



# Activity Report 2021

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## FOREWORD

2021 has been the year of the normalization of operation after the pandemic, even if still coexisting with the pandemic waves and dynamically adjusting the people presence in the facility, prioritizing safety and considering our needs of balancing family and work life.

As usual when going through difficulties, the experience of the pandemic has led us to develop new abilities, as for example in carrying out experiments with a stronger component of automatization and remote control, in the way meetings are organized or how we use new communication tools.

The scientific activity during the whole year has been in full speed. An average number of more than 38 peer-reviewed papers per operating beamline has been published, with a very high average impact factor. The LOREA beamline, dedicated to ARPES, has started the operation, the other beamlines in construction have continued their plans, even if facing in some cases delays driven by providers' difficulties in delivering on time.

And the plans for the future have decisively advanced: the project of the upgrade of the facility to the 4th generation, namely ALBA II, has been continued; the accelerator design status was reviewed in November by an external panel; and what we see as a very important turning point in the whole process, the first funding for ALBA II, has been received for the design and prototyping the arc of the Storage Ring, driving the project to a new phase.



This phase includes the interaction with the whole user community on the scientific case of the upgrade. Workshops and colloquia, as well as a full day dedicated to ALBA II in June, were held along the year and have involved hundreds of scientists in the discussion on which will be the opportunities from the future source.

The Joint Electron Microscope Center at ALBA (JEMCA) has received the first microscope, for molecular biology, headed by the Institute of Molecular Biology of Barcelona (IBMB-CSIC), and has started its installation.

The fruitful collaboration within LEAPS, in the second year of ALBA chairing, has strengthened the European links of our staff and users with the other facilities and the European Commission.

Enjoy the reading.

**Caterina Biscari**  
Director



# Enlarging our services and preparing for the future

ALBA is the Spanish synchrotron light source, providing traditional synchrotron light-based techniques and a growing number of microscopic services and tools for studying and imaging the structure of matter and its behavior.

In 2021, ALBA is operating nine beamlines, and building additional four beamlines covering the complete energy range from infrared to the hard X-ray range with a focus on 100eV to 30keV. The user community of more than 6,000 academic and industrial users per year is forming a mature user program.

In the process of upgrading the light source to the 4<sup>th</sup> generation, ALBA is in an exciting period

of expansion and growth. Focusing on the new imaging capabilities, ALBA is also gradually upgrading the existing beamlines with the goal of providing in future multimodal instrumentation suites; benefitting the wide user base, these suites are specifically tuned to enable the user to address the grand challenges in health, energy, and information technology.

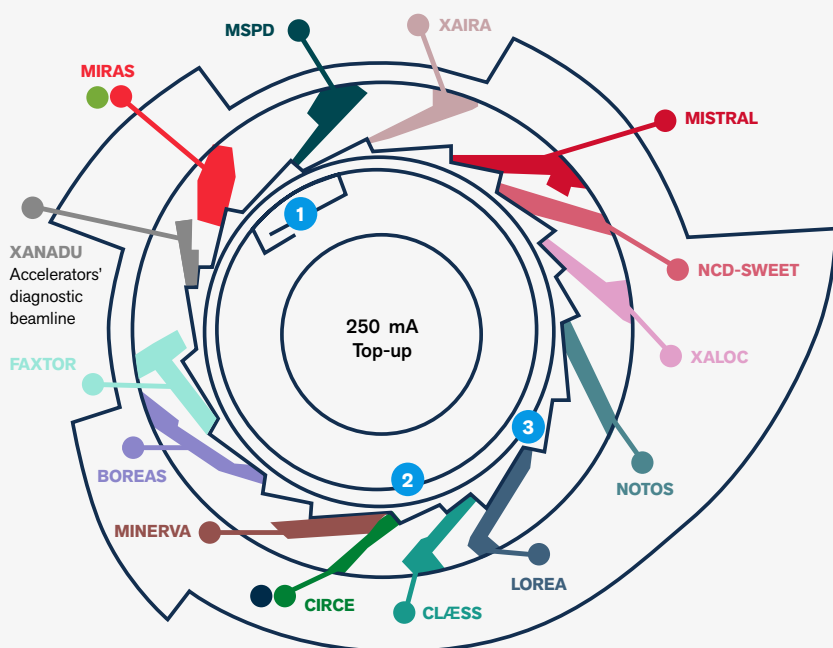


## MAIN PARAMETERS

- **3 GeV Electron energy**
- **268 m Circumference of the Storage Ring**
- **250 mA Electron beam current**
- **Top-up operations within 1% current variation**
- **Beam availability (average last 5 years) 98%**
- **H Emittance 4.6 nm-rad**

- **9 Operational Beamlines**
- **4 Beamlines under construction**
- **17 Experimental set-ups / Endstations**
- **Joint Electron Microscopy Center (first users in 2022)**

- 1 LINAC**  
Electrons are accelerated to 100 MeV
- 2 BOOSTER**  
Electrons reach 3 GeV
- 3 STORAGE RING**  
268 m circumference  
Electrons deliver synchrotron light to beamlines



### DIFFRACTION & SCATTERING

- High energy: **MSPD, NOTOS**
- High pressure: **MSPD**
- Diffraction Scattering: **NCD-SWEET**
- MX: **XALOC, XAIRA**

### IMAGING

- Infrared microscopy: **MIRAS**
- Soft X-ray microscopy: **MISTRAL**
- Photoemission microscopy: **CIRCE**
- Fast X-ray tomography: **FAXTOR**

### OPTICS CHARACTERIZATION

- **MINERVA**

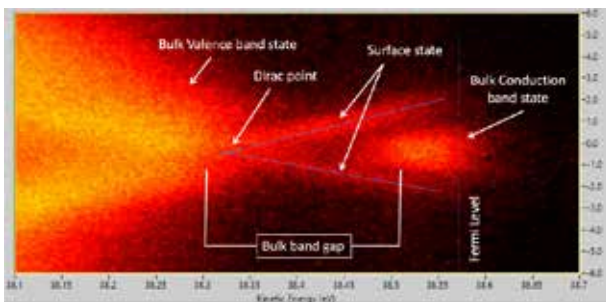
### SPECTROSCOPY

- Infrared microspectroscopy: **MIRAS**
- Absorption and emission: **CLÆSS, NOTOS**
- Angle-resolved photoemission: **LOREA**
- Near ambient pressure photoemission: **CIRCE**
- Magnetic dichroism and resonant scattering: **BOREAS**

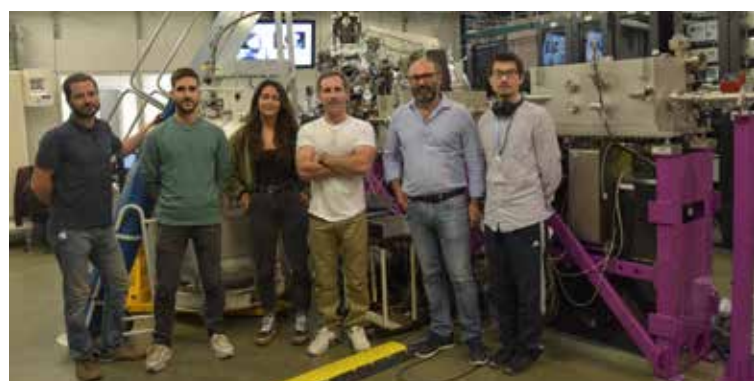
# LOREA, beamline number 9 is now operational

LOREA is dedicated to the study of quantum materials by means of Angle Resolved PhotoElectron Spectroscopy (ARPES). The ARPES technique is the most powerful to determine the band structure of solids and unveil important characteristics of materials to be used in quantum computing, for low energy consumption microelectronics, for superconductors, photovoltaics, and many other devices using the charge or the spin of electrons to transport, store or convert energy.

