was accomplished, to give a robust and crystalline solid catalyst.
- Ligand-free, few-atom Pd Cs in solution that catalyse the α-selective intramolecular Mizoroki–Heck coupling of iodoaryl cinnamates. The α-selective intermolecular coupling is also achieved with Pd Cs encapsulated within fine-tuned and sterically restricted zeolite cavities.
- Pt Cs prepared in water by just adding a biocompatible extremely mild external reductant. The PtCs show 400 times higher antitumoral activity than cisplatin and thousand times higher activity than Pt NPs for various cancer cell lines.

Would you like to participate in the Poster Prize competition?:

Yes

AUSE A - 6/09/22 I / 63

Development and commissioning of a capillary flow cell for quasi-simultaneous in situ/operando XAS-XRD catalysis studies: Oxidative de-ligation of atomically-precise supported metal oxo-cluster catalysts as a showcase study

Author: Wilson Henao[1]

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Registering dynamic changes in short- and long-range atomic ordering of solid catalysts under operando conditions, i.e. during catalytic action under relevant operation settings, is essential for the rational development of this important class of functional materials. Synchrotron radiation X-ray absorption (XAS) and diffraction (XRD) techniques allow such studies, the challenge being to mimic relevant operation conditions and gas-solid hydrodynamics of flow reactors during spectroscopic

studies. A capillary flow cell has been developed through a cooperation between ITQ and ALBA for quasi-simultaneous, in situ, and operando XAS/XRD measurements aimed to be integrated into the recently commissioned NOTOS beamline station, Figure 1a. This versatile cell enables studies under realistic gas-solid operation conditions, i.e. up to 20 bar pressure and 700 ºC temperature, under flow of preset gas mixtures, suitable for numerous catalytic reactions of interest to academy and industry.

The setup comprises a quartz glass capillary with tunable wall thickness and external diameter appropriate for XAS applications (adequate X-ray transmittance at relevant incident beam wavelengths). The sample (dp=100–200 μm) is placed at the center of the capillary aligned with the X-ray beam path and packed within a SiC bed, which contributes to the pre-heating and turbulent hydrodynamics of the gases upstream of the catalyst bed, and fixed with quartz wool plugs, Figure 1b. A hot air gas blower (DGB0001, FMB Oxford) equipped with a Eurotherm regulator and a gas flow controller (typical air flow 450 L/h) is used to heat the sample, delivering an isothermal length of 3 mm along the sample packed-bed when positioned at about 2.5 mm, orthogonal to the capillary's axis. The cell is integrated into a flow gas system with a minimized death volume consisting of four main mass flow controllers able to precisely feed reactive (CO2, hydrocarbons, H2) and inert (He, N2, or Ar) gases with volumetric flows ranging from 0.12-6 mL·min-1 and 0.17-8.5 mL·min-1, respectively. An additional bypass line is connected along with a programable 6-way valve that allows pulse dosing of gaseous reactants of interest with micro-volumetric precision through exchangeable μL-loops, Figure 1c. The cell delivers excellent pressure control under flow conditions up to 20 bar (Figure 1d) and 700 ºC. The major innovation of the design is a high-speed axial rotation capability (<80 rpm) of the capillary in order to minimize artifacts from preferential orientations during XRD experiments.

As a first showcase application, the cell was tested during the oxidative de-ligation of supported transition metal oxo-clusters via temperature-resolved XAS measurements under in situ conditions in static-capillary mode. For this purpose, a series of innovative organometallic complexes ([MCo3O4]Ln, M=Co, Mn, Ru) with a cubane geometry was used as molecular cluster precursors, Figure 2a. The use of these ligand-protected molecular metal clusters bears significant promise toward the fabrication of new solid catalysts bearing highly undercoordinated metal active sites, on atomically precise metal ensembles, capable of lowering the activation energy for the conversion of molecules in catalytic processes of significance for the transition to more sustainable energy and chemical sectors. As summarized in Figure 2b, immobilization of the molecular cubanes was performed in a one-pot process during the formation of the silica matrix via sol-gel route at room temperature (RT) and neutral pH. The obtained [MCo3O4]Ln@SiO2 composite materials were activated in the capillary cell under oxidative thermal treatment up to 450 ºC with a flow of 20%O2/He to decompose the protective organic ligands (Ln). XANES spectra were collected at the Co k and Ru k edges during the heating ramp (5 ºC/min) with a temperature resolution of ca. 10 ºC/spectrum to track changes in the coordination geometry and oxidation state of the metals M=Co, Ru. Following the temperature-resolved XANES experiments, samples were stabilized at 450 ºC for 1 hour and cooled down to RT in order to measure the corresponding EXAFS spectra of the in situ calcined material, as a means to assess the average nuclearity of the metal clusters and coordination environment for Co and Ru atoms. As a strategy to prevent the formation of metal-support compounds, e.g. metal silicates, during the oxidative de-ligation of the oxo-clusters, the silica surface was grafted with thermally stable phenylsilane moieties prior to thermal activation.

In situ temperature-resolved XANES measurements (not shown) collected at the Co k edge during the oxidative de-ligation of the supported [MCo3O4]@SiO2 materials indicated that the local geometry around the Co atoms was progressively distorted towards a less centrosymmetric coordination environment, promoting the dielectric dipole transition from 1s electrons to the p component in 3d-4p hybridized orbitals. Fourier-transform of the k3-weighted EXAFS spectra recorded at the Co and Ru k edges for the as-prepared materials and their corresponding de-ligated counterparts is depicted in Figure 3. After thermal treatment of the supported [MCo3O4]@SiO2 M=Co, Ru samples, the development of multiple scattering shells around Co was observed at radial distances about 1.4 Å (Co-O), 2.6 Å (Co-Co), and 4.7 Å (Co-O-Co) (no phase correction), indicating the structural evolution of the oxo-clusters towards the formation of a spinel-like Co3O4 structure (see reference spectrum, Figure 3a,c), which is particularly desirable to drive selective alkane oxidation reactions. However, when these materials were previously surface-functionalized with phenylsilane moieties ([MCo3O4]@SiO2-syl), only the contribution of the first coordination shell was observed, suggesting the formation of smaller Co3O4 domains with a minor, if any, degree of metal aggregation. Inter-

estingly, when Mn was included into the [MCo3O4] cluster the amplitude of the scattering signals remained quite low pointing to the superior thermal stability of this material, Figure 3b. Conversely, measurements at the Ru k edge revealed the segregation of Ru out of the [Ru(O)Co3O4] cluster lattice and the consequent formation of a separate RuO2 phase (Figure 3d), possibly due to the high vapor pressure of ruthenium sub-oxide species at relatively mild temperatures. These results highlight the importance of unraveling the changes in the nuclearity of metal oxo-clusters as a function of factors such as (i) cluster composition, (ii) nature of organic ligands, (iii) activation temperature, and (iv) support surface functionalization to enable a rational design of these type of atomically precise bimetallic cluster catalysts.

In this contribution, preliminary outcomes of the online commissioning of a new multipurpose capillary cell (assembled to the HRPD-XAS end-station of the NOTOS beamline) are presented to the scientific community and industry. The new instrumentation opens a wide range of in situ and operando XAS/XRD studies on the genesis and usage of solid catalysts in gas-solid catalytic processes under technologically relevant operational conditions.

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No

AUSE B - 6/09/22 I / 2

The role of atomic bond strengths and structural disorder in MXene materials for rechargeable ion-batteries

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Ion batteries are a key technology and play a dominant role in today's world [1]. Extensive research efforts have been dedicated to exploring and developing new cathode materials with higher capacities and lifetimes [2].
Recently, a new family of transition metal carbides and carbonitrides called "MXene"has been synthesized with a layered hexagonal structure and M_{n+1}X_n chemistry, where M is an early transition metal, X is carbon or nitrogen, and n=1, 2, or 3 [3].
MXenes have been found to be promising electrode materials, with capacities close to that of commercially available batteries and an excellent capability to handle high cycling rates [4]. However, studies of correlation of their structural stability and functional properties could help to expand further theirs performances. To address this issue we have performed temperature dependent extended X-ray absorption fine structure (EXAFS) measurements at the Ti K-edge on representative members of the MXene family. Temperature dependent measurements permit to have direct access to the local force constant between the atomic pairs and correlate this information with the battery capacity and ions diffusion rate [5,6]. Presented results address fundamental structural aspects that define the functional properties of electrode materials for ion batteries.

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AUSE A - 6/09/22 I / 5

Structure matters: asymmetric CO ignition at square and triangular Rh steps

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Tracking the active site of catalytic metallic nanoparticles in mandatory for tailoring new catalysts and promote a clean and green environment. The activity of each of the facets of the nanoparticle will differ depending on the orientation and coordination of surface atoms [1], yet isolating their individual activity is typically challenging. Within this context, curved crystals possess several different planes, hence they are ideal for selectively probing different types of undercoordinated atoms [2,3]. Using this methodology, we have studied the CO oxidation on Rh stepped surfaces using a curved Rh(111) crystal. This peculiar sample features the flat (111) surface at the center of the crystal, and an increasing density of either A- (square) and B- (triangular) steps as one approaches each of the edges of the sample.
Preliminary Planar Laser-Induce Fluorescence (PLIF) experiments reveal that the B-side of the crystal ignites earlier during the CO oxidation, mimicking the results obtained using an identical curved Pd(111) crystal [2b], and in clear contradiction with the symmetric ignition observed for a curved Pt(111) sample [3]. Near-ambient pressure X-ray photoemission measurements conducted on the same curved Rh(111) crystal show that prior to the ignition of the whole sample, which is marked by an abrupt CO desorption and CO2 production, the B-steps are partially CO-depleted and oxidized, while the A-steps feature a CO-saturated situation. Therefore, such large asymmetry in the chemical composition of A- and B-steps points to be the reason of the early ignition of the B-steps observed by PLIF.

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Would you like to participate in the Poster Prize competition?:

No

AUSE A - 6/09/22 I / 69

Recent progress on synchrotron radiation based operando characterization of battery materials at Alba Synchrotron

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Operando synchrotron radiation-based characterization techniques applied to energy storage materials are becoming a widespread characterization tool as they allow for non-destructive probing of materials with various depth sensitivities through spectroscopy, scattering, and imaging techniques. Moreover, they allow for faster acquisition rates, variable penetration depths, higher spectral or spatial resolution or access to techniques that are only possible with a continuous tuneable source over a wide photon energy range. Compatibility between the electrochemical cell designs and the experimental set ups may force some specific design features and care has to be taken to ensure that these do not perturb the electrochemical response of the materials under investigation. The use of operando techniques has intrinsic advantages, as they enable the detection of metastable intermediates, if any, and ensure characterization under real conditions avoiding the risk of ex situ sample evolution during its preparation. Operando experiments are thus crucial for both the elucidation of redox mechanisms in new technologies and also understanding of failure and ageing processes for already commercial concepts.
Here we aim to give a general overview of the operando capabilities available at Alba Synchrotron related to battery research, focusing specially on the most recent advancements that have been developed in the last year under the initiative "Synchrotron radiation applied to green energy: superconducting materials, electrochemical storage and catalysis", founded by the Extended Interdisciplinary Thematic Platform (PTI+) European Union-Next Generation EU. Amongst other, we will cover the recent progresses on the implementation of operando synchrotron-based Fourier Transform infrared (SR-FTIR) Microspectroscopy for battery materials at MIRAS beamline, the first XRD&XAS operando experiment conducted at NOTOS beamline, a resume on the preliminary studies realized on a possible future operando setup for operando X-ray microscopy at MISTRAL beamline and status of the future Battery Laboratory that will be operational starting from 2023.

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AUSE B - 6/09/22 I / 54

New pathways to gold chemistry: Electronics at Au centers with non-innocent and ambiphilic ligands

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Transition metal driven chemical transformations in organic synthesis offer the promise of new retrosynthetic strategies for generating novel organic compounds. Efforts are continuously being directed at finding unprecedented reactivity for various transition metals in the hopes of developing, new selectivity, catalytic efficiency and sustainability. Recently gold has garnered significant interest as a

potential redox switchable catalyst with reversible on-demand control of catalytic activity, as well as applications in photo-redox catalysis. Although significant progress has been made in Au chemistry, the focus has largely been on Au(I) and Au(III) complexes. Au(IV) complexes are unprecedented and single-electron processes involving Au(III) complexes are extremely rare. Therefore, we have begun a comprehensive study to explore Au(III) complexes featuring redox active ligands with the aim to access fake Au(IV) complexes and open a new facet in gold chemistry. In the same line we are exploring ligand architectures that can facilitate milder pathways for Au(I)/Au(III) redox catalysis through transition metal –Lewis acid interactions (TM->LA), which impose geometries that promote the 2-electron oxidation of Au(I) complexes. In both cases a thorough understanding of the electronic and coordination environment at the metal center is essential for future development and fine tuning of catalytic properties. As such, X-ray absorption spectroscopy was employed as a direct probe of the ligand influence on the metal center followed by correlation of *in silico* derived with experimentally determined electronic structure.

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No

AUSE A - 6/09/22 I / 50

Effect of Cd pollution on Se-biofortified wheat: competing interactions and influence on the selenium species stored in the grains

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Selenium (Se) plays a vital role in regulating the metabolic activities in humans as it is needed for the thyroid gland functioning, effective immune response, fertility, and detoxification of free radicals.[1] Unfortunately, the Se content in foods depends on the Se present in the cultivation soil which can be very low in certain regions to satisfy the dietary requirements. Indeed, around a billion people worldwide are affected by Se-deficiency with the consequent health issues.[2]
Biofortification of crops with Se is an effective way to incorporate this essential nutrient into the human food chain to overcome Se-deficient diets.[3] Plants can transform inorganic Se species present in soil into organic ones (e.g., seleno-amino acids) which are more bioavailable for humans.[4] However, this metabolization can be altered by the presence of pollutants hindering the benefits of the biofortification process. In that respect, cadmium (Cd) is a common pollutant that presents a global concern since it can be biomagnified in the food chain.[5]
In this study, we have assessed the influence of Cd in Se biofortified wheat plants grown hydroponically, by changing the Se(IV)/Se(VI) ratio in the nutrition solution. Our results show that the Se uptake is reduced under Cd pollution and that the Cd translocation from roots to grains increases in the presence of Se. In addition, the total grain weight is inversely proportional to the level of Cd or Se accumulated in the grains. X-ray absorption spectroscopy (XAS) at the Se K-edge allows identifying selenomethionine (SeMet) and selenocystine (SeCyst) as the predominant Se species forming in grains for the Se treated samples. In the presence of Cd, selenomethylcysteine (SeMeCys) is forming mainly at the expense of SeMet species. μXAS showed that the spatial distribution of the Se and S species is not affected by the Se treatment applied. We conclude that the effect of Cd on Se biofortification mainly affects the total Se translocation and accumulation in grains since SeMet and SeMeCys are similarly bioavailable by the human body. Considering the Se speciation and total

Se accumulation reported, the 50/50 Se(IV)/Se(VI) treatment seems the most effective for wheat Se biofortification.

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No

AUSE Plenary III / **87**

The structure of solid-liquid and gas interfaces: studies with Synchrotron Radiation

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A detailed knowledge of the molecular structure of the interface between material surfaces and gases, and of Electrodes and Electrolytes, is crucial for solving fundamental problems in fields like catalysis, wetting, corrosion, electro-photochemistry, batteries and many others. Until now this has been hampered by the scarcity of surface-sensitive microscopy and spectroscopy techniques that can operate in gas and liquid phases at environmental pressures in the Torr to Atmosphere range. In the last decades my group in Berkeley has developed a variety of techniques and methodologies that break this pressure barrier. I will illustrate the techniques we developed and how we used them to determine the atomic structure of interfaces between metal electrodes (Cu, Au, Pt, TiO2, graphene), soft matter (polymers, biomaterials) in gas and liquid environments, and in the presence of electric fields. The use of Synchrotron-based photon spectroscopies (XPS, NEXAFS, Infrared, and others) combined with of reaction cells with windows transparent to photons and electrons has provided detailed information of the chemical state of electrodes and electrolyte structure in the electrical double layer.

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No

SpLine / **81**

Present and future opportunities at BM25-SpLine at the ESRF

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The main goal of the interdisciplinary and multipurpose Spanish CRG BM25-SpLine beamline at the ESRF is to satisfy the needs of the use of synchrotron radiation in the region of hard X-rays of the Spanish scientific community, with a broad range of interests crossing very different research areas: physics, chemistry, materials science, biology, environmental sciences, and cultural heritage. The Spanish CRG BM25-SpLine beamline is dedicated to structural investigations using hard X-ray scattering mostly in materials science, specialized on the combination of diffraction and spectroscopy techniques.

With the advent of the new EBS-ESRF machine the beamline has been fully upgraded enabling state-of-the art experiments using Grazing incidence X-ray Diffraction, Hard X-ray Photoelectron Spectroscopy and X-ray Absorption Spectroscopy techniques. The increase of brilliance offered by the EBS-ESRF and the upgraded optics and experimental stations enable high energy and angular resolution measurements with low acquisition times, being especially suitable for in-situ and in-operando experiments.

In this presentation, I will give an overview of the present and future capabilities of the BM25-SpLine beamline.

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No

AUSE Thesis Awards / **8**

Growth, characterization and applications of metal oxides on graphitic systems

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Since the discovery of graphene and its impressive properties, the combination of different materials with graphitic systems, such as graphene or graphite, has attracted much attention for different technological applications. Nevertheless, the interface interaction between materials and systems on such nanostructures plays a fundamental role, and can be seen as a direct manifestation of Herbert Kroemer's (Nobel Laureate in Physics, 2000) statement "The interface is the device", beautifully summarizing that their combination essentially results in complex systems that are more than just the sum of the properties of the individual constituents.

This work covers three different cases. The two first consist of a fundamental study of the interactions between CoO and ZnO with highly oriented pyrolytic graphite (HOPG) and graphene supported on polycrystalline copper (G/Cu), respectively. Firstly, by near ambient pressure X-ray photoelectron spectroscopy, we studied the carbon gasification reaction of highly oriented pyrolytic graphite catalyzed by CoOx nanoparticles, giving rise to nanopatterning at lower temperatures than using metallic nanoparticles. This reaction occurs at much lower temperatures because of the weakening of the carbon σ bonds by the initial wetting CoO layer formed at the CoO early stages of the growth on the HOPG surface. In the second place, by combining μ-Raman and X-ray photoemission electron microscopy in the same areas of samples, we have been able to determine the initial chemical, electronic and structural state of pristine graphene grown by chemical vapor deposition on polycrystalline copper, and to infer the complex influence on the ZnO early stages of growth and its interaction with the environment. Finally, the last case consists of the development of free-standing ultrathin (~2 nm) films of Al2O3, which were mechanically robust and transparent to electrons. Their applicability was proved by environmental X-ray photoelectron measurements of air at normal conditions (≥1 bar), demonstrating its potential use in the characterization of solid-gas and solid–liquid interfaces by different synchrotron-based techniques.

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No

AUSE Thesis Awards / 7

Unrevealing the 3D magnetic configuration of nanostructures via x-ray microscopy

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Nanomagnetism is nowadays expanding into three dimensions, triggered by the discovery of new magnetic phenomena and their potential use in applications. This shift towards 3D structures should be accompanied by strategies and methodologies to map the tridimensional spin textures associated. Different lab-microscopy techniques like magnetic force microscopy can be used to explore the magnetic configuration of these nanoobjects. However, these techniques normally do not provide us with information about the 3D configuration of the magnetic moments, which could be crucial in many cases. In this work we combine the use of XMCD-PEEM, X-ray transmission microscopy and micromagnetic simulation to obtain 3D information of the magnetic configuration of in-situ grown single crystal nanometer-thick magnetite islands [1,2] and of magnetic nanowires [3,4].
The experiments have been performed at the CIRCE and MISTRAL beamline of the Alba synchrotron. CIRCE beamline is equipped with a photoemission microscope in which, by taking XMCD images, is possible to acquire nanometer resolution maps of the magnetization of nanosystems. Combining measurements at different azimuthal angles, the full magnetization vector can be determined. MISTRAL beamline is equipped with a transmission X ray microscope operating in the soft X ray range that utilizes photons extracted from a bending magnet source. The angle of the X ray beam with respect to the normal direction to the membrane could be varied by rotating the sample around a vertical axis, typically from +55◦ to−55◦ which allow the acquisition of multiple projections of the magnetization to reconstruct the 3D magnetization. Combining the experimental magnetization maps with micromagnetic simulations, the magnetic configuration of the systems can be completely determined. We will show how the combination of XMCD-PEEM, TXM with imaging and data analysis is a very powerful tool for the study of magnetic configurations of nanometer sized objects.