In 2021, its commissioning reached its final stage. The first ARPES measurement was obtained during the summer 2021. As a first experiment for the new beamline, the chosen sample was made of bismuth-telluride ( $\text{Bi}_2\text{Te}_3$ ), a thermoelectric material capable of converting electricity into temperature difference and vice-versa. Bismuth telluride is a topological insulator, meaning that it is an insulator (or semiconductor) in its bulk state, but it is highly conductive (almost perfectly conductive, with



**Figure 1:** In the first ARPES image of LOREA, one can see the angular band dispersion of  $\text{Bi}_2\text{Te}_3$  in the angular range  $(-6^\circ, +6^\circ)$  as a function of the kinetic energy of the electrons emitted from the sample exposed to photons with 43eV energy. The bulk valence and conduction bands with a band gap of more than 0.2eV, and the surface state showing a linear angular dispersion, converging towards the “Dirac point” placed about 0.3eV below the Fermi Level.



**Figure 2:** Top. Image of LOREA beamline and his scientist leader, Massimo Tallarida. Down: group picture of the team involved in the first official experiment at LOREA (from left to right: Jordi Prat, beamline technician, PhD student David Subires, master student Lorea Sánchez, IKERBASQUE researcher Santiago Blanco from DIPC Donostia, Massimo Tallarida, beamline responsible, and Ji Dai, postdoctoral research associate at LOREA).

linear bands to build a “Dirac cone”) on its surface alone, through the formation of surface states which are resistant to contamination.

At the end of October 2021, the beamline hosted the first official users. They were a research group from the Donostia International Physics Center (DIPC), led by researcher Santiago Blanco. The research group was analyzing the electronic structure of a promising 2D material, based on vanadium and selenium(II) ( $\text{VSe}_2$ ), with great possibilities for spintronics and data storage.



The beamline is co-funded by the European Regional Development Fund (ERDF) within the Framework of the ERDF Operative Programme of Catalonia 2014-2020.

# Beamlines under construction



## **NOTOS. X-ray absorption & powder diffraction**

NOTOS received the first X-ray beam up to the first mirror in the optical hutch in February 2021. During the year, other optical elements have been progressively installed and commissioned and the first monochromatic beam in experimental hutch was detected at the end of July. Starting from the end of September the High resolution Poder Diffraction- X ray absorption (HPD-XAS) station was available allowing the X-ray commissioning of the beamline up to the EH. During the autumn 13-elements SDD detector was received and installed in the available end station. The double channel toroidal crystal for the second mirror was delivered at the end of December.

## **MINERVA. Support beamline for the development of the ATHENA mission (Advanced Telescope for High Energy Astrophysics)**

Many achievements were reached during the year 2021. All the elements of the beamline were characterized and approved by the European Space Agency. The lead hutch hosting the multilayer monochromator was built during the summer shutdown. The front-end was installed during the 2021/2022 winter shutdown. A call for tender for the procurement of the main hexapod and a laser tracker was published in December. Most of the equipment is now in production.

## **FAXTOR. Fast X-ray tomography & radioscopy**

During the year 2021, FAXTOR's project advanced in several aspects. The contracts for the beamline optical elements, including the Double Multilayer Monochromator and hutches were awarded. Advancements in the production of the photon source and front-end were recorded. The end-station Conceptual Design was frozen and the call for the tender of the main components of the end-station, including the sample stage and microscopes, published.

## **XAIRA. Microfocus beamline for macromolecular crystallography**

XAIRA has gone during 2021 from a colourful empty shell, with only the radiation hutches in place, to a complex instrument with the characteristic gear of the synchrotron beamlines. The fluid and electrical services were installed and the racks populated with the hardware required for the vacuum, motion, control, cryogenic and IT subsystems. Importantly, the main optical elements, with the exception of the mirror benders, were installed up to the final focusing stage, already in the experimental hutch. The focusing mirrors were procured and measured to have a figure error of only 100 nrad, while the elements selecting the photon energy, the silicon channel-cut crystal and the pair of multilayers largely complied with the required quality. The rest of the optics, that is, diagnostics, slits and vacuum pipes are ready to be installed next. Overall the optics is assessed to deliver a focused beam in the 1-micron range at the sample position. The end-station has also seen much progress. The custom-made diffractometer was commissioned, showing a runout error of only 70 nm, which could be further reduced by synchronized correction of the rotation axis using fast piezo-motors. The sample visualization system, the beam diagnostics and the temperature conditioning system -which can blow either nitrogen or helium at cryogenic temperature- among other sample environment instruments, are also being manufactured or procured. The photon-counting detector was also procured and is soon to be received. The network and the storage systems are being upgraded to cope with the collected data, which will amount up to 550 9-Mpixel images per second and eventually be the highest data rate at ALBA. The last main beamline instrument to be procured is the automated sample changer.



# ALBA II

ALBA II is the upgrade of the ALBA Storage Ring to a 4<sup>th</sup> generation light source that will deliver higher brilliance and flux. The upgrade requires replacing the Storage Ring accelerator of ALBA including all magnets, vacuum chambers and girders, upgrading the existing beamlines of ALBA and building new long beamlines.

## Initial funding for ALBA II

At the end of 2021, ALBA received 7.5M€ to start designing and prototyping the new accelerators' systems and developing a new nano-positioning laboratory. Funds came from the Ministry of Science and Innovation and the European Union NextGenerationEU through the Recovery and Resilience Plan. The replacement of several accelerator elements with cutting-edge technologies will generate a much smaller electron beam and therefore brighter and more coherent synchrotron light. The development of a nano-positioning laboratory will serve to ensure the

precision and stability at the level of nanometers needed to take full advantage of the probing capacity of the ALBA II light.

## ALBA Colloquium series

To create an open discussion forum in which our user community, the ALBA staff, world experts in synchrotron research and potential future users could exchange experiences, show the current frontier in synchrotron-based characterization and discuss the latest methods, we run during 2021 the ALBA II colloquium series. Sixteen invited speakers participated in these biweekly series,