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No

AUSE Plenary IV / 82

Structure, Dynamics and Regulation of Bacterial Cell Wall. Implications in Antibiotics Resistance

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The bacterial cell wall is an essential gigantic macromolecule that defines the shape of the bacterium and enables the bacterium to resist lysis as a result of its high intracellular osmotic pressure. The main component of cell wall is peptidoglycan (PG) that consists of repeating linear polymers of N-acetylglucosamine (NAG) and N-acetylmuramic acid (NAM) linked together via short oligopeptide chains. Because the cell wall is structurally specific of bacteria, the steps involved in regulation of cell-wall biosynthesis are the targets of numerous antibiotics, including the β-lactams that represent >50% of the available contemporary antibiotic arsenal. The interplay between bacterial cell-wall integrity and the summoning forth of resistance mechanisms to deactivate cell-wall-targeting antibiotics involves exquisite orchestration among cell-wall synthesis and remodeling machineries. In this talk we will present a multidimensional dissection (structural, biochemical, biophysical and preclinical) of some essential bacterial processes pivoting around the bacterial cell wall. These processes are of the outmost relevance in both fundamental and applied sides. Unveiling the molecular basis of these mechanisms paves the way to identification of new drug targets and to develop antimicrobial drugs effective against multidrug-resistant clinical strains and with new modes of action that make the development of resistance less likely.

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AUSE A - 06/09/22 II / 80

BioSAXS: High flux SAXS beamline dedicated to solution scattering at the Australian Synchrotron

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In recent years the Australian Synchrotron received $94.1 million funding from over 20 stakeholders for the construction of new beamlines. The BRIGHT program will expand the beamline infrastructure of the Australian Synchrotron and will increase both its capacity and capabilities. A Small Angle X-ray Scattering (SAXS) beamline is currently being commissioned as part of the BRIGHT program. BioSAXS is due to be available for users from March 2023. The beamline was given a 2 m straight at the storage ring and in order to maximize the photon flux, a superconducting undulator and a double multilayer monochromator were selected in order to monochromatize synchrotron X-Rays between 8-15 keV. The experimental end station consists of an in-vacuum photon counting detector, offering full automation of set up changes and optimised conditions for time-resolved dynamic studies of particles in solution. The BioSAXS beamline will host all types of solution scattering experiments ranging from biological systems to soft matter, chemistry and material sciences. The flux at the sample is expected to be ~5 x 1014 ph/sec and will give the opportunity to users to measure weakly scattering samples and low concentration samples, improving the service and capabilities that are offered to the scattering community in Australia, New Zealand and the Asia-Pacific region.

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No

AUSE B - 06/09/22 II / 22

Unveiling novel temperature scales at the surfaces of 4f-materials by ARPES measurements

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For a long time, rare-earth (RE) intermetallic materials have attracted considerable interest because of their rich and exotic properties including complex magnetic phases, valence fluctuations, heavy-fermion and Kondo behavior and non-Fermi-liquid properties. At the heart of the involved physics is the delicate interplay between itinerant electrons and the lattice of localized 4f states.

In that regard, the class of RE compounds RET2Si2 (T is transition metal atoms) of the ThCr2Si2 type structure attracts considerable attention. Besides their unique bulk properties evolving from an interplay of 4f and itinerant electrons, these materials serve the models for studying exotic physics within the non-centrosymmetric Si-T-Si-RE four-layers surface-silicide block. Within this block, the strength of spin-orbit coupling (SOC) can be tuned by choice of suitable transition metal (T) atoms. It gradually increases by exchanging Co (3d) for Rh (4d) and further for Ir (5d). As a competing ingredient, exchange magnetic interaction may be exploited by inserting elementary 4f magnets like Gd as the RE component. Because the orbital moment of the Gd 4f shell vanishes (L = 0), the pure and large spin moment of Gd will be a strong and robust source of magnetic phenomena. A rotation of the 4f moments to a certain angle relative to the surface normal may be achieved by coupling to a crystal electric field (CEF). To make use of notable CEF effects, a non-vanishing orbital moment L is needed, like for instance in Ho or Dy. Then, this option allows to implement an exchange magnetic field with different strength and orientation at the surface, which competes with the Rashba SOC field and creates additional possibilities to manipulate the properties of the 2D electrons within the considered Si-T-Si-RE system. As the next ingredient, the Kondo effect can be introduced by inserting elements with unstable 4f shell as Yb or Ce. This gives the opportunity to explore the interplay of the 2D electrons with 4f moments within a 2D Kondo lattice in the presence of spin-orbit coupling and a non-centrosymmetric environment.

Our recent experiments have realized the most of such scenarios and demonstrated quite nicely that the Si-T-Si-RE surfaces of the RET2Si2 materials serves as a versatile playground for studying the fundamental properties linked with 4f magnetism and f-d interactions at reduced dimensionality. It represents a kind of construction kit with spin-orbit coupling, Kondo interaction, crystal-electric fields and magnetic exchange with different strengths as building blocks. Their mutual combination gives the opportunity to design systems for different scenarios and to study the physics of 2D electron states in the presence of these competing interactions. The obtained results create a solid platform for the time-resolved studies that are of particular importance for the physics and applications of magnetic materials. The most interesting experimental results, which unveil the novel temperature scales at the surfaces of RET2Si2 as well as of RECo2P2 materials and which are linked with the aforementioned scenario will be presented.

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No

AUSE B - 06/09/22 II / 19

Growth of cobalt iron oxides on Ru(0001) by real-time LEEM and real-time PEEM

Author: Juan de la Figuera[1]

Co-authors: Sandra Ruiz-Gomez ; Anna Mandziak ; Cecilia Granados-Miralles ; Jose Emilio Prieto ; Miguel Aristu ; Alvaro Gonzalez García ; Rafael Navas Rodríguez ; Eva María Trapero ; Guiomar D. Soria ; Adrian Quesada ; Michael Foerster ; Lucia Aballe

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The current quest for spintronic devices might benefit from taking advantage of the properties of highly perfect materials. For example, spinels are oxides with interesting properties that suggest many possible applications based on them. However, growth defects are ubiquitous in spinel thin films. A possible path to obtain highly perfect spinel nanostructures is through growth by oxygen assisted molecular beam epitaxy stopping the growth before island coalescence, where each spinel crystal arises from a single nucleus. We have successfully employed it to grown various spinel

oxides on Ru(0001) single crystals and films, including mixed Ni-Fe [1] and Co-Fe spinels [2]. In particular we have used low-energy electron microscopy to follow the growth at several Co/Fe ratios, complementing it with x-ray absorption spectroscopy analysis of the grown films [3]. However, in a complex multicomponent system, LEEM cannot track the composition evolution of the growth front. In order to follow that evolution, we have acquired PEEM images during the growth at Fe and Co L23 edges by means of photoemission electron microscopy [4]. In this way, we have seen how the composition of the different phases present in the films evolve with coverage.

This work is supported by the Grants RTI2018-095303-B-C51, -A-C52 and -B-C53 funded by MCIN/AEI/10.13039/501100 and by "ERDF A way of making Europe", and by the Grant S2018-NMT-4321 funded by the Comunidad de Madrid and by "ERDF A way of making Europe". C.G.-M. and A.Q. acknowledge financial support from the Spanish Ministerio de Ciencia e Innovación (MICINN) through the "Juan de la Cierva"Program (FJC2018-035532-I) and the "Ramón y Cajal"Contract (RYC-2017-23320), respectively. The experiments were performed at the LEEM microscope at IQFR, CSIC, acquired with funds from the Spanish Ministerio de Economía, Industria y Competitividad (MINECO) through project CSIC15-EE-3056 and the
European Regional Development Fund (ERDF), and at the PEEM station of CIRCE beamline of the Alba synchrotron.

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No

AUSE A - 06/09/22 II / 24

In-situ GIWAXS of thermally-induced co-crystallization in Doped Organic Semiconductor Films

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Among the vast number of organic semiconductors (OSCs) developed in the last decades, [1]benzothieno [3,2-b]benzothiophene (BTBT) derivatives have emerged as one of the best performing materials for p-type organic field-effect transistors (OFETS). However, the understanding and control of molecular doping, as a versatile platform for tuning the optoelectric properties of OSCs, remains a challenge for further advancements in organic electronics.
In this work, we address the structural properties of BTBT films during the sequential deposition of a p-type dopant, 2,3,5,6-tetrafluoro-7,7,8,8-tetracyanoquinodimethane (F_6TCNNQ), with special attention to the comparison of two BTBT derivatives, namely 2,7-dioctyl-BTBT (C_8-BTBT-C_8) and 2,7-diphenyl-BTBT (DPh-BTBT). Grazing incidence wide-angle X-ray scattering (GIWAXS) was performed at the NCD-SWEET Beamline of ALBA in the course of thermal annealing of the films.

Although both BTBT-based films are isostructural, with the (001) plane parallel to the substrate surface and a herringbone packing of the BTBT cores, we find important structural differences upon the deposition of F_6TCNNQ intended to dope the OSC. The deposition of F_6TCNNQ on C_8-BTBT-C_8 results on the formation of a co-crystalline mixed phase at the interface with charge-transfer complex (CTC) properties, which is further promoted by thermal annealing, whereas F_6TCNNQ on DPh-BTBT results in a planar heterostructure, without intermixing of both molecules. These structural differences are expected to be crucial for doping efficiency.

Would you like to participate in the Poster Prize competition?:

No

AUSE B - 06/09/22 II / 52

Rashba-like spin textures in Graphene promoted by ferromagnet-mediated Electronic-Hybridization with heavy metal.

Authors: Beatriz Muñiz Cano[1]; Adrián Gudín[1]; Alberto Anadón[None]; Iciar Arnay[1]; Jose Manuel Díez[1]; Pablo Olleros-Rodríguez[1]; Fernando Ajejas[1]; Matteo Jugovac[2]; Julien Rault[3]; Patrick Le Fèvre[3]; François Bertran[3]; Donya Mazhjoo[4]; Gustav Bihlmayer[4]; Stefan Blügel[4]; Rodolfo Miranda[1]; Julio Camarero[1]; Miguel Angel Valbuena Martínez[1]; Paolo Perna[1]

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Epitaxial Graphene/Ferromagnetic (Gr/FM) structures deposited onto heavy metals (HM) have been proposed for the realization of novel spin-orbitronic devices because of their perpendicular magnetic anisotropy and sizeable Dzyaloshinskii-Moriya interaction, which in turn allow for enhanced thermal stability and stabilization of chiral spin textures [1,2]. In this work we elucidate the nature of the induced Spin-Orbit Coupling (SOC) at Gr/Co interface on Ir by investigating different FM thicknesses [3]. Angular and Spin-Resolved Photoemission Spectroscopy experiments carried out at Cassiopée beamline (Soleil synchrotron), combined with Density Functional Theory calculations show that the interaction of the HM with the C atomic layer via hybridization with the FM is indeed the source of the SOC in the Gr layer. Furthermore, our studies in ultra-thin (2 ML) Co film underneath Gr reveal an energy splitting of $\sim$ 100 meV (negligible) for in-plane (out-of-plane) spin polarized Gr π bands, consistent with a Rashba-SOC at the Gr/Co interface, which is either the fingerprint or the origin of the Dzyaloshinskii Moriya interaction. Interestingly, at larger Co thicknesses ($\sim$ 10 ML), neither in-plane or out-of-plane spin splitting is observed, indicating Gr is almost decoupled from the HM.

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No

AUSE A - 06/09/22 II / 35

Bringing Injection Moulding of Plastics to the SAXS Beamline at ALBA

Author: Geoffrey Mitchell[1]

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Injection moulding is the most common fabrication technology used to shape plastics including recycled plastics. In this technique, molten plastic is injected into a metallic mould under high pressure where it rapidly cools to a solid, thereby preserving the shape and it is then ejected from the mould. The high throughput of this technology has led to its widespread use. The properties of the part critically depend on both the polymer used and the complex processes of flow and cooling within the mould. Analysis using SAXS techniques after moulding reveal complex behaviour which would be easier to understand, optimize and develop, if the data were obtained in real time. This would enable the different processes to be observed separately rather than superimposed as in the final product. This is the objective of the current work. For an amorphous polymer the material solidifies by cooling below the glass transition but for a semi-crystalline polymer, solidification involves crystallization which is strongly affected by the coupled flow and cooling processes within the mould. To develop an understanding of these processes we have set out to design a realistic replica of an industrial injection moulding system, but which would fit on the ALBA NCD-SWEET beam line to allow us to use in situ time-resolved small-angle X-ray scattering techniques to follow the development of structure and morphology of the polymer following the injection stage. There are many challenges in preparing a successful design. Foremost is the restricted space available on the beam line and the need to protect sensitive parts of the beamline equipment from the high temperatures of the mould during the cycle. A second restriction is the weight of the system. The sample translation stage of the NCD-SWEET beamline has a maximum load of 100 kg. The third challenge is the need to design a mould to withstand the pressures within the mould which may reach 200Bar and which provides adequate x-ray transmission without artifacts to enable highly quality time resolving small-angle X-Ray scattering patterns. This presentation will detail the design philosophy we have followed to remain true to industrial practice and which has yield a successful design and we will present the results from experiments performed at the end of last year and discuss the prospects for the future focusing on biopolymers and recycled plastics.

Injection moulding is the most common fabrication technology used to shape plastics including recycled plastics. In this technique, molten plastic is injected into a metallic mould under high pressure where it rapidly cools to a solid, thereby preserving the shape and it is then ejected from the mould. Industrial scale injection moulding can be automated to produce several parts per minute. This high throughput has led to its widespread use. The properties of the part critically depend on both the polymer used and the complex processes of flow and cooling within the mould. Analysis using X-ray scattering technique after moulding reveal complex behaviour which would be easier to understand, optimize and develop, if the data were obtained in real time. This would enable the different processes to be observed separately rather than superimposed as in the final product. This is the objective of the current work. For an amorphous polymer the material solidifies by cooling below the glass transition but for a semi-crystalline polymer, solidification involves crystallization which is strongly affected by the coupled flow and cooling processes within the mould. To develop an understanding of these processes we have set out to design a realistic replica of an industrial injection moulding system, but which would fit on the ALBA NCD-SWEET beam line to allow us to use in situ time-resolved small-angle X-ray scattering techniques to follow the development of structure and morphology of the polymer following the injection stage. There are many challenges in preparing a successful design. Foremost is the restricted space available on the beam line and the need to protect sensitive parts of the beamline equipment from the high temperatures of the mould during the cycle. A second restriction is the weight of the system. The sample translation stage of the NCD-SWEET beamline has a maximum load of 100 kg. The third challenge is the need to design a mould to withstand the pressures within the mould which may reach 200Bar and which provides adequate x-ray transmission without artifacts to enable highly quality time resolving small-angle X-Ray scattering patterns. This presentation will detail the design philosophy we have followed to remain true to industrial practice and which has yield a successful design and we will present the results from experiments performed at the end of last year and discuss the prospects for the future focusing on biopolymers and recycled plastics.

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AUSE B - 06/09/22 III / 48

Two-dimensional ferromagnetic extension of a topological insulator

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As a promising host-system for novel spintronic applications, magnetic topological insulators (TI, MTI's) hosting quantized and spin-polarized transport properties are a highly intriguing research topic. Over the recent years, many design approaches, ranging from magnetic surface coverage over dilute bulk doping up to the use of intrinsic magnetic structures have been tried experimentally, where the key challenge has always been a compromise between strong magnetic order and high crystalline quality [1]. In our work we present the experimental realisation of a novel design approach by magnetically extending the surface of a 3D TI with a 2D layered magnet within the same symmetry class. The magnetic extension approach [2], built up out of the material combination Bi_2Te_3 and $MnBi_2Te_4$ [3] enables a direct overlap between the topological surface state (TSS) density of states and the magnetically active Mn ions, leading to a clear magnetic gap in the TSS as signature of time reversal symmetry breaking while maintaining a highly ordered system.
We present a combined structural and spectroscopic study of this van der Waals heterostructure, facilitating synchrotron based experiments using high resolution angle resolved photoemission (ARPES) x-ray absorption and dichroism (XAS, XMCD) and x-ray diffraction (XRD) on our MBE-grown thin film samples. Together with scanning transmission electron microscopy (STEM) and magnetotransport experiments, we will show a thorough study on the nature of the 2D magnetism in the single sheet of MnBi2Te4, elucidate its direct coupling to the TSS and set the system in perspective to previously studied MTIs and its potential in van der Waals heterostructure design.
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Would you like to participate in the Poster Prize competition?:

No

AUSE A - 06/09/22 III / 18

Towards deciphering Catalytic Mechanisms by Time-Resolved Serial Femtosecond Crystallography at XFELs

Author: Alice Grieco[1]

Co-authors: Miguel A. Ruiz-Fresneda [2]; Juan Luis Pacheco [3]; Rebecca Jernigan [4]; Diandra Doppler [5]; Mukul Sonker [5]; Shahriar Mobashery [6]; Mayland Chang [6]; Petra Fromme [7]; Juan A. Hermoso [1]; Alexandra Ros [5]; Angel L. Pey [8]; Jose M. Martin-Garcia [1]

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Time-resolved serial femtosecond crystallography (TR-SFX) is a revolutionary scientific-technical breakthrough that makes use of the highly-intense, ultra-short X-ray pulses produced at X-ray Free Electron Lasers (XFELs) to study structural dynamics of biological macromolecules in "real time"by using nano/microcrystals under nearly "native" conditions. In our group, we are interested in applying this approach to study the reaction mechanisms of two proteins associated with fatal diseases. Human NQO1 protein, a flavoenzyme associated with cancer, Alzheimer´s and Parkinson´s disease and an attractive target for drug discovery is one. We have recently determined the first structure of NQO1 at LCLS (CA, USA) to 2.5Å resolution using the modulator droplet injector (MDI) developed by Alexandra Ros at Arizona State University (AZ, USA). A careful analysis of our structure has revealed that residues Tyr128 and Phe232, which have been described to play a key role in the function of the protein, show an unexpected flexibility within the crystals. This high-plasticity of NQO1 in the catalytic site provides us with the first structural evidence that the NQO1 functional cooperativity is driven by structural communication between the active sites through long-range propagation of cooperative effects across the NQO1 protein structure. Thus, understanding these functional aspects of NQO1 and its interaction with ligands (substrates and inhibitors) at the molecular level, will be critical to unravel NQO1's role as an antioxidant and a potential target to treat common diseases by advancing in the design of new, more potent, and effective inhibitors that can be used in the clinic. To this end, TR-SFX experiments of the holo-NQO1 in the presence of the substrate NADH at various time delays are ongoing, with the ultimate goal of determining the high-resolution structures of the intermediates involved in the redox reaction mechanism of NQO1.
The second protein of interest to us is the penicillin binding protein 2a (PBP2a) of the methicillin-resistant Staphylococcus aureus (MRSA). PBP2a is used by MRSA as defense shield against beta-lactam antibiotics by an unique allosteric mechanism still not fully understood. We have recently obtained microcrystals of PBP2a and the initial SFX experiments will be conducted at the EuXFEL (Germany) in Fall 2022. For both proteins, NQO1 and PBP2a, it is clear how the setup of TR-SFX experiments is a crucial strategy for providing a new way to explore irreversible reactions and fast conformational changes, leading to generation of molecular movies of dynamic macromolecules in action. SFX at XFELs will represent a very turning point for drug design against cancer and for the design of more potent antibiotics.

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No

AUSE B - 06/09/22 III / 40

Emergent responses in magnetic ring arrays of different lattice arrangements for reservoir computing

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Co-authors: I Vidamour [1]; C Swindells [1]; M Foerster [2]; M. A. Niño Orti [2]; M. C. Rosamond [3]; T Hayward [1]; R Allenspach [4]; A Bischof [4]; D Allwood [1]

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Stochastic behaviour has traditionally been a limiting factor in developing nanomagnetic technology. Recently, we have shown complex probabilistic, emergent behaviour in interconnected nanowire ring arrays [1-3] that is particularly useful for 'reservoir computing'(RC), a highly efficient computation scheme for time domain signal processing [4]. We have also simulated RC with such arrays for recognising spoken digits [2] and anticipate a need to derive additional complex behaviour from the arrays for processing more tasks and data.

Here we vary the lattice arrangements of $Ni_{80}Fe_{20}$ rings (as square, trigonal and Kagome) to achieve alternative responses. Different lattices show rich ground states (for example pinning sites in the trigonal array in Fig. (a)) and can show diverse dynamics. Magneto-optic Kerr effect (MOKE) measurements with in-plane rotating fields (H_{rot}) were used to characterise the arrays [2] and gave the propagating DW state population Nprop (Fig. (b)). The different behaviours are due to interactions at junctions and are seen in X-ray photoemission electron microscopy (XPEEM) images at intermediate fields. The square and trigonal arrays show multiple magnetic states while the Kagome shows vortices. We are now benchmarking computation with these arrays and expect that these varied responses are essential for obtaining additional processing capabilities in reservoir computing.

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Yes

AUSE A - 06/09/22 III / 68

Structural characterization, from synchrotron powder X-ray diffraction data of solid forms of Apremilast, a case of rich isostructural solvatomorphism

Author: Cristina Puigjaner [1]

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Active Pharmaceutical Ingredients (APIs) can exist in different crystalline forms,
demanding a thorough investigation of their solid form landscape during drug discovery. Solvate formation is a common occurrence and in some cases, solvates can serve as intermediates in the production of the optimal form for further development. More challenging is to understand the reason for the formation of isostructural solvates, where the same host incorporates different solvent molecules. Although single crystal X-ray diffraction is the gold standard technique for determining crystal structures, its main limitation lies in the requirement of a single crystal of suitable size, quality and stability which is not always feasible. In the present case, we are studying the rich isostructural solvatomorphic API Apremilast which has been reported to exist in many isostructural solvates. Additional new solvates and cocrystals of Apremilast are reported here and synchrotron

diffraction data of some forms, for which a good quality single crystal has not been obtained, have been recorded on Alba's high resolution MSPD line. These data should be good enough to deal with the structure solution from powders, by using
direct space methodologies of these very similar isostructural forms.

Would you like to participate in the Poster Prize competition?:

No

AUSE B - 06/09/22 III / 26

Bandgap opening in Graphene on Ir (111) mediated by Tellurium intercalation

Authors: Beatriz Muñiz Cano[1]; Daniela Pacilé[2]; Elena Salagre[3]; Enrique García-Michel[4]; Julio Camarero[5]; Manuela Garnica[6]; Miguel Ángel Valbuena[7]; Paolo Moras[8]; Pilar Segocia[4]; Polina M. Sheverdyaeva[8]; Rodolfo Miranda[5]

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Graphene (Gr), in its pristine state, is a semiconductor with a zero band gap and massless Dirac fermions carriers, which conduct electrons like a metal. Nevertheless, the absence of bandgap makes it impossible to control the material's electrons, something essential, for example, to perform on-off switching operations in transistors. Therefore, it is necessary to generate a finite gap in the energy dispersion at the Dirac point (DP). An intense research has been developed to engineer band gaps while preserving the exceptional properties of Gr and different strategies have been proposed, among them, quantum confinement of 1D nanoribbons [1] or the introduction of a superperiodic potential in graphene [2]. Besides, in the context of developing new 2D materials and Van der Waals heterostructures, with new exciting emerging properties, as 2D transition metal chalcogenides monolayers, it is fundamental to know any possible interaction between chacogenide atoms and Gr supporting substrates. In this work, we report on a combined Scanning Tunneling Microscopy (STM), Low Energy Electron Diffraction (LEED) and Angle Resolved Photoemission Spectroscopy (ARPES) study entirely conducted at IMDEA Nanociencia on a new superstructure when Te is intercalated on Gr over Ir(111). Additionally, High Resolution-ARPES measurements were performed at VUV beamline in Elettra Synchrotron. This new superstructure leads to the electronic doping of the Dirac cone (up to ~ 370 meV), while the linear dispersion of massless Dirac fermions is preserved, being the doping level directly related to the ammount of evaporated Te. Very interestingly, our ARPES measurements evidence a large band gap (~ 410 meV) at the DP of graphene Dirac cones, below but close to the Fermi level.

Would you like to participate in the Poster Prize competition?:

Yes

XFEL I / 128

Probing ultrafast structural and electronic dynamics in the condensed phase using X-ray free electron lasers

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X-ray spectroscopy and scattering allow a unique combination of electronic and structural information to be obtained from a variety of different types of samples in many different forms (solid, liquid, gas). The extension of these methods into the time domain has allowed measurement of dynamic processes, for example the tracking the photoinduced charge carriers in a functional material[1],[2] or following the photocycle in a light activated protein[3],[4]. In recent years X-rays have started to become routinely used to measure light-activated processes using a pump-probe scheme, where the sample is photoexcited with light and then probed after a variable time delay using an X-ray pulse. These methods can measure dynamics over a broad range of timescales, allowing them to probe everything from protein dynamics to ultrafast electronic spin-state changes in molecular systems. With the recent development of X-ray free electron lasers (XFELs)[5], time-resolved X-ray techniques have moved into the ultrafast regime, where the timescales of electron and nuclear motion can be accessed using the femtosecond X-ray pulses available from these facilities.[6]
This talk will present an overview of how X-ray techniques are being used at XFELs and the type of information the measurements can provide. The talk will introduce the European XFEL[7], a brand-new, high-repetition rate XFEL facility located in northern Germany, and its'Femtosecond X-ray Experiments (FXE) instrument[8],[9] which is focussed on measuring ultrafast dynamics in the condensed phase. Finally the lecture will present some examples of the types of measurements XFELs can perform and the scientific questions that can be answered using ultrafast X-ray techniques.

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Would you like to participate in the Poster Prize competition?:

No

XFEL I / 106

Novel methods to generate X-ray Transient Gratings

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Nonlinear X-ray wave mixing is a novel area of research that extend the field of nonlinear laser spectroscopy [1] into the short wavelengths regime. Transient grating, a four wave mixing technique, employs two crossed laser beams interacting at the sample to generate an interference pattern. This excitation grating induces dynamics in the sample that transiently changes the index of refraction and evolve over time. The change is detected by a time-delayed third laser beam (probe). Transient grating is widely used in the optical domain to gain information on transport and diffusion processes [2,3] as well as on charge-magnetic and vibrational dynamics [4-6]. However optical wavelengths are limited in the spatial and temporal resolution. With significan efforts, transient grating in the extreme ultraviolet has been demonstrated opening possibility to reach tens of nanometer spatial resolution with element selectivity in solids [7,8]. Extension of transient grating spectroscopy into the X-rays would allow to overcome the limitations of the longer wavelengths thus reaching the ultimate time-spatial resolutions (femtosecond –nanometer) adding chemical specificity. One of the main challenges is the generation of X-ray transient gratings due to the limited X-ray optics and the complexity of the experimental environment. In a series of experiments we have demonstrated the technique by generating X-ray transient gratings via Talbot effect [9] and probing with an optical laser [10] and X-rays at Free Electron Lasers. In this talk I will present the main results obtained in the experiments and explore possible novel methods to generate X-ray transient gratings in the future.

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Would you like to participate in the Poster Prize competition?:

XFEL I / 91

MID, Materials Imaging and Dynamics

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The MID instrument, located in the beamline SASE2 of the European XFEL Facility, has been in operation since 2019. The focus of the MID instrument is ultrafast studies of materials using the High repetition rate and high spatial coherence of the European XFEL accelerator.
The instrument work in a large range of hard x-ray energy ranges from 5 keV to 24 keV. The beam size at the sample position can be tailor from 2 mm to 300 nm (using CRLs) optics. For the longitudinal coherence, the instrument has 2 monochromators Si 111 and Si 220, what allows bandwidths of 10-4 and 6x10-5, respectively. As a plus, the self-seeding available at SASE2 allows to reduce the bandwidth of the photons from the machine to 1.5 eV. The instrument has also a splitting and delay

line (SDL) that is capable of dividing the incoming xrays in two pulses and scan them from -10 to 800 ps. A magnetic pulse environment capable of generating 14 T pulse magnetic fields is available. An optical laser 800 nm with 15 (50) fs
pulse width and a maximum pulse power of 1 mJ is also available for performing pump-probe experiments.
The main detector at the instrument is the single pulse resolve AGIPD, that has a 200 μm square pixel. This detector can work with the 4.5 MHz repetition of the x-ray source and collect 352 pulses by train. The AGIPD detector can be located in WAXS and SAXS configuration and at arrange between 3 and 8 m from the sample. Other detectors available are the Epix, Jungfrau and the scintillator couple Andor Zyla.
The main experimental technique at MID is XPCS (X-ray photon correlation spectroscopy), but experiments of holography, Bragg CDI, ptychography, SAXS, WAXS and pump-probe diffraction have been performed successfully. In the oral contribution some of these experiments will be present to the audience.

Would you like to participate in the Poster Prize competition?:

XFEL I / 41

Ultrafast X-ray and optical time-resolved investigation of CuInS2 quantum dots

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Co-authors: Brener R. C. Vale [2]; V. Fonseca André F. [3]; Lázaro García [1]; Juan F. Hidalgo [4]; Olivia Borrell-Grueiro [5]; Tae Kyu Choi [6]; Tetsuo Katayama [7]; Dongxiao Fan [8]; Shunsuke Nozawa [8]; Luis Bañares [5]; Marco A. Schiavon [9]; Wojciech Gawelda [1]

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The interest in copper-indium-sulfide (CIS) quantum dots (QDs), as heavy metal-free nanomaterials, has increased significantly in the past few years. CIS quantum dots (QDs) have been studied for many applications like photodynamic therapy, solar cells, LEDs, and bioimaging [1]. They show exciting optoelectronic properties, such as broad photoluminescence (PL) with a large Stokes shift and long charge carrier lifetimes. Several mechanisms for the radiative recombination in CIS QDs have been proposed over past years. In this work we aim to understand and confirm the possibility of radiative recombination resulting from an electron in the conduction band and a hole in a so-called confined hole state (CHS) or localized hole [2-3], which is a mid-gap state arising from a defect of Cu+ that can get oxidized to Cu2+ by the hole. The range of possible defects would explain the broad PL and large Stokes shift. In addition, we aim to understand the effects of stoichiometry and Zn doping on the formation process of the CHS.[4] To these ends, the element and oxidation state specificity of X-ray techniques can be a great tool to carry out a more direct observation of such processes, allowing us to confirm the proposed mechanisms. We approached these questions through a combination of laser, synchrotron and XFEL techniques, including our recent results from SACLA XFEL and ALBA. We focused on tracking in real-time the oxidation state changes of Cu via femtosecond-resolved Cu K-edge XANES and comparing the structure of the different samples through steady-state EXAFS. We have complemented our investigation in the X-ray range with time-resolved optical studies

monitoring ultrafast transient absorption and photoluminescence (with fluorescence up-conversion spectroscopy).

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Would you like to participate in the Poster Prize competition?:

No

XFEL I / **107**

Ultrafast dynamics of complex systems at the Alvra Endstation

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The advent of X-ray Free Electron Lasers (XFELs) introduced the possibility to study ultrafast phenomena in the X-ray range, with high temporal resolution and unprecedented peak brightness. This has led to the extension of many established methods into the time-domain as well as the development of new photon-hungry techniques XFELs. These advances have also made it possible to take full advantage of the element and site-specificity of X-ray spectroscopy techniques, such as X-ray Absorption (XAS) and X-ray emission (XES), as well as scattering and diffraction techniques, such as X-ray Solution Scattering (XSS) and Serial Femtosecond Crystallography (SFX), in the study of ultrafast processes in complex molecular systems. In this talk, I will show how this was used to unveil the complete photoinduced dynamics of dilute, biologically relevant heme proteins in physiological conditions, such as Cytochrome C and Myoglobin, as well as present future perspectives in the field of ultrafast X-ray spectroscopy at Free Electron Lasers, and more specifically at the Alvra endstation at SwissFEL.

Would you like to participate in the Poster Prize competition?:

XFEL II / **73**

Opportunities in Non-equilibrium (Bio)chemistry via THz-driven Water Dynamics

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Liquid water is the single most important medium in which highly consequential chemical and biological processes take place. Water is often equivocally regarded as a passive medium. Ranging from an isolated molecule to small clusters and up to bulk, water shows unique and ubiquitous behavior at different temperatures and environments. The main reason is the presence of a strong H-bond network[1], which is why water provides a very dynamic environment to solutes.

The H-bond network plays a crucial role in the vast majority of solvation chemical reactions, such as femtosecond guest-host interactions, folding processes in biomolecules, and non-equilibrium chem-

ical kinetics, which are not light-triggered reactions but kinetically activated. The combination of ultrafast strong-field THz[2] and X-ray sources[3] forges a unique opportunity to drive and visualize water molecular dynamics for in-solvation (bio)chemical reactions to be understood and controlled. First, before its thermalization, investigating the non-equilibrium, femtosecond to picosecond time evolution of the structure of water clusters under strong-field THz radiation renders H-bond network disruptions resembling supercritical-like water structure that may play a crucial chemical role via interactions with the first few hydration shells and beyond. Second, the H-bond network relaxation and thermalization at longer delays (»100s of picosecond) will also yield tunable temperature jumps (T-jumps) from a fraction to hundreds of Kelvin.

In this talk, we will first review recent advancements in THz-driven non-equilibrium in-solution biochemistry. We will also discuss how understanding the ultrafast non-equilibrium and thermalization processes of water under THz excitation could unlock a vast ensemble of physical and biological quantum chemistry in highly disrupted hydration shells that are not possible to study today. Last, we will summarize the scientific and technological challenges ahead to fully capitalize on this generalized framework.

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Would you like to participate in the Poster Prize competition?:

No

XFEL II / 84

Mix-and-probe serial femtosecond crystallography enables the visualisation of an enzyme:substrate complex at room temperature

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Understanding the basis of enzyme catalysis at the molecular level has been a fundamental goal of biochemistry and structural biology. The "recording"of an enzymatic reaction as it happens represents a significant challenge because many of the enzyme:substrate/transition-state/product complexes are transients, making them invisible to standard crystallographic techniques. X-ray free-electron lasers produce ultra-fast femtosecond X-ray pulses *ca.* 10_{12} times more intense than standard synchrotron radiation. Nonetheless, it is critical to develop injector/mixing devices to exploit XFEL capabilities to visualise enzymatic reactions.

In this talk, we will present the application of the concentric-flow electrokinetic injector **[1]** to carry out *mix-and-probe* serial femtosecond crystallography, which allows us to mix unbound enzyme microcrystals with natural substrates and inject them into the path of femtosecond XFEL pulses to obtain structural information of retaining glycosyltransferases. Also, we will present our results using standard synchrotron radiation and quick-soaking of natural substrates into unbound enzyme crystals **[2]** to trap structural snapshots of glycosyltransferases **[3,4]** which allow us to propose a common substrate-assisted S_Ni-type mechanism for all retaining GTs **[4]**.

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Would you like to participate in the Poster Prize competition?:

No

XFEL II / **89**

Femtosecond-to-Millisecond Structural Biology using Synchrotrons and X-ray Lasers

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Providing detailed experimental insights into how proteins change over time and to relate these structural changes to biological function remains one of the major challenges in structural biology. Next generation X-ray sources including diffraction-limited synchrotrons and X-ray Free Electron Lasers offer exciting new opportunities to study protein dynamics by time-resolved pump-probe crystallography.
In the last few years, my group has demonstrated the use of high-viscosity injectors to increase sample efficiency in time-resolved measurements[1]. This allowed us and our collaborators to assemble over 40 structural snapshots of the light-driven proton pump bacteriorhodopsin. In a wide temporal window, we cover the light-induced isomerization of retinal within the first few hundred femtoseconds[2], the following proton release steps within microseconds[3] and the proton uptake reaction in the early milliseconds[4]. Together this provides the most complete molecular view of a membrane pump in action and acts as a template how to approach studies on proteins with increasing complexity. As a first step in this direction, we and our collaborators concluded piloting time-resolved crystallographic measurements at the Swiss Light Source and the Swiss X-ray Free Electron Laser to resolved the structural changes within light-driven sodium pumping[5] and chloride pumping rhodopsins[7]. In our latest work we aimed at increasing the number of proteins that can be studied using pump-probe techniques through the use of synthetic photoaffinity switches[6]. The overarching goal is to map the structural dynamics of protein-ligand interactions in a series of proteins used in optogenetics and photopharmacology.

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Would you like to participate in the Poster Prize competition?:

No

XFEL II / **108**

Tracking phase transitions at extreme conditions of pressures and temperatures using high-energy lasers and XFELs

Co-authors: A. Amouretti [1]; A. Krygier [1]

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Studying matter under extreme conditions is critically important for a wide range of science application including, for example planetary science, astrophysical high-velocity impacts as well as industrial applications. While laser compression is playing a major role in exploring phase diagrams at extreme condition of pressures and temperatures, the associated physical processes and phase transitions mechanism are barely understood. The arrival of XFELs, in complement with synchrotron sources are providing unique new measurements and deeply modifying our understanding of dense matter.
In that context, we present a short overview of recent studies devoted to investigate the solid-solid and solid-liquid transition in laser-shocked iron alloys [1] and iron oxides using X-ray diffraction, X-ray diffuse scattering and X-ray absorption spectroscopy. Experiment were performed at the MEC end-station of the LCLS facility at SLAC (USA), at the EH5 end-station of the SACLA facility (Japan) and at ID24-ESRF (France). Our results show dynamic high-pressure phases that are not identical to those revealed by static diamond anvil cell compression, questioning transition paths, and especially the spin transition mechanism in the case of Fe2O3. Finally, we have also possibly highlighted the reduction of iron in Fe2O3 upon release after a shock at 120 GPa. This observation highlights the rapidity of the redox mechanism under high-velocity impact as suggested by recovered samples from meteorite impacts.
[1] A. Krygier, Physical Review B, 2022

Would you like to participate in the Poster Prize competition?:

ALBA - 07/09/22 / **112**

ALBA Present and Perspectives

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Since the last meeting in 2019, ALBA and its user community has not only seen an exceptional successful operation, despite the difficult working conditions due to COVID and other major changes, but had also experienced a dynamic period of growth and changes. With LOREA and NOTOS being in operation and XAIRA, FAXTOR and MINERVA making excellent progress towards finishing the construction phase, our user program has significantly grown, providing you not only with more available beamtime in hard X-rays spectroscopy and diffraction, but also extended our capabilities to ARPES and strengthening our operando capabilities for chemical and material sciences. With the help of you, the user community, ALBA was also able to start 3Sbar, the first beamline fully dedicated to the upgraded ALBA II and devoted to combined hard x-ray photoelectron spectroscopy (HAXPES) and surface scattering experiments at high gas pressures, potentially benefitting a wide range of the existing user community.
Following the call of politics and society to contribute and fuel the green transformation to create a sustainable and humane economy, ALBA teamed up with the user community to broaden the services from a pure X-ray facility towards an infrastructure which can support your needs to address these complex and, often application driven, challenges with instrumentation and know-how. A cryo-Electron Microscope (cryo-EM) facility for structural biology and a high-resolution materials science Transmission Electron Microscope (HRTEM) will be soon available within the general public user program, significantly extending our suite of tools for structural molecular biology and extending ALBA's materials science microscopy capabilities to sub-atom resolution. A dedicated battery and electro catalysis laboratory with assembly, pre-characterization, and also ageing facilities, combined with a planned new catalysis preparation and staging laboratory will largely strengthen ALBA' s operando capabilities allowing you fast, effective and uncomplicated access to state-of the art characterization facilities. Last but not least, In-CAEM, a major consortium, will significantly broaden the microscopy suite at ALBA, providing a dedicated HRTEM, optimized for operando experiments, and three specialized AFM/STM instruments. All these projects will not only give you the ability to use these high-end instrumentations but also provide experts and potential collaboration partners, supporting you in planning and executing the experiments if needed. With this extension of the services, ALBA is also building out its multi-modal capabilities by developing and providing specialized data pipelines, access to large scale computing capabilities and databases, and by entering the world of big data and data mining.
The talk will provide an overview on the existing user program and will discuss the new exciting developments, including an introduction of our different partners.