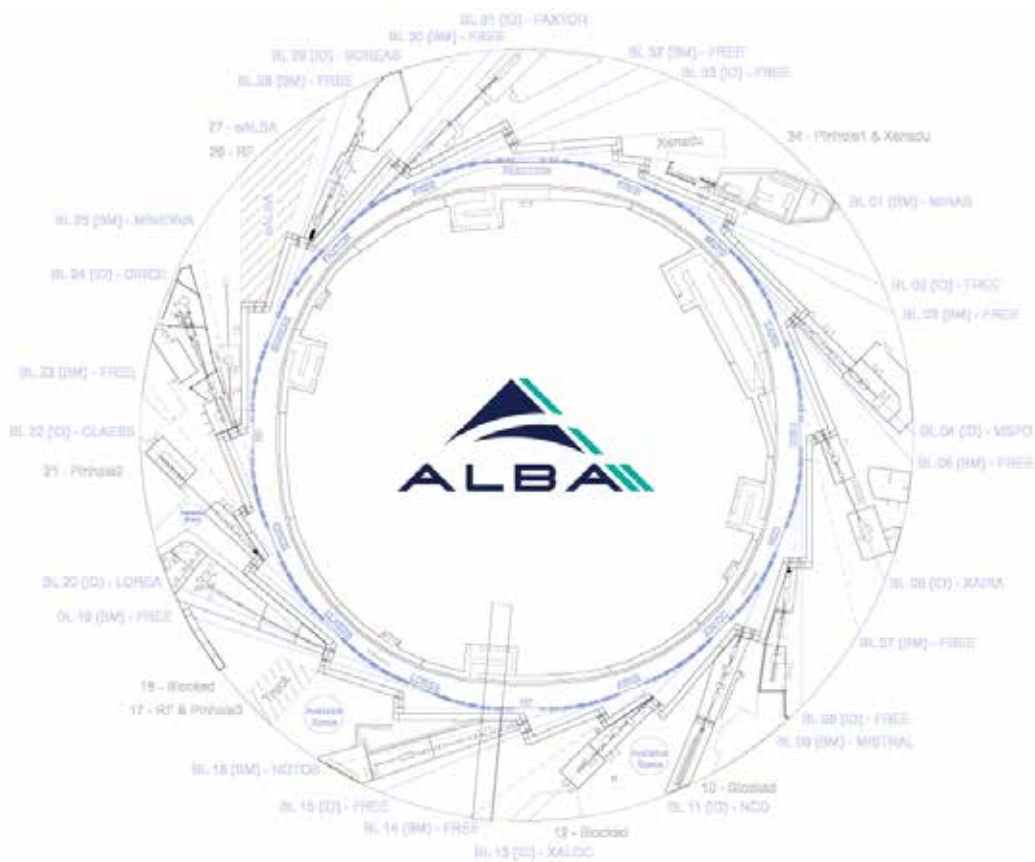
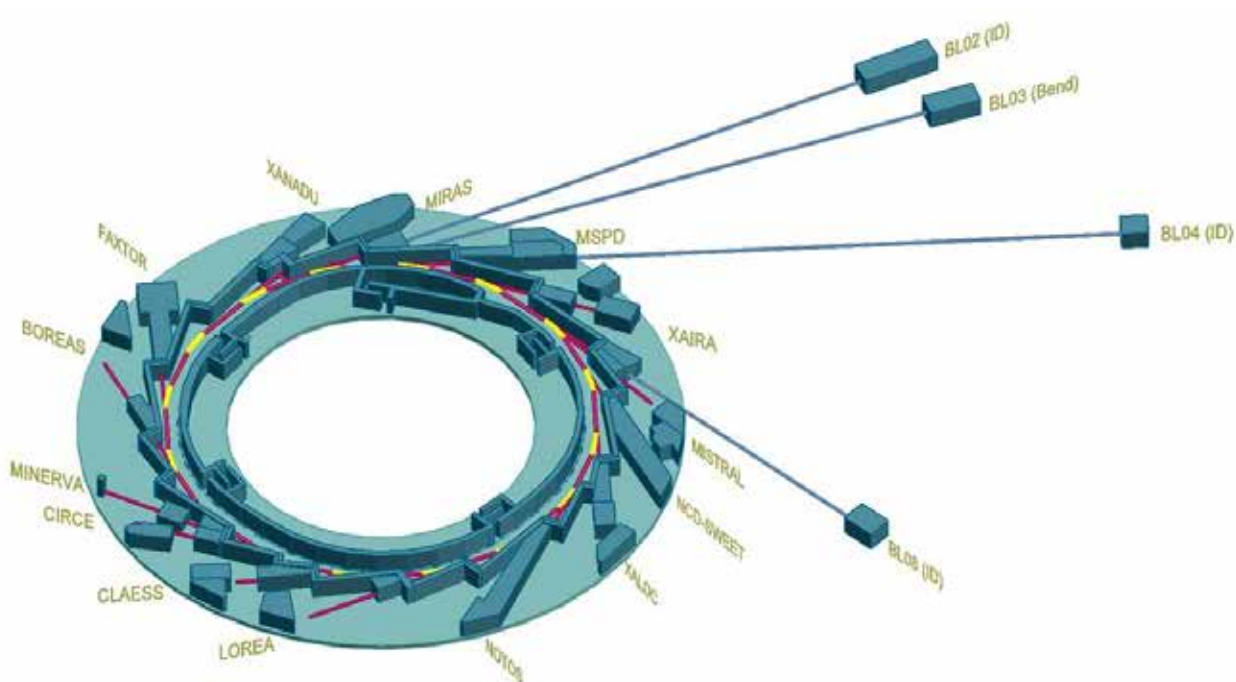


Figure 3: Preliminary design of ALBA II design



**Figure 4:** 3D scheme of the ALBA II accelerators and beamlines, including new long beamlines

with talks of 40 minutes length plus additional 15 minutes discussion. Besides, eight workshops were organized, counting with different experts the same day. Most of the sessions are available in video in this link: <https://www.albasynchrotron.es/en/science-at-alba/alba-ii-upgrade/alba-ii-colloquium>

### ALBA II Day and New Call for Beamlines

The 30<sup>th</sup> of June 2021, ALBA organized an event counting with more than 100 members from the user community for better shaping the ALBA II project needs and priorities. The first session was dedicated to giving an overview on the user perspectives, strategy and mission for academic and industrial communities, the future of the accelerator, the beamlines, and the partnership strategy for ALBA II. The second session was focused on the main strategy fields for the future facility: Health, Information Technology, and Materials & Energy.

### ALBA Colloquium series



**Figure 5:** Snapshot of the some of the participants at the ALBA II day.

The event closed with the launch of a call for new beamlines, where nineteen groundbreaking pre-proposals were received. Three of them were selected to be transformed into a full proposal to start a new beamline in 2022.



# The power of collaboration



**Figure 6:** Left, moment of the symbolic hand-over of the LEAPS Chair for 2022 from Caterina Biscari, ALBA, to Leonid Rivkin, PSI. Right, installing the first electron microscope at JEMCA.

The League of European Accelerator based-Photon Sources (LEAPS) is a strategic consortium, made up of 16 organizations representing 19 light sources across Europe. Its primary goal is to actively promote and ensure the quality and impact of fundamental, applied and industrial research carried out at their facilities.

The ALBA Synchrotron, led by its director, Caterina Biscari, has been deeply involved in LEAPS's activities since the beginning of the collaboration, even though assuming the chair during 2020 and 2021. In the 18<sup>th</sup> LEAPS general Assembly, Lenny Rivkin, Deputy Director of the Paul Scherrer Institut (Switzerland), was appointed the new LEAPS chair from 2022.

In 2021, ALBA has continued contributing to a fruitful exchange and cooperation with other facilities. The LEAPS-INNOV pilot project that promotes open innovation in light sources officially started in April 2021, counting with an

outstanding involvement of ALBA staff. ALBA has been representing LEAPS in many international events during 2021 like the Microscopy Conference 2021, the 3rd International Summit of Synchrotron Radiation Innovation or the global-scale conference on Research Infrastructures (ICRI). The 4th LEAPS Plenary Meeting, organized on-line on October 2021, offered again an exciting opportunity to share the latest of the LEAPS collaboration.

As part of a joint action among 9 research institutions, ALBA has set up the Joint Electron Microscope Center at ALBA (JEMCA) that will host a microscopy platform at its facilities. It will host two new major experimental facilities, one dedicated to materials science, led by the Catalan Institute of Nanoscience and Nanotechnology (ICN2), and another meant for molecular biology, headed by the Institute of Molecular Biology of Barcelona (IBMB-CSIC). This second microscopy arrived at ALBA in 2021 and started its installation with the goal of starting operating for users in 2023.



**Figure 7:** Virtual group photo of some of the attendants at the 4<sup>th</sup> LEAPS Plenary Meeting.

# GOVERNING BODIES

ALBA is funded in equal parts by the Spanish and Catalan Governments. The composition of the governing bodies in 2021 was:

## GOVERNING COUNCIL

**Chair:** Pedro Duque Duque, Minister of Science, Innovation and Universities (January-July 2021), MINCIU, Spanish gov., Diana Morant, Minister of Science and Innovation (July-December 2021), MICIN, Spanish gov.