Would you like to participate in the Poster Prize competition?:

No

ALBA - 07/09/22 / **114**

Catalysis

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ALBA - 07/09/22 / **127**

Resonant x-ray scattering from quantum materials

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We will give a broad overview of recent progress in an experimental effort to understand and control collective quantum phenomena and excitations in metal oxides. Resonant x-ray scattering yields

essential information about interactions between spin, charge, and orbital degrees of freedom at the atomic scale, and is hence a key tool in this effort. We will focus on recent advances in research on copper oxides and ruthenium oxides.

Would you like to participate in the Poster Prize competition?:

No

ALBA - 07/09/22 / **116**

Synchrotron experimental techniques in the post-Alphafold2 age

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ALBA - 07/09/22 / **117**

3Sbar: new opportunities at ALBA

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ALBA II / **110**

Towards ALBA II

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Significant progress in accelerator design, X-ray optics, detection technology, and Information Technology drives worldwide the evolution of synchrotron light sources to the 4th generation, opening new windows to the exploration of inner details of matter, devices, and their functionality. The ALBA II project, initiated in 2021, will transform ALBA into a 4^{th} generation light source, to provide answers for growing research demands caused by the ecological and economical challenges of the 21^{st} century.
The status and perspectives of the project, which is nowadays in the design and prototyping phase, will be presented.

Would you like to participate in the Poster Prize competition?:

No

ALBA II / **88**

ALBA II Accelerator Upgrade Project

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ALBA is working on the upgrade project that shall transform the actual storage ring, in operation since 2012, into a 4^{th} generation light source, in which the soft X-rays part of the spectrum shall be diffraction limited. The project has been officially launched in 2021 and a White Paper presenting the main concepts of the upgrade shall be published in 2022. The storage ring upgrade is based on a 6BA lattice which has to comply with several constraints imposed by the decision of maintaining the same circumference (269m), the same number of cells (16), the same beam energy (3GeV), and as many of the source points as possible unperturbed. The lattice optimization has achieved an emittance of 140pmrad, which is a factor 30 smaller than that of the existing ring, but with an array compactness that presents technological challenges for the magnets, vacuum, diagnostics, RF systems and injection elements designs that are being investigated through an intensive R&D program.

Would you like to participate in the Poster Prize competition?:

No

ALBA II / 118

In-situ Correlative facility for Advanced Energy Materials (In-CAEM)

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Within the Complementary Plans Program in Advanced Materials, a correlative facility for in-situ experiments directly linked to the ALBA Synchrotron will be soon launched launched in Catalonia. Its aim is to enable correlative in-situ (S)TEM, AFM/STM and Synchrotron Radiation (SR) experiments to address some of the scientific challenges of the European Green Deal plan, and thus promote a more sustainable EU economy. Its budget is co-financed by the Ministry of Science and Innovation through MRR funds and by the Department of Research and Universities of the Generalitat of Catalonia with its own funds.

The In-situ Correlative Facility for Advanced Energy Materials (In-CAEM) is conceived as a key tool to address the challenges of materials advanced characterization, down to the atomic scale, analyzed in working conditions/in-situ/ operando, and under controlled environment in gas or liquid.

For example, in advanced catalyst materials for energy applications, which are primarily based on metal-based oxides and nanostructures, small surface changes at the atomic level, such as the presence of dopants, vacancies, holes, or slight differences in atomic structure can strongly influence their final behavior. Current state-of-the-art characterization methods are insufficient for the simultaneous observation of atomic structure and measurement of local physical/chemical properties. The combination of chemical and structural characterization at the atomic scale with in-situ measurements at the nanoscale, based on a powerful combination of electron microscopy and synchrotron techniques on the same nanostructure, will allow a much better understanding of these chemical reactions.

The present proposal includes an electron microscope with in-situ detectors, gas and liquid sample holders for in-situ analysis, the adaptation of existing synchrotron beamlines at ALBA for correlative analyses with TEM, STM/AFM equipment to combine improved Raman spectroscopy (TERS), and various advanced STM/AFM on-site equipment. The project also has an advanced computing system for data storage, data processing, and in-situ data analysis using automated protocols based on artificial intelligence.

In-CAEM is part of the Joint Electron Microscope Center at ALBA, a new infrastructure that has been created in the perimeter area of the ALBA synchrotron with an inter-institutional collaboration model. JEMCA currently hosts two instruments (illustrated in the figures) co-financed by FEDER funds from GenCAT and different research institutes, which share their time of use with external

users who access through a competitive process. In particular the 200 kV CRYO-TEM, dedicated to life sciences, already open to users, managed by the Barcelona Institute of Molecular Biology (IBMB-CSIC) and METCAM, a monochromated and double corrected 300 kV STEM, in the process of being installed, managed by the Catalan Institute of Nanoscience and Nanotechnology (ICN2). In-CAEM follows the EMCA collaboration model, with the participation of different institutes in the construction, start-up and operation, in particular, in addition to the ALBA synchrotron itself, the ICN2, the Institut de Fisica d'Altes Energies (IFAE) , both CERCA centers and members of BIST, and the Institute of Materials Science of Barcelona (ICMAB-CSIC), which together with the ICN2 forms part of the network of centers linked to the CSIC. In-CAEM is complementary to METCAM. Its usage model foresees LongTerm Projects and competitive access and particular attention to industrial users.

ALBA II / **113**

ALBA II Science

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ALBA II is a unique opportunity to create together with you a facility which is fit for the research and development needs of the first half of the 21th century. Well aware of the broad base of ALBA's user community, we used three focus areas, health, energy, and information technology, to analyze the challenges laying ahead of us, to identify the characterization needs, and ultimately develop a holistic concept to fully support the users from these areas but also benefit the full width of the user community by adding individual components to their characterization portfolio.
Each of the examples will feature the needs for developing easy to use multimodal methodologies which fully integrate ALBA II's extended microscopy tools, show the need for fast accessible high throughput facilities with extended energy range in comparison to ALBA, strengthen the operando capabilities often supported by the reduced beam size of the new facility, and last but not least, the systematic integration of big data concepts.

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No

ALBA II / **119**

The future beamlines at ALBA II

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ALBA II / **126**

New Call for Beamlines at ALBA II

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Perspectives of Electronic and Magnetic Structures

ALBA A - 08/09/22 I / 99

Perspectives of Life Science at ALBA

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The Life Sciences scientific program at the ALBA synchrotron has been well established for years, with several beamlines covering multiple techniques widely used in structural molecular and cellular biology. Still, as part of the future ALBA-II upgrade, the program is being further developed to offer new techniques. The existing beamlines are planned to undergo throughout upgrades in the optics and the end-station, and new beamlines are being built. Beyond the traditional portfolio of beamlines, a new super-resolution 3D microscope for correlated ultrastructural cell imaging is currently available, and the first electronic microscope, implemented through a consortium of nearby institutions, will start user operation in few months. Also, the bio laboratories are being completed with a macromolecular crystallography platform, among other equipment. Here we aim to open a discussion about the perspectives of the program and the instruments and services to be conceived and implemented, still to be defined, to optimally boost the scientific capabilities and productivity of the scientific community.

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No

ALBA A - 08/09/22 I / 123

Serial Crystallography ready for XALOC users: from SMX @ALBA to SFX @EuXFEL

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In the new Alphafold2 era, the interest of structural biologists on macromolecular dynamics has increased. Synchrotron Serial Crystallography (SSX) may still be not so known among crystallographers as single-crystal MX, however, the serial data collection of multiple non cryocooled microcrystals opens the door not only to projects including radiation sensitive targets (as metalloproteins) or membrane proteins crystallized in viscous matrices as LCP but also to dynamic pump-probe studies or time resolved measurements. In fact, some of the SSX experiments may also further be completed at FELs using Serial Femtosecond Crystallography (SFX) -where initial SSX information is compulsory- showing the complementarity between both methodologies.

The purpose of this talk is to introduce ALBA users to the current Jet-based SSX implementation at XALOC beamline which mainly comprises an HVE injector, an automated platform for proper jet positioning and a dedicated pump for fine tuning of sample extrusion -controlled with an inhouse developed algorithm-. Several examples collected at the beamline will be presented and general

guidelines to perform SSX experiments at ALBA, provided. Actually, a specific call for Jet SSX proposals have been launched since this last July to better fulfill the needs of the MX community first, at XALOC, but expect to complement it even further with the chance to perform fixed-target SSX at XAIRA soon.

Would you like to participate in the Poster Prize competition?:

No

ALBA B - 08/09/22 I / 38

LOREA: the ARPES beamline at ALBA in operation

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LOREA ('*flower*'in basque language), the ninth beamline of the ALBA synchrotron radiation source, started its operation in 2021 and is dedicated to electronic structure investigation by means of Angle Resolved Photo-Emission Spectroscopy **(ARPES)**.
The beamline covers the photon energy range of 10-1000 eV, with continuously variable polarization, resolving power of more than 10^4 in the whole range, and a spot size of about 10x10 μm^2. The estimated photon flux is 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 energy range. LOREA is suitable for high resolution VUV ARPES investigation in the range of 10-200 eV, Soft X-ray ARPES in the 200-600 eV energy range, and core level spectroscopy, resonant photoemission and X-ray absorption spectroscopy in the whole energy range.
LOREA uses an MBS A-1 hemispherical analyzer with high energy resolution (better than 1meV) and the fast Fermi surface mapping mode. It has been recently upgraded with a spin detector to al-low spin-resolved ARPES.
The 6-axes cryo-manipulator can reach low temperatures better than 7.5K and the sample stage is provided with 4 electrical contacts for I-V characterization of simple devices.
The main chamber of LOREA is connected to a central radial distribution chamber and, through it, to all other vessels, including chambers for in situ UHV deposition and characterization, fast entry load lock and sample storage, docking of vacuum suitcases, docking of STM.
The transfer between chambers is completely automatic, and is based on the tango control system.
This project is co-funded by the European Regional Development Fund (ERDF) within the "Framework of the Smart Growth Operative Programme 2014-2020"

Would you like to participate in the Poster Prize competition?:

No

ALBA A - 08/09/22 I / 124

What can the CryoEM Platform do for you?

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The new Cryo-electron Microscope Platform possess a specialized cryo-electron microscope for structural biology applications, equipped with an automated sample load system and a last generation direct electron detector Falcon IV. The platform will give access to state-of-the-art cryo-EM equipment for structure determination projects using the latest technology and methods.
This equipment will be used mainly to obtain structural information of proteins and macromolecular complexes at atomic resolutions, in order to determine their three-dimensional atomic structure. This information is essential to determine how a protein is capable of carrying out its function at atomic level and the first step in the design of drugs and other molecules of interest in medicine and biotechnology.

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No

ALBA B - 08/09/22 I / 95

Coherent soft x-ray imaging: Uncovering emergent physics with unprecedented spatial and temporal resolution

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Nanometer-scale textures, such as stripe domains and magnetic skyrmions, are ubiquitous in materials in which interactions compete at different length scales. Remarkably, such textures can exist even in a perfectly homogeneous underlying material. Since their energy is translationally invariant, they can move within the hosting material. It is of great fundamental and applied interest to image the emergent dynamics of such textures.
However, the grand challenge in such studies is that they require exceptional spatial and temporal resolution, often beyond the reach of established imaging techniques. Here, I will highlight several scenarios in which holographically-aided coherent x-ray imaging has allowed us to uncover previously inaccessible physics of emergent spin textures at the nanometer scale.
The first example is static magnetic imaging with deep sub-10 nm spatial resolution. Reaching this resolution presents a change of paradigm in x-ray magnetic imaging because it allows to resolve domain walls and not just domains. Thanks to this, we make some highly surprising discoveries in a supposedly well-explored Pt/Co-type material, including the emergence of 3D spin textures near pinning sites.[1]
In my second example I will demonstrate that coherent x-ray magnetic imaging can also be performed with x-ray magnetic linear dichroism contrast, which allows to directly capture the chirality of domain walls and which is also suitable for imaging of antiferromagnetic materials. At beamline BOREAS at ALBA, this technique has allowed us to directly image Bloch line defects in skyrmions in bulk DMI DyCo films.[2]
Finally, I will show that coherence also allows to massively enhance the temporal resolution. The example I will show is the direct imaging of thermal fluctuations between highly degenerate magnetic stripe domain states. Such fluctuations are very common in nature, especially in disordered or imperfectly ordered systems at the nanometer scale. Yet, they are notoriously difficult to access by direct imaging because pump-probe techniques cannot be employed. The challenge can be traced back to seemingly a fundamental dilemma between temporal and spatial resolution. I will show that coherent imaging can overcome this dilemma, by allowing to identify the underlying state of a scattering pattern at much lower photon count as required for the reconstruction of a real-space image. This approach, which we coin Coherent Correlation Imaging, allows us to uncover an intricate network of more than 30 recurring magnetic states and dynamics that is governed by a surprising

interplay of attractive and repulsive pinning.[3]
I will conclude with a wish list for new high coherence sources such as ALBA-II.

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No

ALBA A - 08/09/22 I / 10

Application of |ρ| - based direct methods to the solution of anomalous scatterers substructures from SAD data of protein crystals

Authors: Jordi Rius[1]; Xavier Torrelles[2]

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Owing to the importance of the *SAD* technique, |ρ|-based direct methods in the form of the recent *SMAR* (= SM,|ρ|) phasing algorithm incorporating the inner-pixel-preservation (*ipp*) procedure [Rius, J.& Torrelles, X. (2021) Acta Cryst A77, 489-493] have been adapted to the determination of anomalous scatterers substructures. Their applicability has been tested on a series of representative experimental data sets, mostly retrieved from Protein Data Bank. The suitability of the data sets is indicated by two main indicators. The dominant anomalous scatterers are either SeMet or S atoms, or metals/clusters incorporated by soaking. The test results indicate that the adapted *SMAR* algorithm (*S-SMAR*) solves the substructures of the protein crystals quite efficiently provided that the Fourier peaks of the anomalous scatterers have spherical symmetry at the working resolution.

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(and Feder)

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No

ALBA B - 08/09/22 I / 97

Interaction of alkali metals and Graphene: a LEEM/PEEM study

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One of the most common approaches to introduce improvements for graphene future technological applications is the intercalation of atoms or molecules through graphene. Among the different studies that have been done, the intercalation of alkali metals have been proven to be very appealing to engineer the band structure of graphene. In particular, lithium and more recently sodium also stand out due to their direct application on graphene ion-batteries. In this sense, our work focuses on a novel approach to intercalate lithium[1] and sodium[2] through graphene by means of photon irradiation. A thin film of LiCl or NaCl previously grown on top of graphene is irradiated with soft X-ray photons leading to a cascade of physico-chemical reactions. Upon the salt photodissociation we find fast chlorine desorption and a complex sequence of alkali intercalation processes. The full sequence of processes has been studied in real-time by a multi-technique in-situ characterization in the PEEM/LEEM end station of Circe at ALBA Synchrotron.

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Would you like to participate in the Poster Prize competition?:

No

ALBA A - 08/09/22 I / 45

Peptide Amphiphilic-Based Supramolecular Structures Interaction with Liposomes

Author: Ramon Pons[1]

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We have used SAXS to investigate the incorporation of several peptide amphiphiles to vesicles. These modified peptides have been shown to have amphiphilic properties. Vesicles have distinct SAXS features that provide information about the electronic density across the bilayer. We have adopted a multiple Gaussian description of the bilayers using several constrains to keep the number of fitting parameters to reasonable figures. The presence of multilayers is dealt with the use of a modified Caille description as detailed by G. Pabst et al (Pabst, G.; Rappolt, M.; Amenitsch, H.; Laggner, P. Phys. ReV. E 2000, 62, 4000-4009). Asymmetric description of the bilayers has been achieved by adding perturbations to the basic symmetric description using several strategies: keeping the number of Gaussians in the description but with different parameters at each side of the bilayer (width, position and intensity as possible changes) or adding additional contributions at one or other side of the bilayer. Studying a series of compounds, we have been able to propose several modes of interaction of amphiphilic peptides with bilayers.

Would you like to participate in the Poster Prize competition?:

No

ALBA A - 08/09/22 II / 101

High-sensitivity quantitative X-ray phase-contrast imaging for biomedical applications

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Phase-contrast X-ray imaging uses the refraction of X-rays to generate the contrast. It has been demonstrated to provide superior soft-tissue contrast in comparison to conventional attenuation-based X-ray imaging. However, quantitative imaging of biomedical soft tissue at high spatial resolution and high image quality still remains challenging. Some existing methods require assumptions on the composition of the specimen (e.g., single material and low attenuation) to retrieve the phase information and show less sensitivity in resolving small changes in electron density within the sample. Specimens violating these assumptions become impossible to image. Within a long-term proposal at the imaging beamline P05 at PETRA III (DESY, Hamburg), we successfully designed and built an imaging setup based on 2D Talbot array illuminators (TAI) (Gustschin et al., 2021) and a speckle-tracking technique (Unified Modulated Pattern Analysis, UMPA) (Zdora et al., 2017), which overcomes these challenges. Our method accurately extracts the electron density distribution with higher sensitivity than comparable techniques and is compatible with a wide energy range. Here, we will review the potential of this new quantitative imaging method by highlighting the recent results on biomedical applications.

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Would you like to participate in the Poster Prize competition?:

No

ALBA B - 08/09/22 II / 92

The Chemistry and Material Science section at ALBA

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The Chemistry and Material (CHEMAT) section is administratively one of the three scientific sections of CELLS-ALBA Experiment Division. It presently encompasses 4.5 operating beamlines (BL04-MSPD, BL11-NCD-SWEET, BL16-NOTOS, BL22-CLAESS and BL24-CIRCE-NAPP) and two laboratories: (Chemistry and High Pressure). Already foreseen is the integration in the section of the new beamline 3sbar (operative in 2026), and two new laboratories: battery lab BATTlab (operative 2023) and catalysis lab CATlab (foreseen 2024).
The idea of this administrative structure is to promote and bring synergy in scientific field aspects

against purely technical ones, targeting essentially the ALBA strategic scientific lines which are Catalysis and Energy related materials, but maintaining high level scientific activity in High Pressure, Polymer, Strongly Correlated Electron systems and Functional materials, topics which remains highly demanded by the Spanish user community. A multi techniques approach will be developed, intensively involving the above mentioned beamlines, some others depending on fields, eg BL01-MIRAS and BL09-MISTRAL for battery, BL01-MIRAS and BL31-FAXTOR for catalysis, as well as the upcoming InCAEM environmental TEM. Methodology, data processing, extensive laboratory support and possibility of remote and fast access mode is considered as part of the overall CHEMAT vision.

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ALBA B - 08/09/22 II / **83**

A retrospective view of synchrotron radiation in polymer science at ALBA and a dream for the future

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Scattering techniques have been widely used for studying the structural heterogeneity of soft condensed matter in general and polymers in particular. Simultaneous Small Angle X-ray Scattering (SAXS) and Wide Angle X-ray Scattering (WAXS) is a well suited technique for investigating phase changes or conformational rearrangements on a length scale ranging from 1 to 500 nm. Static or time resolved measurements can be performed with simultaneous SAXS and WAXS area detectors. Investigation of thin films at different length scales is also possible by using grazing incidence geometry, GISAXS and GIWAXS. Some examples of the application of these techniques, available at NCD-SWEET beamline, will be given: the study of structure-property relationship in fully biobased polymers for packaging1, the investigation of nanostructured thin films2, as well as the structure developed in polymers during "operando"3-D printing3.
Finally, as a dream for ALBA II, it will be show how a Resonant Soft X-ray Scattering (RSoXS) beamline, devoted to soft condensed matter, can complement the scattering techniques available at ALBA4.

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Would you like to participate in the Poster Prize competition?:

No

ALBA A - 08/09/22 II / **100**

Applying soft X-ray tomography to support therapeutic development for Muscular Dystrophies

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Our aim was to apply high resolution and precision techniques to investigate the efficacy of gene editing to revert the cellular and biochemical phenotype of cells harbouring collagen VI mutations which give raise to a severe form of Muscular Dystrophy. Soft X-ray tomography can provide new structural and complementary results given that no sectioning is required, thus preserving the ultrastructure of the cell and the possibility to obtain qualitative and quantitative information from whole cells.

Would you like to participate in the Poster Prize competition?:

No

ALBA B - 08/09/22 II / 103

Operando X-ray diffraction and absorption spectroscopy to better understand battery materials

Authors: Damien Saurel[1]; Marcus Fehse[1]; Marine REYNAUD[2]; Henri Anne[1]; Iciar Monterrubio[1]; Maria Angeles Cabañero[None]; Montse Casas Cabanas[1]; Montserrat Galceran[1]; Morgane Giner[1]

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Li-ion and Na-ion batteries operate thanks to reversible intercalation reactions of the intercalant cation (A = Li^+ or Na^+) with the host compound (A_xH) used as the active material of the positive electrode (often referred as "cathode"). These intercalation reactions typically exhibit two types of reaction mechanisms: (i) homogeneous reactions (single phase or solid solution), which involve the formation of a non-stoichiometric compound whose insertion content x in A_xH continuously varies throughout the intercalation domain $x_{min} \geq x \geq x_{max}$; or (ii) heterogeneous reactions (multi-phase) which involve the nucleation and growth of a second phase A_yH (where $y \neq x$) as a result of the compositional changes occurring within the electrode. In single-phase reactions, the host structure does not suffer from major structural changes other than a continuous variation in volume to accommodate the change in composition, which is generally considered to be more favorable for fast diffusion than the moving interface found in two-phase reactions. On the other hand, depending on the rate at which these intercalant reactions occur (*i.e.* depending on the rate imposed to the battery for the charge and/or discharge processes), the electrodes materials are driven away from the equilibrium conditions, which can provoke significant differences in their reaction mechanism, for example changes on the phase transitions sequences.
In this talk, we will illustrate how operando powder X-ray diffraction (XRD) and absorption spectroscopy (XAS) experiments provide valuable insights for the understanding of the reaction mechanisms in electrode materials such as Li-rich layered oxides [1], the high-voltage spinel $LiNi_{0.5}Mn_{1.5}O_4$ [2] and the Na-ion triphylite (olivine-type) $NaFePO_4$ and $NaFe_{0.8}Mn_{0.2}PO_4$ cathode materials [3,4].

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Would you like to participate in the Poster Prize competition?:

No

ALBA A - 08/09/22 II / 9

The potential of synchrotron-based cryo-X-ray phase contrast imaging of myocardial biopsies

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Co-authors: Anne Bonnin [2]; Vishwanie Burdham-Mahadeo [1]; Thomas A Treibel [3]; Andrew C Cook [1]

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Cardiomyopathies are serious heart muscle (myocardial) abnormalities which can lead to life-threatening complications such as heart failure, cardiac arrest, and sudden death. Myocardial biopsies obtained from surgical septal myectomies are essential for confirming diagnosis of cardiomyopathies. Owing to the recent advancements of synchrotron radiation-based X-ray phase contrast imaging (XPCI), detailed histological information of myocardial microstructure can be achieved ex vivo and non-destructively. However, synchrotron-based cryogenic (cryo-) XPCI of biological samples, which has not yet been perfected, is a technique of interest due to its ability to preserve biological samples. This is because this technique requires minimal tissue processing and therefore maintains DNA and RNA integrity which are paramount for downstream genomics and proteomics applications. In order to establish optimal conditions for imaging, cryopreserved myocardial biopsies from mouse models [Brn3b (Pou4f2) knockout and wild-type mice] were used to mimic the clinical myectomy biopsies for imaging with cryo-XPCI at the Swiss Light Source TOMCAT X02DA beamline. To test the effects of the beam on the samples post-scanning, DNA and RNA were extracted from the samples for integrity assessment. This data was then used to design a novel protocol for clinicians performing surgical septal myectomies from cardiomyopathy patients to minimise sample degradation and maximise the potential use of these precious biopsies for synchrotron-based cryo-XPCI for future genomics and transcriptomics analyses. Overall, this pilot study demonstrated the potential of synchrotron-based cryo-XPCI of myocardial biopsies from pre-clinical animal models and invaluable human myectomies.

Would you like to participate in the Poster Prize competition?:

Yes

ALBA B - 08/09/22 II / 86

NOTOS at ALBA: Versatile XAS and XRD for operando experiments

Authors: Carlos Escudero[1]; Giovanni Agostini[2]; Dominique Heinis[2]; Jordi Prat Albert[2]; Josep Nicolàs Roman[2]; José Ramón García Molinero[2]; Nil Serra Peinado[2]; Oriol Vallcorba Valls[2]; Roberto Javier Homs Puron[2]; Álvaro Baucells Costa[2]

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NOTOS at the ALBA synchrotron light source is a beamline devoted to XAS, XRD, and metrology applications in the energy range 4.5 –30 keV. In addition to the capability to perform XAS and XRD investigations, the beamline will allow combination of XAS and XRD experiments in the same beamtime. NOTOS has been designed to study the electronic structure, short and long range order by XAS and XRD for wide range of scientific disciplines: chemistry, catalysis, energy science, nanomaterials and condensed matter, environmental science. In addition to typical applications mentioned above, it will be focused on in situ and *operando* measurements on heterogeneous catalysis and electrochemistry.
The X-ray source is a bending magnet and the optics consist of a cylindrical mirror, Double Crystal Monochromator and double channel toroidal mirror, which delivers the beam to the experimental stations. The photon flux at the experimental stations is in the order of 10^{11}(ph/s/0.1%BW) in the whole energy range with high order harmonic rejection better then 10^4.
Two different stations will be available in the EH. The first one consists of a 2.0 x 0.8 m table open to perform metrology measurements and suitable to XAS investigation in transmission and fluorescence mode and it is open to future developments in function of needed identified with users community. The second station is equipped with a two circle diffractometer where 10-channel Ge(111) analyser detector and Mythen detector have been mounted. Three ion chambers and 13-elements SDD detector will allow the combination of XAS measurements in transmission and fluorescence configuration. For both the stations a setup to handle reactive gas fully integrated in the beamline control system will be available.
The beamline started the operation with the users at the end of April and some example of experiment performed in the first user operation will be reported.
This project is co-funded by the European Regional Development Fund (ERDF) within the pluriregional operational program of Spain (POPE), 2014-2020.

Would you like to participate in the Poster Prize competition?:

No

ALBA A - 08/09/22 II / 102

Chemical modulation of microtubule structure in neurodegenerative diseases

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Microtubules (MTs) are dynamic filaments involved in many essential cellular functions including those needed for cancer cell growth. Taxanes are MT stabilizing agents and the most successful antitumoral drugs targeting MTs. However, despite their mode of action is the stabilization (i.e., do not destroy the filament structure), they produce a paradoxical neurotoxic effect by inducing axon degeneration. This has been related to MT structural modifications upon drug binding. Alternatively,

the laulimalide/peloruside binding site also promotes stabilization, but have not been exploited in clinics. We have found that differently to the taxane site, the stabilization mechanism involves exclusively lateral interactions and entails changes on the inter-PF angle. Importantly, some compounds do not modify MT upon binding when compare to native ones. This feature, together with the low cytotoxic effect found, open the possibility of exploiting these compounds in neurodegenerative diseases, where MT structure and function are compromised due to other primary cellular alterations.

Would you like to participate in the Poster Prize competition?:

No

ALBA B - 08/09/22 II / 27

On the use of XALOC BL for the characterisation of materials prepared under supercritical CO2 conditions

Author: A. M. Lopez-Periago[1]

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During the last few years, the supercritical fluids and functional materials group (SFFM) at ICMAB, have been researching on the preparation of metalorganic materials using an unconventional technique based on supercritical CO2 technology (scCO2) as solvent.

In the field of coordination polymers and metal-organic-frameworks (MOFs), scCO2 is widely known for being used for the post-synthetic activation, or cleaning steps agent, however scCO2 can go further, as it can be used for the synthesis of these materials.

Thus, using this approach, we have widely proven that single molecules as well as 1D, 2D or 3D coordination polymers or MOFS can be prepared through the reaction of the right choice of building blocks.

On the other hand, scCO2 precipitation approach is generally governed by heterogeneous nucleation involving supersaturation of the reactants followed by nucleation and further crystal growth. However, in scCO2 nucleation generally dominates crystal growth, leading to the precipitation of very small crystals, which cannot be resolved by conventional diffractometers.

Under these lines, synchrotron radiation at ALBA though XALOC BL have been crucial for the determination of the structures of the materials precipitated in scCO2.

Herein, we report the scCO2 synthesis of single molecules, adducts and coordination polymers, based on the reaction between metals of the first transition row and nitrogen-based ligands. In all cases, the structure determination was carried out through single crystal diffraction using synchrotron radiation at ALBA.

Acknowledgements.

This work was supported by the Spanish Ministry of Science and Innovation MICINN through the Severo Ochoa Program for Centers of Excellence (SEV-2015-0496 and CEX2019-000917-S) and the Spanish National Plan of Research with projects CTQ2017-83632, PID2020-115631GB-I00. ALBA synchrotron is acknowledged for the provision of beam-time.

Would you like to participate in the Poster Prize competition?:

No

ALBA B - 08/09/22 III / 129

Operando experiments for catalysts

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Would you like to participate in the Poster Prize competition?:

ALBA A - 08/09/22 III / 98

The mysteries of magnetism and structure in the layered magnet chromium triiodide

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Chromium triiodide (CrI3) was the first layered van der Waals material to demonstrate the persistence of a sizable ferromagnetic hysteresis down to the monolayer [1]. This observation was accompanied by a striking transition from a layered ferromagnetic to a layered antiferromagnetic order as the number of layers of the crystal approached the two-dimensional limit [2]. The discovery of layered-dependent magnetism in CrI3 motivated a wealth of fundamental studies seeking the origin of this phenomenon. Although this effect can be underpinned by the differences of the spin superexchange coupling in the distinct layer stacking alignments found in bulk and few-layer cystals [3, 4], CrI3 still hosts deep conundrums. First and foremost, a clear explanation of why bulk CrI3 exhibits a layer-stacking structural transition to a rhombohedral low-temperature phase whereas few-layer samples do not is still missing. Secondly, the exact crossover point in terms of the number of layers appears to be, surprisingly, in the mesoscopic scale, but is currently unknown. In addition, there exists other controversies regarding the presence of a peak at 50 K in the in-plane magnetization curve [5] and the coexistence of different structural phases in bulk single crystals of this material [6]. In this talk, I will provide experimental insights regarding the magnetic states and crystalline phases of CrI3 beyond the reported monoclinic/rhombohedral stacking dichotomy, showcasing a far more intricate scenario than the one currently understood.

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Would you like to participate in the Poster Prize competition?:

No

ALBA A - 08/09/22 III / 96

3D Magnetic Vector Imaging: towards Experimental Micromagnetism

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The study of the three-dimensional behaviour of the magnetisation vector field at the nanoscale is of paramount importance for the magnetism community. The access to this information provides the fundamental information necessary to properly understand the physics and phenomena present in magnetic systems. In general, the actual methodology to study the magnetisation states at the nanoscale is based on the combination of 2D magnetic imaging and micromagnetic simulations/modelling. However, the recent development of 3D magnetic vector imaging techniques [1,2,3] allowing for a direct characterisation of the 3D magnetisation configuration with no prior assumptions [4,5,6], is opening the way towards a change of paradigm and the realisation of Experimental Micromagnetism. In this talk the idea behind the vector magnetic imaging methodology will be presented as well as its application to different X-ray based magnetic imaging techniques.

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Would you like to participate in the Poster Prize competition?:

No

ALBA B - 08/09/22 III / 85

Experiments of CO_2 adsorption in zeolites and structural stability of carbonate phases at high-pressure and temperature conditions using synchrotron X-ray diffraction

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High-pressure and high-temperature techniques are used to strongly modify the atomic interactions of matter while in situ synchrotron X-ray diffraction characterizes the samples. This has enabled reliable experimental studies in a wide range of P-T conditions, like those presented here. Firstly, I will present the results of two CO_2-loaded pure-silica zeolites where the content of adsorbed CO_2 molecules and the location of these guest molecules in the porous frameworks were accurately determined. Subsequently, I will show experimental results that, combined with DFT calculations, accurately constrain the P-T phase diagrams of several naturally-occurring carbonate minerals in the 0-20 GPa pressure and 300-1000 K temperature ranges. In particular, the compressibility, thermal expansivity, the anisotropy and the evolution of the atomic environments was determined. Novel dense carbonate phases were found and fully characterized. These results offer new insights into the high-pressure high-temperature chemistry of carbon dioxide and carbonates, with implications in geophysics (deep carbon cycle) and the potential design of efficient CO_2 capture strategies.

Would you like to participate in the Poster Prize competition?:

No

ALBA B - 08/09/22 III / 94

Future of high pressure at Alba

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Alba synchrotron is going towards an important upgrade, Alba II, impacting the future characterization capabilities offered to the user community. In this framework, the high-pressure program is one of the Alba scientific programs that has to compete with other scientific areas serving wide user community. Thus, it is critical that HP techniques fit in the big picture of Alba II and the participation of the user community and its input will definitely be an important asset for developing the HP program.
In this presentation, I will show the current status of the HP research in Alba, the facilities involved in this framework and what we need to address in order to develop the program. In particular, I will address the limitations that hamper the HP users coming to Alba and how we can enhance the characterization capabilities correlated with the future upgrade of Alba.

Would you like to participate in the Poster Prize competition?:

No

ALBA A - 08/09/22 III / 90

Magnetic and electronic properties of 2D metal-organic networks

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Molecular magnetism is an emerging field with potential for technological applications as high-density information storage, quantum computing and spintronics.[1] 2D metal-organic networks are of especial interest since they allow the ordering of magnetic atoms in regular patterns. These systems are highly versatile with endless possible combinations of organic linkers and metallic atoms. We have investigated two kinds of systems: lanthanide metal-organic networks and π-conjugated networks.
By one side, molecular systems based on lanthanides are especially promising due to the fundamental properties of lanthanides. Their strong spin-orbit coupling can lead to a high magnetic anisotropy while the strong localization of 4f states reduces the hybridization with surfaces increasing spin lifetimes.[2] Our pioneering investigations of metal-organic networks coordinated Er and Dy show that it is possible to tailor the magnetic properties and electronic of lanthanides by a proper choice of molecular linkers and metallic centers.[3],[4] The orientation of the easy axis of magnetization and the intensity of the magnetic anisotropy are strongly dependent on the metallic center and the molecular linker.
On the other side, π-conjugated metal-organic networks coordinated with 3d metals can present

exotic quantum phases as superconductivity,[5] flat-band,[6] and quantum spin liquid.[7] The conjugation also enhances the coupling between magnetic moments and can lead to antiferromagnetic ground states. We have employed conjugated molecular linkers coordinated with Co to prepare metal-organic networks that present very narrow band-gaps. The experimental results are compatible with antiferromagnetism and one of the investigated systems also presents a large unquenched orbital magnetic moment, unprecedented in 2D transition metal-organic networks.

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Would you like to participate in the Poster Prize competition?:

No

ALBA A - 08/09/22 III / 74

XPEEM Imaging of Magneto-acoustic Waves at GHz Frequency

Author: Muhammad Waqas Khaliq[1]

Co-authors: Oliver Amin [2]; Alberto Hernández-Mínguez [3]; Blai Casals [4]; Marc Rovirola [5]; Khalid Omari [6]; Sandra Ruiz-Gomez [7]; Simone Finizio [8]; Kevin Edmonds [2]; Lucia Aballe [1]; Miguel Angel Niño Orti [1]; Joan Manel Hernàndez [5]; Ferran Macia [5]; Peter Wadley [2]; Michael Joachim Ulrich Foerster [1]

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Magnetization oscillations in thin films with spatial variations at the nano- and microscale are interesting in the development devices for high-speed and low-power signal processing compatible with existing technology. Surface acoustic waves (SAWs) are an alternative to magnetic fields in the excitation and control of magnetization dynamics, which use electric fields in order to induce magnetoelectric and magneto-elastic effects [1]. Casals et al. employed 500 MHz SAWs to create long range magnetization waves in Ni thin films [2]. More recently we have extended this method to include antiferromagnetic CuMnAs. For the observations we used PhotoEmission Electron Microscopy (PEEM) with magnetic contrast based on x-ray magnetic linear dichroism (XMLD), and the SAW excitation synchronized with the x-ray illumination.
Wadley et al. demonstrated the control of antiferromagnetic (AFM) domains in CuMnAs by electrical currents [3]. In principle, alternative switching methods such as the magnetoelastic effect should be equally possible but are so far relatively unexplored in AFM materials. We have for the first time detected antiferromagnetic magneto-acoustic waves in epitaxial CuMnAs films excited by SAW in the GaAs substrate. On the other hand, exciting magneto-acoustic waves at higher frequencies, approaching the intrinsic ferromagnetic resonance frequencies, can lead to higher amplitudes, larger propagating distance of magnons and increased phonon-magnon interaction. For ferromagnetic Ni thin films on LiNbO3 we have already increased the frequency into the GHz range.
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Would you like to participate in the Poster Prize competition?:

No

ALBA B - 08/09/22 III / **44**

Hierarchical organization in biodegradable polymer films by SAXS, USAXS and synchrotron FTIR imaging

Authors: Christopher Garvey[1]; Martin Kreuzer[2]; Jan Ilavsky[3]; Marianne Impéror-Clerc[4]; Stéphane Rouzière[4]; Bronwyn Laycock[5]

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Poly(lactic) acid (PLA) is a biodegradable biopolymer which suffers from poor mechanical properties and high cost. The addition of polyethylene (PE) introduces a toughening effect which dramatically improves these material properties. Here we report on initial characterization of films produced by blown film extrusion and the re-organization of films as static loads are applied. The measurements utilized are synchrotron based FTIR microspectroscopy and the polarization analysis capability of the MIRAS beamline at ALBA together with a combination of synchrotron (ALBA, NCD-SWEET and Advanced Photon Source, 9ID) and lab based X-ray scattering. The extended range of scattering vectors of our X-ray scattering measurments characterizes length scales typifying molecular scale packing of polymer chains but also the organization around the micron scale phase separation of PE and PLA. While X-ray scattering is able to provide insight into organization of craze formation in films, orientation of PE semi-crystalline lamellae and their phase separation it is ill suited to provide information on the poorly ordered PLA. As the films were stretched, visually dark bands appeared in the films. X-ray scattering provided evidence of a reinforcing effects of the phase separated PE. The poor performance of the pure PLA films is associated with the crystallization of PLA as evidenced from the appearance of broad SAXS peak typical of semicrystalline lamellae in the pure PLA films. This feature was poorly visible or absent in the blend films. These bands were associated with chemical and orientational heterogeneity. Polarized FTIR microspectroscopy measurements showed a dichroic behavior for the PLA/PE blend films in the fractured regions, indicating an alignment of PLA and PE with respect to the stretching direction in the presence of PE. The dichroic signal is much weaker for the PLA films. The results show that the presence of PE supports an alignment of the PLA chains without crystallization.

Would you like to participate in the Poster Prize competition?:

No

ALBA A - 08/09/22 III / **75**

Tuning charge and spin interactions at hybrid organic/metal and organic/topological insulator interfaces

Authors: Aitor Mugarza[1]; Alessandro Barla[2]; Cesar Moreno[3]; Marc G. Cuxart[4]; Miguel Ángel Valbuena[5]; Corneliu Nistor[6]; Inhar Imaz[7]; Jeremy Hieulle[7]; Luca Persichetti[6]; Pierluigi Gargiani[8]; Pietro Gambardella[6]; Roberto Robles[9]; Sergio O. Valenzuela[1]

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Interfacing materials with different functionalities is an efficient way to manipulate their respective properties and promote the emergence of novel phenomena. Controlling interfacial interactions is however a complicated task in most cases. In that respect, the tunability offered by ligand chemistry in organic materials is an interesting asset that can be exploited at hybrid interfaces [1,2]. Here we present two examples where the molecular strategy is employed to tune the interactions of localized transition metal ions with underlying spin-degenerated electrons in non-magnetic metals, and with spin-textured electrons in topological insulators. In both cases, we obtain a comprehensive picture of the phenomenology by combining scanning tunnelling microscopy/spectroscopy, X-ray absorption and magnetic circular dichroism, angle-resolved photoelectron spectroscopy, and ab-initio calculations.