**Vice-Chair:** Ramon Tremosa, Minister of Business and Knowledge (January-May 2021), Gemma Geis, Minister of Research and Universities, (May-December 2021), Catalan gov. GENCAT.

### Members:

- Rafael Rodrigo Montero, Secretary-General for Science Policy Coordination, MINCIU (January-July 2021)
- Raquel Yotti, Secretary-General for Science, MICIN (August-December 2021)
- José Ignacio Doncel Morales, Deputy Director for Singular Scientific and Technical Infrastructures, MICIN
- Carmen Castresana Fernández, General Director of Research Planning, MINCIU (January-July 2021)
- Gonzalo Arévalo, General Director of Research Planning, MICIN (August-December 2021)
- Francesc Xavier Grau i Vidal (January-July 2021), Esther Morales (July-December 2021) Secretary for Universities and Research, GENCAT
- Joan Gómez i Pallarès, Director-General for Research, GENCAT
- Javier Lafuente Sancho, Rector of the Universitat Autònoma de Barcelona (UAB)

**Secretary:** Luisa María Rodríguez Garrido, State Lawyer, MICIN

**Guest:** Caterina Biscari, Director of ALBA

## EXECUTIVE COMMISSION

**Chair:** Francesc Xavier Grau i Vidal (January-July 2021), Esther Morales (July-December 2021), Secretary for Universities and Research, GENCAT

### Members:

- Rafael Rodrigo Montero, Secretary-General for Science Policy Coordination, MINCIU (January-July 2021)
- Raquel Yotti, Secretary-General for Science, MICIN (August-December 2021)

• José Ignacio Doncel Morales, Deputy Director for Singular Scientific and Technical Infrastructures, MINCIU

• Joan Gómez i Pallarès, Director-General for Research, GENCAT

**Secretary:** Luisa María Rodríguez Garrido, State Lawyer, MICIN

**Guest:** Caterina Biscari, Director of ALBA

## SCIENTIFIC ADVISORY COMMITTEE

Board of internationally renowned experts in the field of synchrotron radiation, who participate in the strategic scientific direction of the ALBA Synchrotron with the aim of ensuring the quality and relevance of the research performed and developed at ALBA.

**Chair:** Beatriz Roldan, Director and Head of the Department of Interface Science at the Fritz Haber Institute (Germany).

### Members:

- Reinhard Brinkmann, Lead Scientist at the DESY Accelerator Division (Germany)
- Valerie Briois, ROCK Beamline Manager at Soleil Synchrotron (France)
- Carlo Carbone, Research Director at Consiglio Nazionale delle Ricerche, Istituto di Struttura della Materia (Italy)
- Peter Cloetens, responsible of ID16A - Nano-imaging beamline at ESRF (France)
- Andrew Dent, Physical Science Coordinator at Diamond Light Source (United Kingdom)
- Tiberio Ezquerro Sanz, Head of Soft and Polymeric Matter Group at Instituto de Estructura de la Materia-CSIC (Spain)
- Gwyndaf Evans, Principal Beamline Scientist for VMXm at Diamond Light Source (United Kingdom)
- Pedro Fernandes-Tavares, Project Leader for the Storage Rings at Max-IV Laboratory (Sweden)
- Michael Wulff, ID09 Beamline Manager at the ESRF (France)

# HEALTH & SAFETY

Victor Garrido, head of the Health & Safety Office



**Figure 8:** The Radiation Protection Group checking the radiation levels at NOTOS beamline.

It is highly important today still recovering from COVID-19 pandemic effects all over the world, to keep a positive mindset to overcome all difficulties through this moment. Projects like ALBA II, with a deep impact in our community, or the creation of our OPS (Own Preventive Services) can help us to see the glass half-full.

Apart from the regular activities of the Health & Safety Office, the approval of this new prevention model (called OPS) by the Governing Council in July 2021 has been one of the huge challenges achieved. Staff resources have been increased by two new members, improving capabilities to face these new challenges. The selection and acquisition of a specific measurement equipment has allowed us to analyse environmental labor pollutant and others physical parameters. We can consider 2021 as a transitional time to be completed in 2022 with an external audit.

The SPS (Safety Prevention System) has been created to implement several functionalities in our People Portal as the work positions assignment. The health monitoring protocols to appoint visits has been another of the big projects initiated in 2021 and still developing during the following year together with risk assessments design and corrective measure planning functionalities. At the end of 2021, Psychosocial reassessments and the

Health Surveillance Survey have been initiated to define future strategies based on their results.

A HAZOP (Hazard and Operability study) for new BL16-NOTOS had been put into practice in September 2021. The development of the results for this study has been the precursor of a new set of experiments at ALBA. On the other hand, the Radiation Protection Service has focused on ensuring the correct radiation levels around new beamlines during 2021. The first half of the year, LOREA and NOTOS continued their evolution towards becoming operative.

The area surrounding LOREA's hutch was classified as watched area and measurements were performed around the monochromator and beyond. BL20-LOREA has been classified as public access area and has the regulator permit to operate.

MINERVA's hutch and PSS system were installed during the summer shutdown in port 25, next to CIRCE beamline.

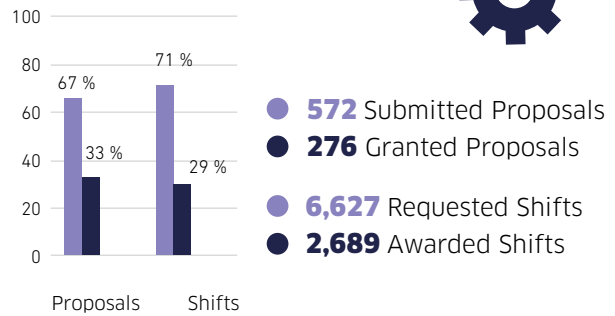
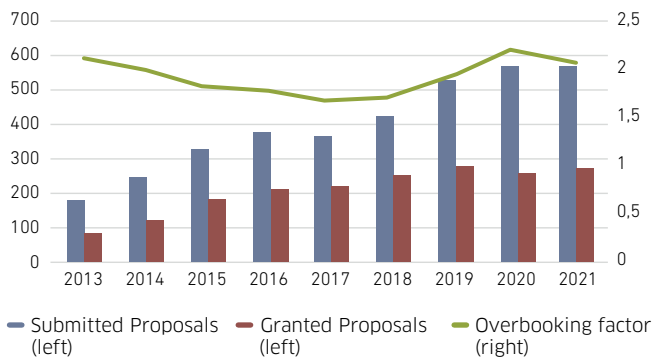
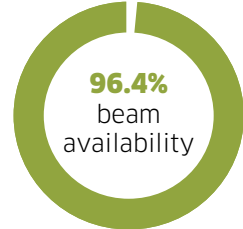
For 2022, the Health & Safety Office is prepared for the upcoming commissioning phases of XAIRA and MINERVA. Finally, the radiation measurements performed around the rest of the facility ensure that the levels of radiation outside the shielding enclosures are below public level as usual.



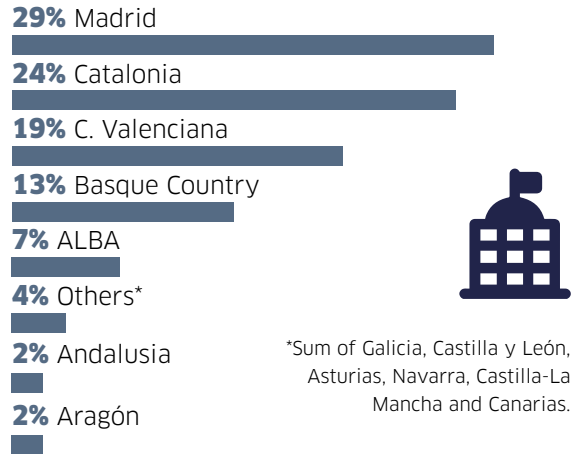
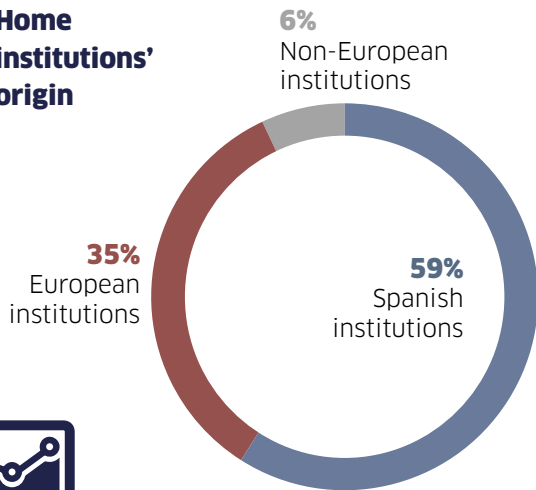
# KEY FIGURES IN 2021

Serving our user community

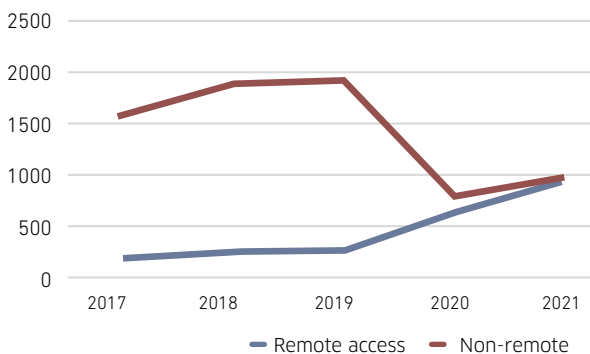
**5,848 operation hours**  
**4,646 hours for beamlines**  
**76.3 hours Mean Time Between Failures**  
**2.73 hours Mean Time to Repair**



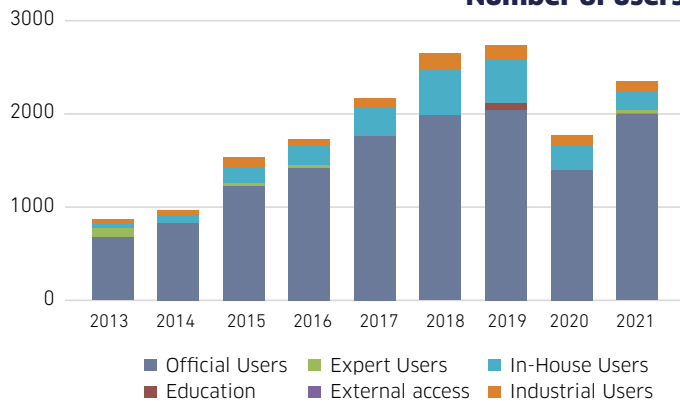
## Home institutions' origin



## Remote access

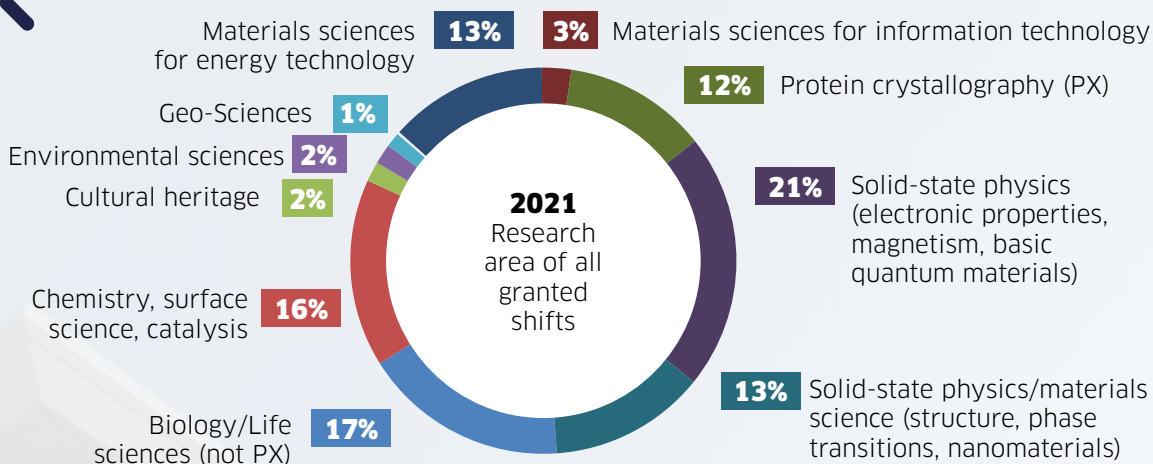


## Number of users

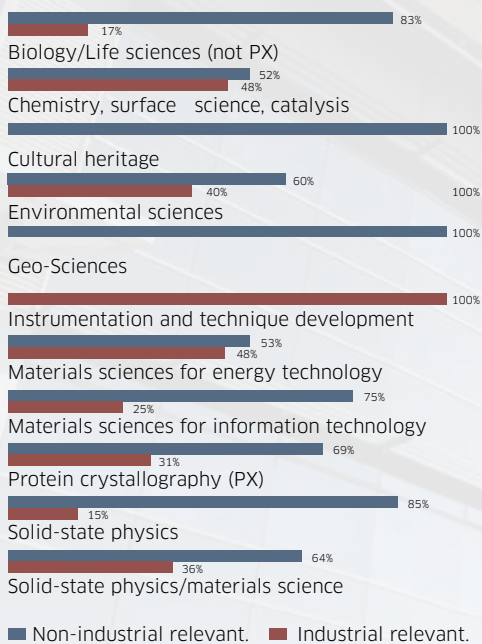




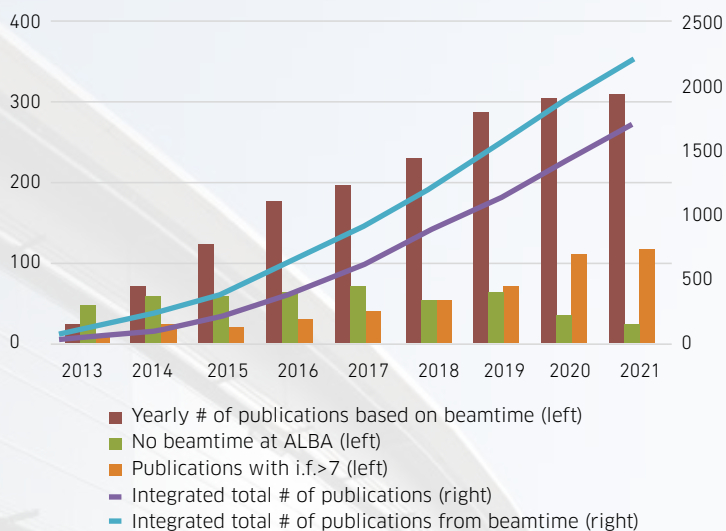
## Research area



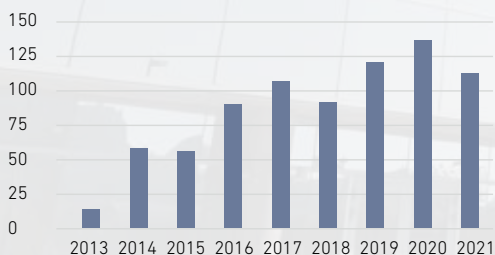
## Granted proposals by research area & industrial relevance