For molecular films on topological insulators, the tunability of ligands is exploited to tune the interaction of Co ions with the underlying topological surface state (TSS), going from the strongly interacting regime where the TSS is quenched in the first quintuple layer [3], to the weakly interacting regime where both the TSS and the Co magnetic moment are preserved [4]. The ultimate test of the tunability of interfacial interactions by ligand chemistry is carried out in a study of the Kondo interaction on a spin-degenerated metallic substrate [5]. Here, by varying the ligand configuration, we are able to depart from the mixed-valence configuration to the Kondo regime and smoothly modulate the exchange interaction between the spin of the ion and that of the metallic electron gas. Altogether, the different organic/inorganic interfaces cover the whole interaction window, from the strong (mixed-valence), to the intermediate (Kondo), and finally weak (decoupled) regimes.

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Would you like to participate in the Poster Prize competition?:

No

List of posters presented during the conference / 93

Synchrotron X-ray Diffraction studies of Metal Organic Frameworks (MOFs) at high-pressure

Authors: Alba San José Méndez[1]; Gregor Kieslich[2]

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Metal-Organic Frameworks (MOFs) are functional materials where the interconnection of inorganic coordination and organic linker chemistries provides a virtually unlimited chemical parameter space to investigate material responsiveness through chemical-structural changes. Their open network structure gives MOFs an extraordinary structural flexibility that often results in a large structural response to pressure (P) as an external stimulus, revealing a variety of material properties of large academic and technological relevance such as negative linear and area compressibility, mechanical energy storage and barocalorics amongst others. Identification of crystal chemistry principles to explain the interrelation between composition, structure and P-responsiveness of a MOF is key for synthesizing MOFs with potentially new and useful P-responses. In parallel, the discovery of electrically conductive MOFs raises fascinating questions of how the conductive pathways are affected by P-induced structural changes –an untouched research area with promising opportunities in applied and academic research.

Following structural changes as a function of hydrostatic P demands the use of high-P powder X-ray diffraction (HPPXRD) cells, which are ideally operated at synchrotron light sources. Such experiments deliver information about the mechanical properties and thermodynamic stabilities of MOFs thereby providing the data basis for the application and optimization of MOFs as barocalorics, or as piezochromatic sensors, to name a few. However, existing HPPXRD cells come with limitations such as difficult and time-consuming sample loading procedures, a poor P-control in the low-pressure range relevant for soft material research, i.e., P < 1 GPa, or a restricted maximum achievable P often insufficient to fully reflect the chemical diversity of MOFs. Additionally, simultaneous electrical conductivity measurements at high-P still involve a remarkable experimental challenge. To fully harness the potential of this research area, the development of new experimental techniques tightly coupled to chemical synthesis is key. In this contribution, we will discuss the required features of a prototype HPPXRD setup for further advancing in high-P research of MOFs and soft materials, clarify and improve existing structure-property relations that determine the mechanical properties of MOFs at high-P and provide proof-of-principle studies related to the high-P dependency of charge transport properties in electrically conductive MOFs.

Would you like to participate in the Poster Prize competition?:

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STRUCTURAL EFFECTS OF THERMAL PROCESSING ON RED SEAWEEDS FOR THE PRODUCTION OF BIO-BASED FOOD PACKAGING MATERIALS

Authors: Amparo López Rubio[1]; Antonio Martínez Abad[2]; Vera Cebrian Lloret[3]; Marta Martínez Sanz[4]; Juan Carlos Martínez Guil[5]

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This study evaluates the use of whole seaweed biomass to obtain bio-based films for food packaging applications in a more sustainable and energy efficient way. To this end, four different species of agarophytes (Gelidium sesquipedale, Gracilaria chilensis, Gracilaria tenuistipitata and Gracilaria verrucosa) were minimally processed by melt blending combined with compression moulding, investigating the effect of the composition and cell wall structure of the different species on the final performance of the films. The seaweed biomass was mainly composed of carbohydrates (35-50%), but

significant amounts of proteins, ashes and lipids were also detected. Temperature-resolved SAXS experiments evidenced the distinct behaviour of the different seaweeds upon thermal processing, with those species with higher cellulose content (G. sesquipedale and G. verrucosa) presenting a greater interfibrillar packing density and thermal resistance. The higher cellulose content of G. sesquipedale resulted in stronger films with high water vapour barrier capacity, while the higher agar content of G. chilensis improved its elongation capacity. The results from this work evidence the potential of red seaweed biomass to generate food packaging materials in a cost-effective and environmentally friendly way and show the great utility of SAXS to investigate the effect of cell wall nanostructure on the processability and properties of the obtained materials.

Would you like to participate in the Poster Prize competition?:

Yes

List of posters presented during the conference / 43

Revealing mechanism of the ultrafast growth of superconducting epitaxial thin films by in-situ X-ray synchrotron diffraction: from design/installation to measurements

Authors: Elzbieta Pach[1]; Jordi Aguilar Larruy[1]; Daniel Sanchez[2]; Diana Garcia[1]; Lavinia Saltarelli[1]; Albert Queraltó[3]; Víctor Fuentes[1]; Eduardo Solano[4]; Marc Malfois[4]; Xavier Obrados[1]; Teresa Puig[1]

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Investigation on the preparation of efficient and flexible high temperature superconducting materials (HTS) is one of the puzzles to be solved for the Energy Transition goal. One of the important parts of this development is focused on the cost-effective, scalable methods of synthesis of such materials.

Nowadays, HTS based on REBa2Cu3O7 (RE=Y or Rare Earth, REBCO) are manufactured as long, flexible conductors deposited on metallic substrates using thin film technologies, the so-called coated conductors (CC), which are rather expensive. Our approach is to use an innovative method, called Transient Liquid Assisted Growth (TLAG) [1], a non-equilibrium process based on epitaxial crystallization from a transient melt at very high growth rates (100 nm/s, 100 times larger than conventional methods). This process is compatible with low cost, scalable chemical solution deposition methods and allows to grow high temperature epitaxial superconducting films.

However, in order to achieve a deep understanding of such a fast growth process of REBCO films, determine the phases´ evolution and the kinetic phase diagrams that would permit to better control their properties, a new methodology had to be developed. This goal is being achieved through fast acquisition of in-situ X-Ray diffraction data during the TLAG process at the NCD-SWEET synchrotron beamline of ALBA light source in Spain. For that purpose, a unique portable system was developed using a fast heating XRD furnace with controlled atmosphere capable to tune temperature up to 1000 ºC and total pressures from 10-5 bar to 1 bar with controlled oxygen partial pressure and flow rate synchronized with simultaneous acquisition of 2D XRD images at 105 ms/image and 18 keV. Additionally, the system allows for simultaneous analysis of the volatiles with mass spectrometry and in-situ electrical conductivity that permits to follow the phase transformation from the insulating precursor phases to the metallic superconductor phase at the growth conditions.

The ultrafast process of TLAG required very fast time responses of all the systems and accurate time synchronizations. Results on the epitaxial nucleation and growth mechanism of the REBCO

phase on STO single crystals and metallic substrates, and TLAG phase evolutions process will be discussed.

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Would you like to participate in the Poster Prize competition?:

Yes

List of posters presented during the conference / 17

A tensile stage for synchrotron-based infrared microspectroscopy at ALBA

Author: Martin Kreuzer[1]

Co-authors: Carlos Manuel Falcon Torres [1]; Domingo Alloza Castillo [1]; Llibert Ribó Mor [1]; Gabriel Vicent Jover Mañas [1]; Ibraheem Yousef [1]

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For the study of thin films and fibres under load, a uniaxial tensile stage has been developed. The stage has been designed with several key features for tensile load experiments at synchrotron-based polarised infrared microspectroscopy endstations. One of the advantages compared to commercial available stages is its compact design (<20 mm thickness) and the large field of view on the sample for transmission experiments (75 mm x 20 mm). The unique design allows placing the stage at the focal position of an infrared microscope with typically small working distances of only around 10.5 mm, using one of the highest magnification objectives (36x, NA= 0.52) allowed by the IR microscope optical design. In addition, the stage was designed in a way that it is possible to rotate between -15° and +193° in the sample plane, in order to rotate the sample relative to the fixed polarisation direction of the incoming infrared light from the synchrotron source. This feature allows performing synchrotron-based polarised FTIR microspectroscopy for the analysis of vibrational band orientation in stretched samples. Furthermore, the stage can be sealed for atmospheric control of the sample.
Preliminary in situ tensile load experiments conducted at MIRAS beamline of the ALBA synchrotron were done using 3D printed polymer thin films and fibres as test samples. The samples could be mapped in transmission geometry under tensile load achieving the highest spatial resolution between 3 to 10 microns. Making use of the polarised synchrotron-based infrared light, it was also possible to show the alignment of different vibrational bands parallel and perpendicular to the stretching direction. The experiments highlight the unique instrumentation capabilities of the tensile stage for in situ measurement of chemical distributions and molecular orientations as a function of sample displacement and applied load. The stage is now part of the user program at MIRAS, the infrared microspectroscopy beamline of ALBA.

Would you like to participate in the Poster Prize competition?:

No

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On the origin of large magnetic anisotropy in ε-Fe2O3

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The epsilon phase of Fe_2O_3 is a ferrimagnetic polymorph that stands out for a remarkable magnetic anisotropy (K_u~2·10^5 J/m3) and sizeable remnant magnetization at room temperature (~50 kA/m)[1] making it appealing for applications in magnetic recording and electromagnetic applications in the range of millimetre waves [2]. Moreover, ε-Fe_2O_3 is also interesting from a more fundamental point of view, featuring low-temperature magnetoelectric properties [3] and three distinct zero-field magnetic orders between 10 K and its paramagnetic state above ~850 K [4]. Such a rich phase diagram has much to do with its non-centrosymmetric structure (*Pna21*), more complex than for other ferric oxides, with four different Fe sites in the asymmetric unit cell: three in an octahedral (O_h) and one in a tetrahedral (T_d) local symmetry [1].

Despite having attracted increasing attention over the last decades, the intriguing magnetic order in ε-Fe_2O_3 is still poorly understood. Here we present recent results of temperature-dependent X-ray and neutron diffraction, X-ray absorption spectroscopy (XAS) and X-ray magnetic circular dichroism (XMCD) experiments that provide new insights into the origin of magnetic anisotropy in ε-Fe_2O_3 and ⊠-$(Fe_{1-x}Cr_x)_2O_3$ in the form of nanoparticles (NPs) and thin films. The Fe^{3+} with Cr^{3+} substitution is very revealing due to its expected isovalent and magnetic isotropic character. Although trivalent iron could be thought as behaving in a similar way, a nonzero orbital angular momentum m_L value has been proposed for the Fe2 crystallographic site, which might act as the primary source for the magnetic anisotropy responsible of the gigantic coercive field. Thus, depending on the preferential entering sites for Cr in the ε-Fe_2O_3 structure, a systematic reduction in m_L and a weakening of the spin-orbit coupling along the series may be expected. Our XMCD investigation has addressed this controversy.

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The CIRCE-PEEM: past, present and future

Authors: Ana Martínez Carboneres[1]; Antonio Camps Giménez[1]; Michael Joachim Ulrich Foerster[1]; Fernán Saiz Poyatos[1]; José María Álvarez Fernández[1]; Miguel Angel Niño Orti[1]; Muhammad Waqas Khalioq[1]

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We present an overview of the status and capabilities of the PhotoEmission Electron Microscope (PEEM) at the CIRCE beamline of the ALBA synchrotron. The PEEM instrument, which can be also used with an electron gun (Low Energy Electron Microscopy (LEEM) and micro-LEED), is a versatile, multipurpose surface and thin film characterization platform. The Synchrotron irradiation (Photon energy and polarization) gives access to a variety of chemical, electronic and magnetic contrast mechanism coupled to the high spatial resolution (down to 20 nm lateral, 1-10 nm in depth) of the microscope. Spectroscopy techniques (e.g. XAS, XPS) can be applied to selected nanoscale regions.
The CIRCE-PEEM offers many different sample environment options, for example application of small magnetic fields or electric signals through the sample. We review examples from user operation and highlight more recent developments. Finally we present possibilities of future upgrades in the context of ALBA-II.

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Current status and upgrades of the MX beamline XALOC

Author: Fernando Gil Ortiz[1]

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XALOC is a tunable MX beamline, in user operation since 2012, located at the 3rd generation synchrotron ALBA (Barcelona). It has been designed to deal with automatable X-ray diffraction experiments of micrometer-sized crystals, including a variety of crystal sizes, unit-cell dimensions and crystals with high mosaic spread and/or poor diffraction. The aim for a reliable all-in-one beamline is equaled by the aim to maximize ease-of-use and automatization. Mail-in data collection is in routine operation. A double gripper mounted at the CATS sample changer allows sample interchange in less than 20 seconds. Unipucks and EMBL/ESRF pucks are acceptable with a capacity of up to 6 Unipucks and 3 ESRF pucks. In addition, MXCube allows new features like loop autocentering, helical data collection and mesh scan showing the results in a heat map. ISPyB is fully operative for sample tracking/experiment reporting used through a web browser (https://ispyb.cells.es/). Automatic data processing with autoPROC, EDNA and XIA2/DIALS is carried out through the ALBA HPC. Furthermore, automatic data processing for small molecule users has recently been implemented. Other software like Dimple, PanDDA or Archimboldo is also available. The beamline allows "in-situ"diffraction and serial crystallography experiments have been carried out successfully. Drug discovery is already feasible although with some limitations. Several options of user access are available including a continuous call, open to new proposals throughout the year, providing beamtime within a few weeks. Spanish and Portuguese users are fully funded while dewar transport expenses are covered for the rest of the EU users Current possibilities and important upgrades that will become available during 2022-2023 will be presented.

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Water-cooled Double Multilayer Monochromator for the BioSAXS beamline at the Australian Synchrotron

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The Multilayer Monochromator for the BioSAXS beamline at the Australian Synchrotron is intended to provide high monochromatic flux into the experimental station. A vertical bounce arrangement using a single Ru/B4C multilayer stripe will deliver a flux of up to 5 x 10^14 photons/s with a 1% bandwidth off an undulator insertion device. A side clamped water-cooled solution is used to dissipate the heat load, this arrangement was chosen to improve the instrument stability as the required cooling performance is achieved without the use of liquid nitrogen.

We present the design, manufacturing, and testing factory efforts to deliver a high-performance Multilayer Monochromator for the BioSAXS beamline. The cooling analysis, motion, and stability testing, as well as the multilayer design and simulation performed in conjunction with the optic supplier, and multilayer metrology performed on BL11 beamline at ALBA Synchrotron show the instrument and the BioSAXS beamline is ready to take beam enhancing the SAXS capabilities at the Australian Synchrotron.

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Hard X-ray micro-tomography at the Spanish Synchrotron Alba

Author: Alberto Mittone[1]

Co-authors: Klaus Attenkofer [1]; Carles Colldelram Peroliu [1]; Josep Nicolàs Roman [1]; Alessandra Patera [1]; Llibert Ribó [1]

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ALBA is a third generation 3-GeV synchrotron radiation facility built near Barcelona. Since 2012, it serves worldwide academic and industrial users. At the present day its portfolio includes nine operating beamlines, with an additional five, one that will soon enter into operation, and four that are in the design/construction phases, that will expand its capabilities. Among these new beamlines, one is a micro-tomography beamline, the BL31-FAXTOR, which is currently under construction. The beamline will serve different communities, including material science, biomedical, paleontology, earth science, cultural heritage etc.
FaXToR - Fast X-ray Tomography & Radiography beamline, will provide users with beams with an energy range between ~10 keV and ~70 keV. The maximum achievable beam size expected is 35×12 mm2 (HxV) at the entrance of the sample, which is located at 35 m from the source. The beamline will be fed by a short in-vacuum multipole wiggler with an expected flux of ~6x1013ph/s/0.1%BW at 30 keV (250 mA storage ring current). Users will have the possibility of working in the end-station with both a filtered white beam and a beam obtained from a Double Multilayer Monochromator. At the start of operations, the spatial resolution (in terms of image pixel size) will range between ~0.5 μm and ~10 μm, thanks to the presence of different detection systems. The design of the endstation allows the possibility of acquiring imaging simultaneously at two different spatial resolutions if required. The possibility of performing dynamical studies with a temporal resolution < 1 s (per tomography) is foreseen. Both phase-contrast imaging (laplacian and differential) and absorption-based imaging techniques in radiography and tomography modes will be accessible during the experiments. The beamline is expected to present a high data throughput and will use state-of-the-art CMOS fast detectors, therefore particular care is required in order to cope with the computing requirements.

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Discovering Morphology Mapping with 3D printing at the NCD-SWEET Beamline at ALBA

Author: Paula Pascoal Faria[1]

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Direct digital manufacturing is a family of technologies which enables products to be manufactured directly from a digital definition without the use of specialized tooling or molds. Fused deposition modelling and stereolithography are probably the most common and widely used of these transformation technologies. These have developed out of techniques to rapidly produce prototypes of products from design or marketing ideas. Since their development, the range of materials used has widened to include materials from which actual products can be produced and which exhibit the properties required. Although there have been many advances in 3D printing technology, most of the focus has been on producing in hi-fidelity shapes from a digital definition. Little attention has been placed on developing technology to focus on other aspects beyond the simple form of a product. This work seeks to readdress this area.

Here, we focus on the use of 3D printing to produce plastic parts. Essentially, a thin strand of molten polymer is extruded onto a moving build platform in a defined manner to build up a structure layer by layer. As with any polymer processing technology, the process conditions will influence the polymer morphology and structure upon cooling which, in turn, will impact the properties. As part of a major project to fully understand all aspects of 3D printing, we performed small-angle X-ray scattering experiments on parts prepared in this manner on the NCD-SWEET beamline at the ALBA Synchrotron Light Source in Barcelona, Spain. We designed and built a 3D printer which can be mounted on the ALBA NCD-SWEET beamline so we can follow the structural development in real time. We will show examples of how the printing parameters affect the structure and morphology, we will describe the experiments which have been performed, and we will discuss the type of information we have been able to extract. We will show how the results we obtain can be used to optimize 3D printing technology and the materials used, and how this approach can be used to produce patterns or variations in properties by printing different morphologies –morphology mapping. In short, we will show how we can print properties, and not just shape and this will greatly extend the capabilities of 3D printing.

This work is supported by the Fundação para a Ciência e Tecnologia (FCT) through the Project references: MIT-EXPL/TDI/0044/2021, UID/Multi/04044/2013; PAMI-ROTEIRO/0328/2013 (N° 022158), Add. Additive-POCI-01-0247-FEDER-024533 and UC4EP PTDC/CTM-POL/7133/2014). These experiments were performed at NCD-SWEET beamline at ALBA Synchrotron with the collaboration of ALBA staff.

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No

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Operando XAS Studies on Aqueous Zn-MnO2 Batteries

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Manganese-based (such as MnO2) cathodes have been attracting enormous attentions in aqueous Zn metal battery, thanks to its low-cost, suitable potential and considerable capacity. However, the electrochemical mechanism remains unclear, being ascribed to co-insertion/conversion with Zn2+, Mn2+, H+, or even precipitation of an intermediate products (Zn4SO4(OH)6·xH2O, ZHS), which is retrained by differing complicate structure of Mn in aqueous electrolyte and that might only be observable by real-time characterizations. Herein, operando XAS technique is used to probe the electronic and local structure of Mn and Zn during several consecutive cycles with the intention to shed some light on the underling the ambiguous mechanisms that govern the reactions. α-MnO2 are employed as the cathode in a 1M ZnSO4 + 0.2M MnSO4 electrolyte with a Zn metal anode. The XANES region of Mn K-edge shows a reversible shift of ca. 5 eV upon consecutive cycling, which is consistent with the formation of Mn (III) species upon reduction. Furthermore, the EXAFS indicates significant weakening of the nearest Mn-O shell at ca. 1.4 Å and strengthening of Mn-Mnegde in [Mn4+/3+O6] structures at ca. 2.6 Å during extended cycling. Meanwhile, Zn-K edge shows little change in all charging and discharging states. Hence, a mutual conversion reaction might be referred to between Mn (III) and Mn-ion (II) at the potential windows of 1.2-1.6 V.