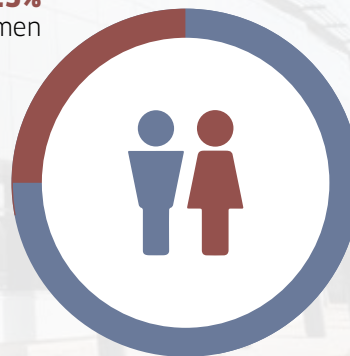
## Publications



## Deposited structures in the Protein Database



25% Women



75% Men



213 Staff Members

18 different nationalities

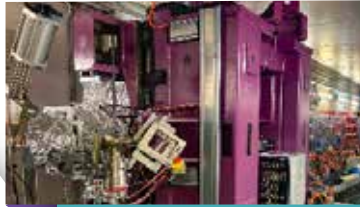
# 2021 AT ALBA



## JANUARY

### ALBA builds a new beamline in collaboration with the European Space Agency

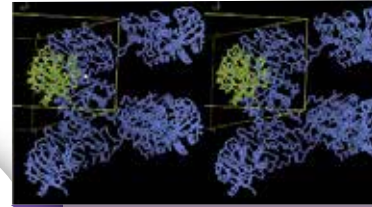
MINERVA will be the 13<sup>th</sup> ALBA beamline and will be used to support the ATHENA mission, the Advanced Telescope for High Energy Astrophysics that will reveal new insights about hot and energetic universe.



## FEBRUARY

### Milestone reached! XAIRA's undulator installed

This is the longest undulator ever installed at ALBA, with a magnetic length of 2.3 metres and housing 115 magnetic periods. XAIRA is a microfocus beamline, dedicated to challenging Macromolecular Crystallography (MX) experiments.



## MARCH

### ALBA hosts virtually the HERCULES School

From 15 to 18 March, 19 participants of the European HERCULES 2021 school could delve into a wide variety of synchrotron techniques with the help of ALBA scientists. This course, running since 1991, was held virtually combining theoretical and practical sessions.



## APRIL

### In-person visits again at the facility

ALBA started to host progressively at its facilities in-person visits, after the restrictions imposed by the pandemic. Among them, the State Secretary for Global Spain, Manuel Muñiz Villa, and Eurodeputy from Esquerra Republicana de Catalunya (ERC) Jordi Solé visited us during this period.



## MAY

### ALBA successfully showcased its synchrotron techniques to the agrifood industry

The ALBA Synchrotron actively participated in the Smart Agrifood Industry congress organized on the 25 and 26 of May by secpho, the Deep Tech cluster from South Europe, using their innovative virtual platform Secpholand. Several connections with companies were made during the event.

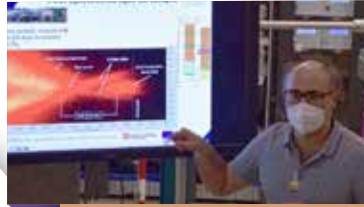




## JUNE

### **ALBA II Day Webinar: the ALBA upgrade project**

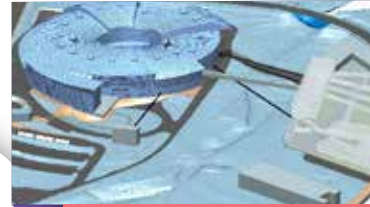
The user community of the ALBA Synchrotron was called to participate in a webinar session the 30 of June. Users were able to learn about the status of the ALBA II project and how to contribute to its success. A call for new beamlines was open.



## JULY

### **First Angle Resolved Photoelectron Spectroscopy (ARPES) measurement at LOREA**

The first ARPES measurement was a fundamental step in the commissioning of the LOREA beamline. The chosen sample was bismuth-telluride, a thermoelectric material capable of converting electricity into temperature difference and vice-versa.



## SEPTEMBER

### **Initial funding for the ALBA II upgrade**

The ALBA Synchrotron received 7.5M€ to start developing and prototyping the new accelerators' systems for transforming ALBA into a 4<sup>th</sup> generation synchrotron facility. These funds are part of the Recovery and Resilience Plan within the framework of the NextGenerationEU.



## OCTOBER

### **ALBA hosts the workshop on accelerator operations**

The 12<sup>th</sup> edition of this workshop was held virtually from 5-8 October 2021, promoting an excellent forum where to exchange ideas and best practices among worldwide experts in accelerators. This workshop, which was initially to take place in 2020, focused on the impact of the pandemic in the way accelerators are run.



## NOVEMBER

### **ALBA, awarded by the "Amics UAB" association**

In a ceremony held at the UAB Casa Convalescència in Barcelona, the ALBA Synchrotron was recognized by the "Amics UAB" association with an award addressed to institutions that work for improving the services provided at the Universitat Autònoma de Barcelona (UAB).



## DECEMBER

### **The Cryo-EM for biological applications arrives at ALBA**

Owned by a consortium of several institutes in the Barcelona area and led by the IBMB-CSIC, the cryo-EM was installed at ALBA at the end of 2021. This instrument has been co-funded with ERDF funds.

# Life sciences and soft condensed matter

Judith Juanhuix, Head of the Life Sciences and Soft Condensed Matter section (Experiments Division)

Year 2021, remembered as the second year after the COVID pandemic outbreak in the future history books, has seen a clear evolution of the methods and processes to operate our instruments which, ultimately, has led to the highest scientific output of the ALBA history in spite of the circumstances. A number of factors have contributed to this success, the main one being the excellent response of all ALBA staff, and in particular that of the Life Sciences section. Scientific, technical and administrative staff performed the extra tasks required since the pandemic outbreak in March 2020 to keep the experiments and services running all year long, from introducing new protocols to performing complex sample preparations and experiments on behalf of the research groups. In summary, all beamlines of the section were adapted to safety conditions changes upon the evolution and were operating remotely when required. From the outbreak, tens of COVID-related experiments have been carried out at XALOC (macromolecular crystallography), MISTRAL (soft X-ray tomography) and NCD-SWEET (small-angle X-ray scattering). As a result, the Life Sciences beamlines and laboratories have been studying a large variety of samples, from protein crystals to single cells and tissues. The beamtime offered by the Life Sciences Beamlines could also be made compatible with materials sciences, chemistry and magnetism user programs.

New instruments and techniques have been developed during year 2021. A setup for jet-based serial crystallography has been implemented at XALOC beamline, and is currently available to academic and industrial users. MISTRAL has completed the assembly of a Cryo 3D-SIM instrument for correlative microscopy in cryo conditions and improved tomographic data collection rate, and is ready for user program once protocols and personnel are appointed. Finally, MIRAS beamline (infrared microscopy and spectroscopy), in collaboration with the SISSI beamline at the Elettra synchrotron, has implemented a setup to study live cells. First

results using these three setups have already been published in top journals.

New instruments also come into operation. The first Cryo-electron microscope (CryoEM), owned by a consortium of several institutes in the Barcelona area led by the IBMB-CSIC, has been installed at ALBA. This 200 kV microscope, equipped with a field emission gun, an automated sample exchanger and a state-of-the-art direct electron detector, is being commissioned. This configuration has been shown to have a great potential for single particle analysis. The CryoEM will host first experiments with academic users on the first half of 2023. The two new beamlines under construction within the section have also seen significant progress. The microfocus macromolecular crystallography beamline XAIRA has finished the installation of the in-vacuum undulator and front-end, and is currently installing the optics. The hard X-ray tomography and radioscopy beamline FAXTOR, coming next, is also starting installation of the first elements. All these instruments are well supported by close-by biological laboratories with a total area of 230 m<sup>2</sup>, available to academic and industrial users upon demand. The equipment includes a full-equipped mammalian cell culture lab with biosafety level 2 capabilities, an automatic dispenser for protein crystallization compatible with LCP techniques, and a new FPLC system.

Finally, a very significant progress has been made in defining the scientific strategy of the Life Sciences program, to be implemented within the ALBA-II upgrade. Notably, two scientific reviews, the Structural Macromolecular Biology Review and the Structural Cell and Tissue Biology Review, were essential to critically assess the guidelines of the long-term strategy for the Life Sciences instruments and user program, which will include new instruments as well as the extensive upgrade of the existing ones. Also, a dissemination workshop and a number of seminars were held during 2021 to receive the feedback of the Spanish and international scientific communities.

# Synchrotron light unveils the efficacy of a new nanomaterial for cardiac fibrosis

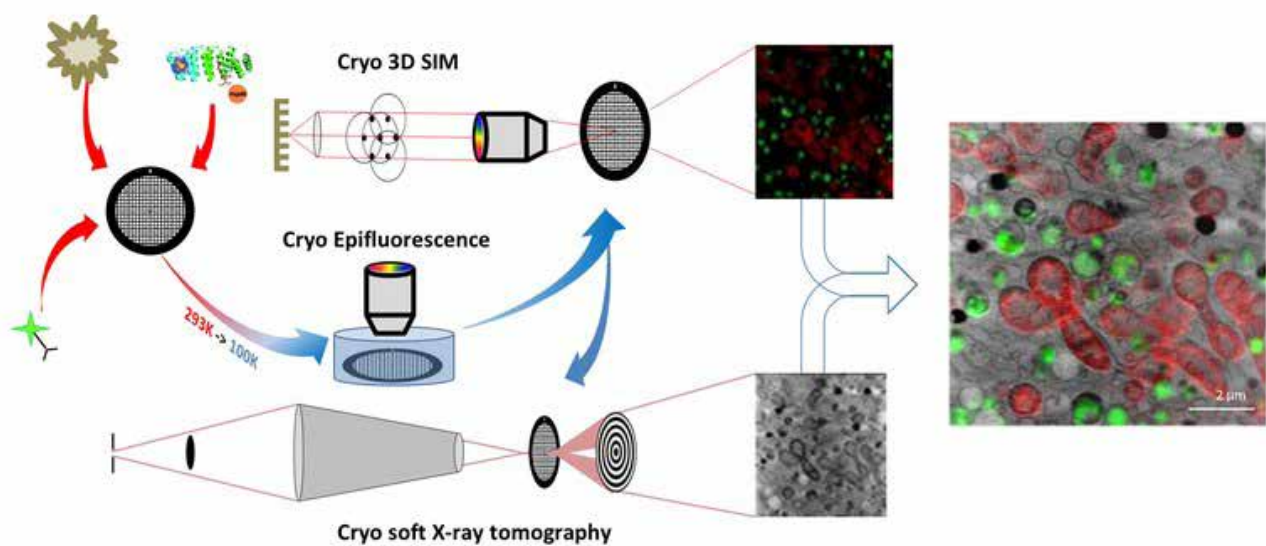
Experiments performed at the ALBA Synchrotron revealed, for the first time, the location of a novel hybrid nanomaterial designed to inhibit the collagen overproduction after a myocardial fibrosis event and the induced morphological changes in the cells. Obtaining this high-resolution 3D information of cells is crucial for developing pre-clinical studies of novel therapeutic agents.

A collaboration between ALBA Synchrotron PhD student Johannes Groen and researcher Eva Pereiro and the groups of Aitziber L. Cortajarena (CIC BiomaGUNE, San Sebastián) and Ana V. Villar (IBBTEC, Santander) have visualized for the first time in 3D the exact location and how a nanomaterial drug behaves in whole cells. This drug is a therapeutic protein-nanomaterial hybrid specifically designed to inhibit the collagen overproduction after a myocardial fibrosis event.

Cardiac fibrosis is a health condition that negatively influences the progression of many heart diseases and affects millions of people worldwide. It promotes the pathological increase of collagen deposition at the site of injury and the production of a scar, which can result in the disruption of

tissue function in the worst cases. The most common causes of cardiac fibrosis are ischaemia, infarction, cardiomyopathies, hypertension and myocarditis, which require short- and long-term follow-up due to pump dysfunction and myocardial stiffness. These pathologies are closely related to an unhealthy diet or lifestyle, advanced age and stress, among others.

There is no preventive or curative treatment for cardiac fibrosis, although a number of therapeutic agents prescribed for other cardiovascular disorders have been shown to exert beneficial effects on it. In most cases, it is only possible to reduce myocardial fibrosis once the underlying cardiovascular disease has been alleviated, mainly with invasive and life-threatening surgery.



**Figure 9:** Cryo-3D correlative fluorescent light and soft X-ray tomography (CLXT) approach: cryo-3D structured illumination microscopy (cryo-3D-SIM) and cryo soft X-ray tomography (cryo-SXT).





**Figure 10:** Johannes Groen, whose PhD work was carried out at the MISTRAL beamline of the ALBA Synchrotron.

Reducing fibrosis could save lives by improving the prognosis of patients with cardiovascular pathologies. Using a new approach, researchers combined cryo-3D correlative fluorescent light and X-ray tomography to locate, for the first time, the nanomaterial and to obtain high-resolution information on the cellular morphological changes after treatment, proving the antifibrotic properties of the drug.

First, the intracellular location allows to understand what possible routes are used to enter the cell, secondly, how the cell deals with a specific agent and finally, what are the effects induced by the treatment on the structural morphology of the cells. The samples were prepared at the ALBA Synchrotron and travelled to the B24 beamline at the Diamond Light Source (UK) to acquire 3D fluorescent data using their cryo-3D structured illumination microscopy (cryo-3D-SIM) setup. Then, at the MISTRAL beamline of ALBA, a cryo soft X-ray tomography (cryo-SXT) was performed, which allowed to study whole cells without the need to stain or manipulate the samples.

In addition, the full workflow in cryogenic conditions maximized efficiency by maintaining sample integrity and quality between both experiments, which was crucial to locate for the first time a protein-nanomaterial hybrid in whole cells.

Cryo-3D-SIM confirmed the presence of the therapeutic agent in treated cells, detecting it through its fluorescence signal, whereas cryo-SXT revealed the ultrastructural environment and subcellular localization of the nanomaterial with high spatial correlation accuracy. Indeed, the protein-nanomaterial hybrid was found, after overnight treatment, in multivesicular bodies associated with endosomal trafficking events by confocal microscopy. Moreover, this approach allowed assessing the cellular response towards the treatment: a clear reduction in collagen production was confirmed, but substantial differences between NIH-3T3 cells and primary fibroblasts were noticed, the latter being more resilient to the treatment. Finally, the small metallic cluster of 4 to 12 atoms, in addition to its function as a stabilizing and tagging module, possibly has an effect on the cellular morphology, which still needs to be further investigated.

The results obtained in this study pave the way for the introduction of nanomaterial-based drugs and nanomedicine into the clinic as they reinforce the usefulness of imaging techniques for evaluating cellular structure after the application of specific treatments.

**REFERENCE:** Johannes Groen, Ana Palanca, Antonio Aires, Javi Conesa, David Maestro, Stefan Rehbein, Maria Harkiolaki, Ana Victoria Villar, Aitziber L. Cortajarena and Eva Pereiro. *Chemical Science* (2021). <https://doi.org/10.1039/D1SC04183E>

# Chemistry and materials science

François Fauth, Head of the Chemistry and Materials Science Section (Experiments Division)

The year 2021 still remained marked by the COVID induced pandemic situation which for academic user experiments resulted in many remote access experiments due to travel restrictions and sometimes severe limitations in sample environment offer, particularly for those experiments requiring hazardous gas setups. However all allocated beamtime in proposal round 2021-I and 2021-II could be conducted on MSPD (43 accepted out of 98 proposed), NCD-SWEET (52/78, but 20% beamtime allocated for Life Sciences), CLAEISS (43/89) and CIRCE-NAPP (12/45, only half of the beamtime is distributed to NAPP endstation). Those numbers do not only demonstrate the intense academic user activity but highlight as well the severe over subscription for beamlines of the Chemistry and Material Science section. Though 6 proposal were accepted on NOTOS, they could not be performed because of delay in critical components delivery. They will be scheduled in the second semester 2022 when the beamline will be operational.