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Determination of chemical profiles of normal and tumoral cell lines treated with DOX-loaded ACP nanoparticles by Synchrotron-based Fourier Transform Infrared Microspectroscopy

Authors: MARÍA DEL CARMEN ELIZABETH DE LAMA ODRÍA[1]; Juana del Valle-Mendoza[2]; Imma Martínez-Rovira5[3]; Ibraheem Yousef [3]; Jordi Puiggalì[4]; Luis Javier del Valle[4]

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El abstract se encuentra en el documento adjunto
Find the abstract document in the attachment

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Tuning the orientation of the magnetic spiral by doping in YBaCuFeO5 multiferroic

Author: Arnau Romaguera[1]

Co-authors: Xiaodong Zhang [2]; Ruyong Li [1]; Javier Herrero-Martín [3]; Francois Fauth [3]; Oscar Fabelo [4]; Jose Luis García-Muñoz [1]

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The layered perovskite YBaCuFeO5 is considered one of the best candidates to high-temperature spin-driven multiferroics. In RBaCuFeO5 perovskites (R: rare-earth or Y) A-site cations are fully ordered and their magnetic properties strongly depend on the preparation process [1,2]. They exhibit partial cationic disorder at the B-site that generates a magnetic spiral stabilized through directionally assisted long-range coupling between canted locally frustrated spins [3]. Moreover the orientation of the magnetic spiral can be critical for its magnetoelectric response. We have synthesized and studied YBaCuFe1-xMxO5 doped samples, with the aim of increasing spin-orbit coupling effects, and found that the overall Fe/Cu cation disorder at the B-sites can be increased by doping without changing the sample preparation process [4,5]. In YBaCuFe1-xMnxO5 samples prepared under the same conditions, the T-x magnetic phase diagram have been constructed in the range 10K-500K combining magnetometry, XAS, synchrotron X-ray and neutron diffraction techniques. The tilting angles of the spins in the collinear, θcol , and spiral phases, θspiral, barely vary with temperature. In the collinear phase θcol is also independent of doping. In contrast, the presence of Mn produces a progressive reorientation of the spin rotation plane of the magnetic helix in the incommensurate non-collinear phase, capable to transform the helicoidal spin components into cycloidal ones, which may critically impact the ferroelectric and magnetoelectric response of the material. These findings are of interest for engineering and developing this family of potential high-temperature multiferroics.

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Effects of A-site order on the Mn local structure and polar phases of magnetoelectric REBaMn2O6 (RE: La, Nd, Sm and Y)

Authors: Gloria Subias-Peruga[1]; Javier Blasco[2]; Vera Cuartero[3]; Sara Lafuerza Bielsa[4]; Laura Simonelli[5]; Giulio Gorni[None]; Joaquín García[1]; Miguel Castro[3]

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The relationship between Mn local structure and the polar and magnetic phases of A-site ordered REBaMn2O6 [1-3] and disordered RE0.5Ba0.5MnO3 (RE: La, Nd, Sm and Y) manganites has been investigated combining high energy resolution fluorescence and total fluorescence detected X-ray absorption at the Mn K-edge, to overcome the interference of the RE L-edges [4]. The extended k-range EXAFS spectra were measured at the CLAESS beam line of the ALBA synchrotron using the CLEAR spectrometer. An abrupt loss of local distortions of the MnO6 only occurs when the A-site ordered samples develops long-range ferromagnetic non-polar phases (RE=La). With decreasing the A-site ionic size (RE=Nd, Sm), a competition between ferromagnetism and charge localization appears, resulting in the development of a local distortion of the MnO6 octahedron in the low temperature polar phases. For the smallest A-site atom, YBaMn2O6, the local distortion of the MnO6 octahedron already exists at temperatures above the polar charge-ordered phase and vary little with temperature below the transition. This polar local distortion in REBaMn2O6 (RE: Sm, Y) is a bit less than half of the expected for a 1:1 Mn3+-Mn4+ order, i.e. ~0.3-0.5 e-. On the other hand, the A-site disorder weakens the ferromagnetism, favouring the presence of local distortions of the MnO6 octahedron. For the smaller A-site atoms (Sm, Y), a large local distortion of the MnO6 octahedron that is temperature-independent prevents the development of any magnetic order in the A-site disordered RE0.5Ba0.5MnO3 perovskites.
In conclusion, both a large difference in the ionic size of A-site cations and A-site disorder are proven to be detrimental for the development of long-range ferromagnetism in REBaMn2O6 (RE: La, Nd, Sm and Y) by favouring the electronic localization. Moreover, entropy contents in connection with the EXAFS results indicate that the mechanism of the polar structural transitions in ordered REBaMn2O6 (RE: Sm, Y) can be mainly associated with an order–disorder phase transition.

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Acknowledgements. We thank the Spanish Ministerio de Ciencia, Innovación y Universidades (Projects No. RTI2018-098537-B-C22 cofunded by ERDF from EU) and Diputación General de Aragón (Project E12-20R) for financial support.

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Tuning the hexagonal warping of topological surface states in Rare-Earth surface doped magnetic topological insulators

Authors: A. Barla[1]; Adriana I. Figueroa[2]; Beatriz Muñiz Cano[3]; Aitor Mugarza[4]; Ji Dai[5]; Julio Camarero[6]; Kevin García[2]; Manuel Valdividares[5]; Marc G. Cuxart[2]; Massimo Tallarida[5]; Miguel Ángel Valbuena[3]; Pierluigi Gargiani[5]; Rodolfo Miranda[6]; Sergio O. Valenzuela[4]

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Topological insulators (TIs) are materials of particular interest because of their exceptional features stemming from their conducting, topologically protected surface states. The combination of topological properties and magnetic order can lead to new quantum states of matter as the quantum anomalous Hall effect (QAHE) [1]. Recent discoveries as the first antiferromagnetic topological insulator MnBi2Te4 [2] have opened a new perspective for realising these quantized topological effects in intrinsically magnetic stoichiometric compounds. However, such system has a complex seven-layer structure that heavily depends on sophisticated and complex growth methods, resulting in variations in the density of structural defects that can lead to drastic changes, as the opening or not of an intrinsic magnetic gap at the Dirac point [3]. As an alternative strategy, ***we explore the effects of Rare Earth (RE) elements as surface dopants on TI substrates***, investigating their magnetic properties and their influence on the topological surface state (TSS). In principle, RE large magnetic moments could be relevant in order to maximize an eventually magnetically induced gap which would host the spin-polarized currents. Additionally, RE magnetic moments large size can also inhibit substitutional sites, reducing the multiplicity of adsorption configurations. Particularly, we report a study on, in the first place, the magnetic anisotropy of RE (Er and Dy) single atoms on Bi2Te3, which has been investigated by X-Ray Magnetic Circular Dichroism (XMCD). Then, by means of Angle Resolved Photoemission Spectroscopy (ARPES) measurements the effects of the RE surface dopants on the TSS have been explored. More precisely, the deposition of Er and Dy on Bi2Te3 and Bi2Se2Te substrates has been analyzed, reflecting how it is directly affecting the TSS of these TIs. Especially relevant are the changes induced in the Fermi surface (FS) of the different systems investigated, noticeably affecting the hexagonal warping (see attached Figure), which is an indirect indication that RE magnetic impurities can significantly act on the spin texture of the TSS, reducing out-of-plane spin component and possible scattering channels derived from the hexagonal warping [4]. This study has been carried out entirely at the ALBA synchrotron, at BOREAS (XMCD measurements) and LOREA (ARPES) beamlines.

Figure: FS evolution of Bi2Te3 single crystal (left) with 10% of Er coverage (right).

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Iron-Manganese crystalline phases in ancient Lead Glazes

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Iron and Manganese oxides are commonly used to colour and decorated lead glazes since medieval times. Original raw pigments react, dissolve, and recrystallize into new crystalline compounds during firing. Their nature, size and distribution depend on the composition of the pigment, glaze and ceramic ground, method of application and thermal paths. Their presence gives direct information on the technology of production and may be related to the final colour and appearance. Therefore, the analysis of crystalline phases in ancient glasses has been demonstrated very useful for determining ancient techniques.

Hematite and melanotekite crystals were found inside iron lead glazes and kentrolite, bixbyite and braunite inside manganese lead glazes. Fe plus Mn combined compounds in glazes had not been studied in detail before. High-Temperature Synchrotron Radiation X-Ray Powder Diffraction experiment was performed to determine the iron and iron-manganese compounds formed during the heating and during cooling of a near eutectic high-lead glass composition. Calcite, dolomite and kaolinite were also added to study their role in the iron-manganese compounds formed. To expand the firing temperature range above the range accessible in the HT-PXRD experiment (928℃) the same mixtures were also fired in the laboratory following the same thermal protocol at temperatures (690℃-1020℃) and were analysed by Scanning Electron Microscopy (SEM).
The kinetic profile of the experiment is designed to provide the right sequence of iron-manganese phases formed during heating and cooling. Bixbyite ((FeMn)2O3), barysilite ((Pb,Mn,Fe)Si2O7), kentrolite-melanotekite (Pb2(FeMn)2Si2O9), hematites (Fe2O3) and braunite (Mn7SiO12) are formed in Fe Mn lead Glazes. Kentrolite-melanotekite and braunite crystallise with different crystal habits during heating and cooling. If dolomite is present a pyroxene ((CaMg,Fe,Mn)2Si2O6) is formed. If calcite is present, ganomalite (Pb3(Ca,Mn)2Si3O11), margarosanite (Pb(Ca,Mn)2Si3O9) and wollastonite ((Ca,Mn)SiO3) are formed in Mn Lead glazes and andradite Ca3(Fe,Mn)2Si3O12 in Fe Mn lead glazes. Wollastonite can incorporate enough manganese to transform into bustamite ((Mn,Ca)3Si3O9) at high temperatures. This leaves less manganese available for the crystallisation of kentrolite and braunite.

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No

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Vortex chirality observation in trilayer disks of Fe/Al/Co using X ray resonant magnetic scattering

Author: Javier Ignacio Diaz Fernández[1]

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X ray Resonant Magnetic Scattering (XRMS) was used to understand the magnetic behavior of a 2-dimensional square array of trilayer ellipsoidal disks of submicrometer size (800 nm) deposited on Si. The disks were made of Fe (14 nm)/Al (3 nm)/Co (17 nm) by magnetron sputtering and lithographied by laser interferometry. The experiment was done in MARES end-station, in BL29 at the ALBA synchrotron. Thanks to the chemical and chiral symmetry sensitivity of XRMS [1], not only the magnetic hysteresis loops of the Cobalt and the Fe layers were distinguished, but also their chiral asymmetries. The hysteresis loops obtained at different Bragg angles far from the specular direction were investigated, demonstrating the sensitivity of the experimental technique to accurately determine the chirality of the vortex and their creation and annihilation fields in each of the two layers. The technique was applied in combination with magnetic reflectivity in the same end-station, which gave information about the quality of the magnetic interfaces, crucial to understand the magnetic interaction between layers.

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Site-specific X-ray magnetic circular dichroism in high quality Mn_3Ge ferrimagnetic epitaxial films

Author: Charles Guillemard[1]

Co-authors: Victor Palin [2]; Claudia De Melo [3]; François Bertran [4]; Pierluigi Gargiani [1]; Manuel Valvidares [1]; Stéphane Andrieu [3]

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Ferrimagnetic tetragonal Mn-based Heusler compound family Mn_3G (G=Ga, Ge) has attracted much attention in the last decade due to the strong magneto-crystalline anisotropy along the c-axis [1], small magnetic moment [1] and high spin polarization [2], thus standing as a good candidate for non-volatile and efficient high density magnetic random access memories. In this family of materials, two inequivalent Mn sublattices are coupled antiparallelly and give rise to a ferrimagnetic arrangement with a small overall magnetic moment. However, some theoretical and experimental studies pointed out some problems of reproducibility between samples, and a possible moment canting at one Mn site [3], owing to the magnetic frustration occurring in this compound. The full magnetic characterization of those compounds is very challenging but necessary to demonstrate their high potential for information storage applications.

Figure caption: X-ray magnetic circular dichroism at Mn L_3 edge as a function of the applied field and the corresponding vertical line profiles.

In this study, the epitaxial growth of Mn_3Ge thin films will be presented together with a structural and chemical ordering characterization, demonstrating the high quality of the films. Then, X-ray Absorption Spectroscopy and X-ray Magnetic Circular Dichroism (XMCD) measurements are conducted and allow us to unveil the magnetic ground state. In particular, the dichroic signals of both Mn sublattices can be distinguished at the Mn L_3 edge, as shown in figure \ref{fig}. XMCD measurements as a function of the applied magnetic field and the angular incidence of the X-rays both support a normal collinear ferrimagnetic ground state with one Mn sublattice having a very large magnetic anisotropy.

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Yes

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STRUCTURAL CHARACTERIZATION OF BIOLOGICAL SELENIUM NANOPARTICLES BY X-RAY ABSORPTION SPECTROSCOPY AND ELECTRON MICROSCOPY

Author: Miguel Angel Ruiz-Fresneda[1]

Co-authors: Maria Victoria Fernandez-Cantos [2]; Jaime Gomez-Bolivar [1]; Pier Lorenzo Solari [3]; Mohamed Larbi Merroun [1]

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A wide diversity of microorganisms has been recognized to enzymatically reduce toxic selenium forms (SeVI and SeIV) to non-toxic elemental selenium (Se0). The Se0 formed is usually produced in form of nanoparticles (NPs) with a wide array of shapes (spheres, nanorods, nanowires, etc.) structures (amorphous, monoclinic, trigonal, etc.), and sizes, which influence their environmental behaviour and industrial applications. The local chemical structure of these NPs of interest can be characterized by synchrotron-based analytical techniques such as X-Ray absorption spectroscopy (XAS) and electron microscopy. In the present study, selenium NPs synthesized by the cells of the bacterium Stenotrophomonas bentonitica after exposure with SeVI and SeIV were analysed with these techniques. The near-edge structure (XANES) region of the Se reduction products showed that the local coordination of Se is dominated by Se0 for both initial sources of Se. The extended fine structure (EXAFS) spectra indicated the presence of one Se-Se coordination shell at a bond distance of about 2.33–2.34 ± 0.02 Å and 2.35-2.37 ± 0.003-0.004 Å for SeIV and SeVI as initial source, respectively. According to the literature, the bond distance around 2.33-2.34 correspond to amorphous Se (a-Se), while the bond distances of 2.35-2.37 Å could correspond to a mixture of a-Se and trigonal Se (t-Se). Further characterization of the selenium NPs with electron microscopy coupled to electron diffraction (ED) and Fast Fourier Transform (FFT) showed a crystallization process of a-Se nanospheres to t-Se crystalline nanostructures. The results presented herein showed the potential of S. bentonitica for bioremediation purposes and a green and cheap methodology to produce selenium NPs of substantial interest for industrial and medical applications.

Would you like to participate in the Poster Prize competition?:

Yes

List of posters presented during the conference / 30

Structural characterization of a mitochondrial intermembrane domain

Author: Ramiro Illanes Vicioso[1]

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Our object of study is a human protein anchored at the mitochondrial inner membrane. This protein consists of three domains whose function is still unknown. The N-terminal domain (N) spans through the intermembrane space, whereas the C-terminal domain (C) faces the mitochondrial matrix, both regions being connected by a transmembrane helix embedded in the inner membrane. Several constructs of both the N and C domains were generated to obtain stable protein fragments suitable for expression and crystallization. However, only a few N-terminal constructs were soluble, but most of them aggregated during purification. Construct N4 showed the highest expression levels in Escherichia coli and could be reasonably purified. Nevertheless, once pure, N4 had a high tendency to precipitate, which led us to explore new approaches to improve its stability. We will present the re-design approaches of the constructs to improve solubility and solve aggregation and precipitation.

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Yes

List of posters presented during the conference / 34

Novel Biaxial Deformation Stage for Natural Rubber for SAXS/WAXS

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Co-authors: Barbara Lamolinara [1]; Paula Pascoal Faria [1]; Artur Mateus [1]; Geoffrey Mitchell [2]; Fabio Gamerio [1]

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Applications of natural rubber often involve biaxial deformation, yet most testing of rubber takes place using uniaxial deformation, despite the fact that, biaxial extension provides a more exacting test of theoretical models. In this work, we design and develop a novel equi-biaxial deformation stage which enables in-situ and time resolving small-angle X-Ray scattering and wide-angle X-ray scattering to be obtained during deformation. We use this system to study the strain induced crystallization of natural rubber in equi-biaxial mode, which takes place at uniaxial extensions typically greater than 4. The stage involves deforming a flat clamped circular disc of natural rubber about 1mm in thickness using compressed air into a hemispherical bubble, the pole of which exhibits equi-biaxial deformation. As this is a transmission device we are able to measure the absorption of the rubber sheet whilst it is being deformed to evaluate the thickness and hence the equi-biaxial extension ratio. We present preliminary results and describe the performance operation of the stage.

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Yes

List of posters presented during the conference / 70

BL06-XAIRA, the new microfocus beamline for MX at ALBA: status and scientific opportunities

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Co-authors: Nahikari González Martínez De Lapera [1]; Carles Colldelram Peroliu [1]; Igors Sics [1]; Jordi Marcos Ruzafa [1]; Josep Campmany Guillot [1]; Josep Nicolàs Roman [1]; Judith Juanhuix Gibert [1]

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BL06-XAIRA beamline at ALBA synchrotron light facility, foreseen to perform the first experiments by the end of 2023, will be dedicated to microfocus macromolecular crystallography, complying with a long-standing request from the scientific community and complementing the available MX capabilities of BL13-XALOC beamline.
The beamline is designed to support a broad range of biomedical structure determination methods and, more specifically, to cater for three main scientific cases: i) microfocus MX experiments, such as projects producing crystals with micrometric sizes, reduced diffracting power or requiring complex

data collection strategies; ii) fixed-target serial crystallography (SSX) experiments; and iii) anomalous phasing and elemental characterization.
XAIRA will provide a highly stable X-ray beam with a micrometric size (3 × 1 μm2 FWHM at 1 Å wavelength), adjustable to the users' needs, down to 1×1 μm2 and up to at least 10 × 10 μm2.
A novel dual monochromator design developed inhouse allows the photon wavelength to be selected within the 4.0 –14 keV energy range, using either a double multilayer monochromator, for high photon fluxes over 3·1013 ph/s, or a channel-cut monochromator, for extra beam stability at >3·1012 ph/s. The photon source, a 2.3m-long, 191.9 mm magnetic period in-vacuum undulator is the longest installed at ALBA.
Another distinctive element of the beamline is the chamber enclosing the whole end station, which allows experiments to be performed either in air or in helium atmosphere, both at room temperature or cryogenic conditions. The helium environment not only can drastically reduce the background noise, thus increasing data quality for the whole energy range, but also prevents flux loss at low energies, providing the optimal conditions for anomalous phasing experiments achievable in general-purpose beamlines.
A vertical single-axis diffractometer will allow for "traditional"oscillation data collection from samples on pins, meshes and small chips, while a dedicated sample rastering stage will also be available for non-oscillation data collection from large SSX chips.
XAIRA will be equipped with a pixel-array photon-counting detector capable of data acquisition at a maximum frame rate of 1 kHz. In combination with the high flux provided by the multilayer, this will enable time-resolved SSX experiments in the millisecond regime.
The state-of-the-art detector, in combination with an automated sample mounting system with a dewar capacity for over 450 samples and automated data analysis capabilities, grant XAIRA the necessary high throughput to allow rapid sample screening and data collection of crystals.
XAIRA is currently under construction; the optical system is currently being commissioned and the beamline will see first light in the forecoming months.

Would you like to participate in the Poster Prize competition?:

No

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Fast X-ray micro-tomography with a multi-scale approach at the ALBA synchrotron

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The BL31-FaXToR is the new beamline currently under construction at the third generation synchrotron facility ALBA, dedicated to hard x-ray micro-tomography. The beamline will provide the opportunity to perform 3D imaging within sub-seconds time resolution, working under mono- or white-beam conditions. Absorption and phase-contrast (mostly based on free propagation and grating interferometry) image contrast modalities [1] will be available to the user community.
This work focused on the innovative FaXToR experimental station. The hutch mostly includes: the beam conditioning table (holding a custom fast shutter), the tomography stage, and the detection optics table. Its novel design is foreseen in view of a beamline operative for multi-resolution dynamic X-ray imaging prone to a range of applications. The fast shutter, whose in-house design is currently ongoing, will be installed on the beam conditioning elements table. Its role will be to minimize the unwanted radiation exposure on the sample and other sensitive elements and to reduce the eventual artefacts linked to process dynamics by adequate synchronization with the detection camera. Samples will be located on the top of the rotary head of the tomography tower, capable to

reach up to 800 rpm at its maximum speed. The stage presents a flexible design and it is equipped with slip rings, allowing the use of complex sample environments. The peculiar optics table includes a dual detection system and a multipurpose platform. The two indirect detection optics, based on the combination of X-ray scintillation screens and visible optics lens systems will be provided of different magnifications, selectable according to experimental needs. Their distances with respect to the sample stage can be set remotely. FaXToR will make use of CMOS detection technology [2] to satisfy the requirements in terms of image quality, efficiency and speed. The multi-purpose platform will host a set of in-situ devices and will accommodate future upgrades of the beamline.
The beamline IT infrastructure will be dimensioned in order to be able to cope with a maximum data flow of 10 GB/s towards ALBA high-performance computing system. Existing software packages like [3], [4] will be used for the data reconstruction, analysis [5] and visualization [6].

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No

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Synchrotron X-ray diffraction study of novel orthovanadates, $Ca_{10.5-x}TM_x(VO_4)_7$, in broad temperature range

Author: houri rahimi mosafer[1]

Co-authors: Wojciech Paszkowicz [2]; Roman Minikayev [1]; Marek Berkowski [1]; Andrew Fitch [3]

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Calcium orthovanadates and orthophosphates substituted with various cations attract researchers' attention because of opportunity of their application in various fields, especially in optoelectronics, biomedicine and in chemistry in connection with their catalytic properties. Parent compounds $Ca_3(XO_4)_2$, X = V or P, are known to crystallize in R3c space group. The unsubstituted $Ca_3(XO_4)_2$ crystals can be modified by replacing a small fraction (typically up to ~10%) of Ca atoms by other ones, of valences from +1 to +4, without a change of structure, forming novel materials of modified properties; for the case of a divalent transition metal (TM) substituent, their formula is routinely written as $Ca_{10.5-x}TM_x(VO_4)_7$. The structure of such substituted crystals is similar to that of

whitilockite related material. Their complex structure including five independent sites (M1-M5) for Ca (and substituting) cations, with polyhedra arranged according to an unusual columnar architecture. Understanding of site occupation preference by transition metal atoms is one of main issue for consideration of such compounds.
Thermal expansion Studies regarding transition metal substituted to $-Ca_3(PO_4)_2$ (β-TCP) or $Ca_3(VO_4)_2$ (TCV) have not been reported, neither for orthovanadates nor orthophosphates except for $Ca_{10}Co_{0.5}(VO_4)_7$ and $Ca_{10}Cu_{0.5}(VO_4)_7$ [1]. The phenomenon of thermal expansion has been studied only for some whitlockite related materials incorporating monovalent and/or trivalent substituents, for instance $Ca_9Y(VO_4)_7$ [2], $Ca_{9.33}K_{2.33}(VO_4)_7$ [3], $Ca_9Gd(VO_4)_7$, and $Ca_{10}K(VO_4)_7$ [4]. Most of these results have been obtained by dilatometric methods.
In this presentation, the structure of whitlockite related TCV oxide is studied at non-ambient temperatures. The high resolution X-ray powder diffraction experiments were performed at ID22 at ESRF. In addition, the structural properties of novel calcium orthovandates, $Ca_3(VO_4)_2$, with Ca atoms partially substituted by transition metal (TM^{2+}), investigated at room and non-ambient temperature based on powder diffraction measurements.
Inspection of the non-ambient-temperature diffraction patterns indicated that the structure does not change with temperature, as confirmed by the Rietveld refinements, the sample maintained the trigonal structure (R3c space group) in the temperature range studied, 4 –1173 K,. This observation is in line with the high temperature Raman scattering studies for TCV (performed in temperature range 298 - 1483 K); the only ferroelectric-paraelectric phase transition is reported to occur at a considerably higher temperature, Tc = 1383 K [5]. In this work, the lattice parameters and unit cell volume of $Ca_{10.5-x}TM_x(VO_4)_7$ are determined as function of temperatures. Moreover, the Rietveld analysis allowed for investigation of temperature variation of both, the site preference of the substituting transition metal atoms and the interatomic distances.

We are grateful to the Polish Ministry of Education and Science for financing the access to ESRF, decision number: 2021 / WK / 11.

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Yes

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The role of casein in the carbonation of transferred Romanesque mural paintings

Authors: Núria Oriols[1]; Salvador Butí[2]; Nati Salvadó[2]; Trinitat Pradell[3]; Núria Jiménez García[3]; Judith Juanhuix Gibert[4]; Ibraheem Yousef[4]

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Fresco paintings are made of lime or dolomitic mortars [1,2]. The mortars dry reacting with the atmospheric CO2 and produce, depending on their nature, different calcium carbonate polymorphs. Casein was widely used in antiquity as a binder or glue in different painting techniques. Since the beginning of the 20th century it has also been applied to artwork restoration thanks to its adhering capability. In particular, casein mortars, lime/dolomitic mortars mixed with milk or cheese casein, have been extensively used, due to their compatibility and good adhesive properties, to stick mural paintings, previously removed from the original wall, onto a new background. During the mortar carbonation process, materials which were unintentionally introduced in the inner layers of the paintings, coming from milk or cheese (e.g. fatty acids), can react, producing new substances such as calcium soaps. These materials modify the original nature and structure of the painting and consequently, may affect its chemical stability.
Our main objective was to understand how the presence of casein modifies the carbonation process and if this affects the stability of the paint. The historical samples studied belong to one of the most important collections of European Romanesque mural paintings. The paintings were detached at the beginning of the 20th century from the churches of Santa Maria de Taüll, Sant Climent de Taüll and Sant Romà de les Bons in the Pyrenees, and preserved ever since at Museu Nacional d' Art de Catalunya (MNAC in Barcelona) [3]. The historical paintings and fresco replicas prepared in the laboratory were analysed by optical microscopy (OM), scanning electron microscopy with a focused ion beam (FESEM-FIB), synchrotron-based micro infrared spectroscopy (SR-μFTIR) and X-ray diffraction (SR-μXRD) (XALOC and MIRAS beamlines).
The data obtained indicates that the presence of casein enhances the stability of amorphous calcium carbonate, calcium hydroxycarbonates and vaterite, one of the crystalline calcium carbonate polymorphs. In addition, a good adherence between the original painting and caseinate mortar has been verified. Finally, we have observed that the stability of the painting layer is not affected by the reattachment process.

Acknowledgements:
The project received financial support from MINECO (Spain), grant PID2019-105823RB-I00 and Generalitat de Catalunya, grant 2017 SGR 0042. The μSR-XRD and μSR-FTIR experiments were performed at BL13 XALOC and BL01 MIRAS beamlines respectively, at ALBA Synchrotron Facillity with the collaboration of ALBA staff. We acknowledge Museum Nacional d'Art de Catalunya MNAC and the collaboration of conservators and curators, especially to thank Mireia Mestre and Paz Marquès.

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No

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Electronic and magnetic structure of Ru and Mn in new potential multiferroic materials Ca3Mn2-xRuxO7 (x<=0.5) by X-ray Spectroscopy

Authors: Vera Cuartero[1]; Javier Blasco[2]; Sara Lafuerza[3]

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$Ca_3Mn_2O_7$ was proposed as a prototypical multiferroic material in which the ferroelectric and the ferromagnetic ground state arise from the same elastic lattice instability, providing an indirect but high magnetoelectric coupling mechanism.[1] In order to further tune the functional properties of this system towards multiferroicity at room temperature, we have applied chemical doping substituting Mn by Ru.

The electronic and magnetic states states of Mn and Ru atoms in the $Ca_3Mn_{2-x}Ru_xO_7$ ($0.05 \leq x \leq 0.9$) series have been investigated by soft X-ray absorption spectroscopy (soft XAS) and X-ray magnetic circular dichroism (XMCD) at the Mn $L_{2,3}$ and Ru $L_{2,3}$ edges, measured at BL29-BOREAS beamline, and by high-energy resolution fluorescence detection (HERFD) XAS and X-ray Emission spectroscopy measured at ID26 (ESRF) .

The spectral shape of Mn $L_{2,3}$ XAS closely resembles those of the $CaMnO_3$ [2], with a dominant feature at 642.3 eV with a very narrow low-energy shoulder at 640 eV, implying that manganese predominantly exists in a Mn^{4+} oxidation state in the $Ca_3Mn_{2-x}Ru_xO_7$ system, in agreement with HERFD-XAS at Mn K edge measurements. For the higher Ru concentrations, a slight shift to lower energy of the main peak is observed, suggesting an increasing amount of Mn^{3+}. We estimate a ratio of Mn^{3+}/Mn^{4+} of 0.15, which demonstrate that the Ru doping increases the concentration of Mn^{3+}, maybe related to the introduction of oxygen vacancies, similarly to the behavior reported for Ru doped $Ca_3Ti_2O_7$.

According to the sum rules applied to Mn XMCD, the Mn magnetic moment increases with increasing the Ru content for $x \geq 0.3$, although the values are substantially lower than expected if the samples were fully ferromagnetic (~3 Bohr magnetons). However, the evolution of the estimated total magnetic moments with the Ru content agree quite well with that of M_S measured at 50 K and an applied magnetic field of 5 T with SQUID. For $x \geq 0.3$, the total magnetic moments deduced from the sum rules are slightly higher than the M_S values. Furthermore, the Mn XMCD data measured in remanence provide evidence supporting a canted antiferromagnetic ground state for Ru contents $x \geq 0.7$. A very weak Ru $L_{2,3}$ XMCD signal is observed, of opposite sign to the Mn $L_{2,3}$ XMCD, indicating that the direction of the small net Ru 4d magnetic moment is antiferromagnetically coupled to the net Mn 3d magnetic moment. Also, according to the spectral shape, we can conclude that only the $t_{(2g)}$ orbitals contribute to the XMCD signal. This result correlates well with the presence of either Ru4+ low spin ($3d^4$; $t_{(2g\uparrow)}{}^3$ $t_{(2g\uparrow)}{}^1$), in agreement with HERFD-XAS measurements at Ru L_3 (detected at the maximum of Ru L-alpha line).

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Would you like to participate in the Poster Prize competition?:

No

List of posters presented during the conference / 55

Nylon 7,10: Real time X-ray diffraction and FTIR microspectroscopy studies on a novel odd-even polyamide

Authors: Matteo Arioli[1]; Juan Carlos Martínez Guil[2]; Ibraheem Yousef[2]; Jordi Puiggalí[3]; Lourdes Franco[3]

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See attached document.

Would you like to participate in the Poster Prize competition?:

Yes

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Fast 3D magnetization recovery of 2D magnetic structures

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Co-authors: Lucía Aballe [2]; John Fullerton [3]; María Vélez [1]; Jose Ignacio Martín [1]; Andrea Sorrentino [2]; Eva Pereiro [2]; Salvador Ferrer [2]; Carlos Quirós [1]; Aurelio Hierro-Rodriguez [1]

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In the actual paradigm, where it is possible to grow magnetic nanostructures with 3D magnetization configuration, more complex structures appear, such as vortexes, skyrmions or hopfions. In order to visualize these new configurations, new magnetic imaging techniques different from the conventional 2D approach are mandatory. With X-ray Magnetic Circular Dichroism (XMCD) in X-ray transmission microscopes, it is possible to access the vector magnetization field within arbitrary magnetic systems down to tens of nm resolution [1-2]. To obtain the full magnetization field, different projections where the sample is rotated with respect to the X-ray beam are needed since we are only sensitive to the magnetization component along the X-ray beam. However, recording all the projections needed for an accurate reconstruction consumes a lot of time (usually a vector tomography experiment with 240 different projections requires 24 –28 hours of beamtime).
Here we present a fast method to reduce dramatically the acquisition time needed for accurate magnetization vector reconstruction specific for quasi two-dimensional magnetic structures, heterostructures and continuous films which are of interest for spintronics. The algorithm combines the transmission images to obtain first the electronic charge and, then, the magnetic configuration fitting the Bourguer-Lambert-Beer equation particularized for XMCD [3].
To validate our method, we performed measurements of 40 nm thick Py microstructures at the MISTRAL beamline of the ALBA Synchrotron. Even though 30 projections were taken, we have proven that with only 6 projections it is possible to reconstruct the magnetization thus greatly reducing the acquisition time.
Work supported by Spanish MCI (PID2019-104604RB/ AEI/10.13039/501100011033) and Foundation for the Promotion of Applied Scientific Research and Technology in Asturias (GRUPIN21 AYUD /2021/51185).

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Yes

List of posters presented during the conference / 37

Analysis of the dysprosium M5 circularly polarized X ray absorption spectrum to detect magnetically uncoupled rare earth atoms to TM in TM-RE amorphous alloys

Author: Javier Ignacio Diaz Fernández[1]

Co-authors: Jose María Alameda [1]; Manuel Valvidares [2]; Pietro Gargianni [2]; Cristina Blanco [3]

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The circularly polarized absorption spectrum of Dy M5 in DyCo4.5 amorphous alloys was decomposed in its spectral components related to transitions to states with the dysprosium angular moment parallel, antiparallel and perpendicular to the applied field [1]. This was done taking advantage of the atomic-like behavior of the 4f electrons, and the fact that, due to their large orbital moment in dysprosium, the parallel and antiparallel spectral components have very small overlap, being easily deconvoluted from the XMCD related spectrum. The intensity of the deconvoluted components in the analyzed dysprosium M5 spectra at RT and 2 K did not match the expected deduced from the magnetic moment values obtained from the XMCD sum rules. This indicates that the spectra must be formed by dysprosium atoms in different magnetic states, which are attributed to those related to strongly coupled to cobalt, and those uncoupled or weakly coupled to cobalt. A model is proposed that place most of the uncoupled dysprosium atoms at the surface of the alloy, as photoemission spectroscopy measurements done in similar samples proved, indicating rare earth segregation at the surface. This is also coherent with the surface sensitivity of the method used to detect the absorption spectra (TEY). The proposed spectral deconvolution analysis can be extended to other rare earths like Tb and Nd, whose orbital moment in their 4f orbital is not zero. The method is specially sensitive to detect if the rare earth has more than a single magnetic state in the analyzed material. The measurements were done in BL29, in the HECTOR end station, at the ALBA synchrotron.

[1] J. Díaz and C. Blanco. Phys. Rev. B 104, 054439 (2021)

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Cubic Rashba effect and 2D-ferromagnetism at the iridium-silicide surfaces of antiferromagnetic GdIr2Si2 and mixed-valent EuIr2Si2

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Cubic Rashba effect and 2D-ferromagnetism at the iridium-silicide surfaces of antiferromagnetic GdIr2Si2 and mixed-valent EuIr2Si2

Two-dimensional (2D) electron states at the surface of RT2Si2 compounds (R = lanthanide, T = transition metal) with ThCr2Si2 structure have proven to be ideal model systems for studying the joint action of spin-orbit (SOI) and exchange interactions on itinerant electrons [1-5]. Those surface states are predominantly situated in the Si-T-Si-R surface block and subject to Rashba-type spin splittings which can be manipulated by ordered 4f moments.
Here, we present our combined angle-resolved photoelectron spectroscopy (ARPES) and density functional theory (DFT) studies on the Si-terminated surface of compounds with T = Ir, which are of particular interest because Ir leads to a large SOI. We found that in the paramagnetic phase the surface states are characterised by a huge energy splitting of the highly spin-polarised bands and an exotic triple-winding spin structure along the constant-energy contours induced by the so-called cubic Rashba effect [4]. Upon ordering of the 4f moments below the Si-terminated surface, the emerging exchange coupling of the surface-state spins to the localised lanthanide moments modifies the spin structure, leading to pronounced asymmetries in the band dispersion. Surprisingly, these asymmetries were not only found for the antiferromagnet GdIr2Si2 [5], but for the valence-fluctuating EuIr2Si2, too [3]. The latter allowed us to unveil unusual 2D ferromagnetic properties and related temperature scales of the iridium-silicide surface of EuIr2Si2, which is non-magnetic in the bulk. Moreover, a short overview on additional results from complementary experimental techniques like photoelectron diffraction and magnetic dichroism experiments on the 4f shell is given [6].

[1] A. Chikina et al., Nat. Comm. 5, 3171 (2014)
[2] A. Generalov et al., Nano Lett. 17, 2 (2017)
[3] S. Schulz et al., npj Quantum Mater. 4, 26 (2019)
[4] D. Yu. Usachov et al., Phys. Rev. Lett. 124, 237202 (2020)
[5] S. Schulz et al., Phys. Rev. B 103, 035123 (2021)
[6] D. Yu. Usachov et al., Phys. Rev. B 102, 205102 (2020)

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ExPaNDS - The benefit of Open Data

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We would welcome the opportunity to take part in the presentation abstract session to highlight "The benefits of Open Data".

Using Photon and Neutron (PaN) sources to investigate samples of matter at molecular or atomic level apply to extremely diverse science domains, ranging from chemistry and life science to palaeontology and art history. The scientific community represented by PaNOSC for European Research Infrastructures (RIs) and ExPaNDS for national RIs is extremely wide-ranging rich, as it embraces over 30,000 researchers, but due to the diverse character of their sciences it is also extremely fragmented.

ExPaNDS is the European Open Science Cloud (EOSC) PaN Data Service. The ambitious project will create enormous opportunities for the Photon and Neutron Research Infrastructures (PaN RIs) and through their findings for humankind across the globe. This will be achieved through the collaboration and federation of 10 national PaN RIs from across Europe based on the EOSC services in partnership with EGI, and will become a game-changer for the scientific user community. ExPaNDS will make the majority of PaN RIs data 'open'following the FAIR principles (Findable, Accessible, Interoperable, Reusable) according to the user's needs, and to harmonise efforts to migrate facility' s data analysis workflows to EOSC platforms enabling them to be shared in a uniform way.

The goal of our projects and the EOSC is to make data from publicly funded research in Europe Findable, Accessible, Interoperable and Reusable (FAIR). Fostering FAIR data practices will allow other facilities and their users to benefit from the valuable data produced thanks to our light and neutron sources. By reusing data, it is possible to plan experiments and simulations that will produce more than was originally imagined.

ExPaNDS sees EOSC as an opportunity to generalise the adoption of FAIR data practices at our PaN RIs that will enable data sharing, the reuse across a wider community and the provisioning of services for remote data analysis. We will map all relevant data catalogues to ensure that our scientific research communities have access to both the raw data collected that is linked to the experiments at their facility, and the relevant peer review articles produced as a direct result of their usage.

We are keen to engage with scientists who are interested in "Open data", those who believe that open data will provide new opportunities for our PaN community and science in general. Those wanting to support that open data could be freely used, re-used and distributed to advance knowledge and help to combat 21st century problems. We would also like to showcase a number of use cases which highlight exactly these benefits of open data.

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No

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Distribution of antiferromagnetic domains in Fe-doped NiO thin films on Ru(0001)

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Antiferromagnetic (AFM) oxide materials in low-dimensional geometries, either in nonmagnetic or magnetic environments, display a rich variety of magnetic behavior. They are very interesting materials to investigate the fundamental physics of finite-size effects in magnetic systems. Despite the limited applications in current technology, AFM oxides are important reference and model systems for studying the interface coupling phenomena that are ultimately exploited in devices such as spin-valves. Furthermore, they are the current focus for next generation of spintronic devices.

Here we demonstrate a route for preparing high quality ultrathin ternary transition metal oxide films on a metallic substrate. Nickel oxides with a small content of iron have been grown on Ru(0001) by oxygen-assisted molecular beam epitaxy at elevated temperatures (1150 K). The nucleation and growth is observed in real time by means of Low Energy Electron Microscopy (LEEM. This enables the optimization of the growth parameters. A comprehensive characterization is performed combining LEEM and LEED for structural characterization and PEEM (PhotoEmission Electron Microscopy) with synchrotron radiation for chemical and magnetic analysis via X-ray Absorption Spectroscopy and X-ray Magnetic Linear Dichroism (XAS-PEEM and XMLD-PEEM, respectively).

We have been able to obtain high quality 2D islands with atomically flat surfaces and a low density of defects. The high crystalline and morphological quality result in optimized properties with respect to films grown by other methods, such as magnetic domains whose size are larger by several orders of magnitude. The spin axis orientation from a single domain area has been extracted applying vectorial magnetometry.

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LEAPS & ESUO

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