Scientific output was exceptionally high in 2021: 83, 48, 42 and 10 peer-review publications on MSPD, NCD-SWEET, CLAEISS and CIRCE-NAPP, respectively. Such numbers coupled to performed experiments reveal a 1 to 1 experiment/ publication ratio which appears as a clear sign of maturity and efficiency of all operating beamlines of the section. Looking

more specifically at the 16 Science highlights of these beamlines, we identify topics on energy-related materials and catalysis to be the main contributors. To be mentioned finally is the PhD thesis defense of MSPD-ICMAB and CLAEISS-UAB students which were financed through DOC FAM, a H2020-MSCA-COFUND project.

Instrumental maintenance, development and upgrade was pursued despite limited resources, essentially focused on new beamlines construction. It should be mentioned however the automatization of pressure control and continuous monochromator scan on CIRCE-NAPP, monochromator crystals cleaning on CLAEISS, purchase of new slits on NCD-SWEET and a humidity control device on MSPD.

Finally, the most intense scientific activity of the section peaked in September with the Chemistry and Material Section review. During one and a half days, the up to now and future scientific activity of the section was reviewed by a panel of external experts. This review was conducted within the context of preparing to ALBA II upgrade and contributed in fruitful exchange of the scientific staff of the section. Beside this review, workshops on Catalysis, High-Pressure and Ambient Pressure X-ray Photoelectron spectroscopy, as well as Colloquium on various scientific fields covered in the section were organized by the section staff.

# Scientists discover a new extra-large pore zeolite with promising applications in the chemical industry

The new zeolite, named ZEO-1, shows a three-dimensional system of interconnected extra-large pores (around 10 Å), the highest observed in stable zeolites after 80 years of research. It could work as a catalyst in fine chemistry for the production of pharmaceutical intermediates, in controlled substance release, for pollution abatement or as a support for the encapsulation of photo- or electroactive species. Experiments at the MSPD beamline of the ALBA Synchrotron were key to determine the accurate structure of ZEO-1.

An international research team, led in Spain by CSIC scientist Miguel A. Camblor, has discovered a stable aluminosilicate zeolite with a three dimensional system of interconnected extra-large pores, named ZEO-1.

Zeolites are crystalline porous materials with important industrial applications, including uses in catalytic processes. The pore apertures limit the access of molecules into and out of the inner confined space of zeolites, where reactions occur. The research, published in *Science*, proved that ZEO-1 possesses these “extra-large” pores of around 10 Å (1 angstrom equals one ten billionth of a meter), but also smaller pores of around 7Å, which is actually the size of traditional “large” pores.

Because of its porosity, strong acidity and high stability, ZEO-1 may find applications as a catalyst in fine chemistry for the production of pharmaceutical intermediates, in controlled substance release, for pollution abatement or as a support for the encapsulation of photo- or electroactive species (they react to light or an electric field).

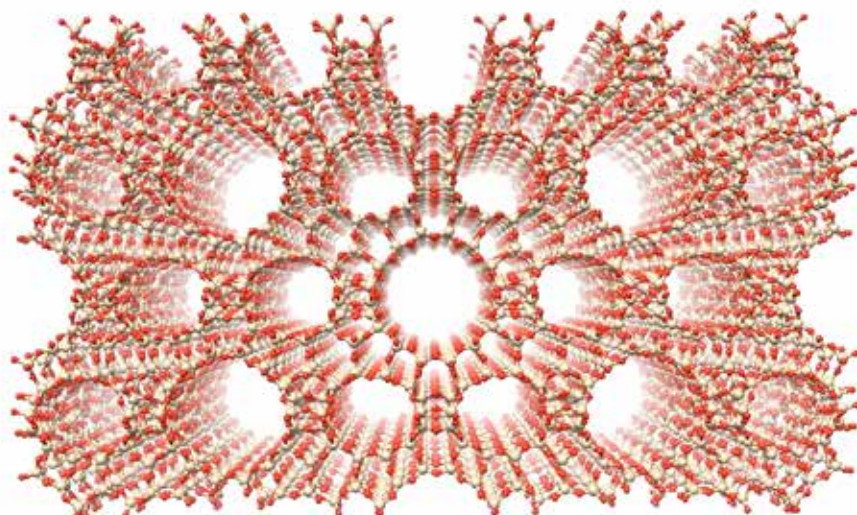
“The crossings of its cages delimit super boxes, open spaces that can be considered nanoreactors to carry out chemical reactions in their confined space”, explains Miguel A. Camblor, researcher at the Instituto de Ciencia de Materiales de Madrid - CSIC.

To prove that this new zeolite may be useful in applications involving bigger molecules, researchers measured the adsorption to the inner surface of the zeolite of the dye Nile red - a big molecule. Moreover, they tested its performance in fluid catalytic cracking of heavy oil, a process the world still relies on to produce fuels. In both processes, the new zeolite performed better than the conventional large pore zeolite used nowadays. The zeolite was discovered following a high-throughput screening methodology. The structure solution was challenging because the zeolite has a very complex structure, with a small crystal size (<200nm) but an exceedingly large cell volume.

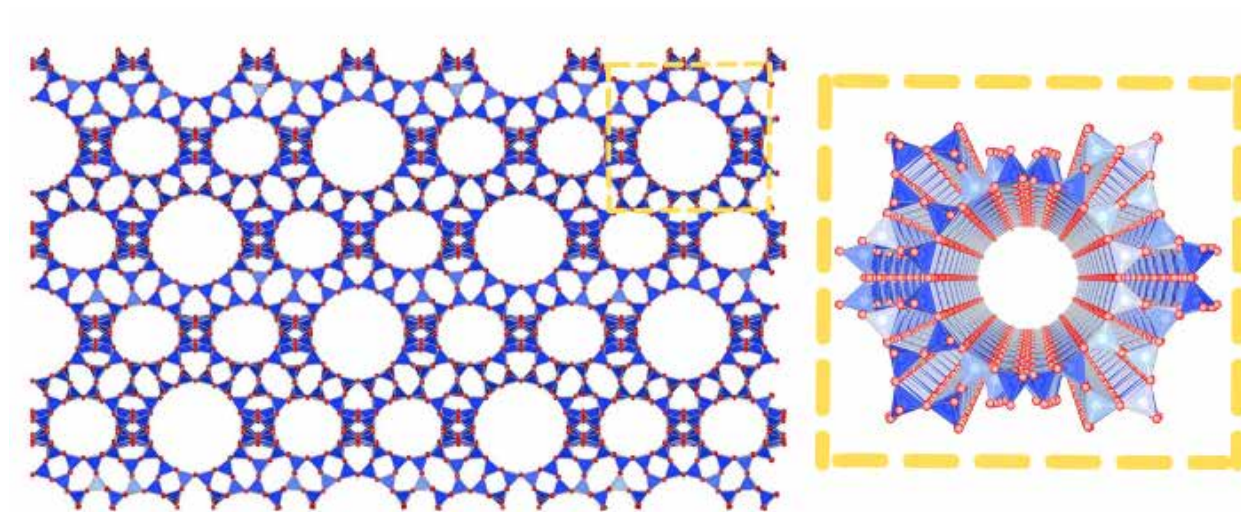
“The combination of electron diffraction data with synchrotron powder X-ray diffraction data collected at the MSPD beamline of the ALBA Synchrotron and the Argonne National Laboratory (USA) made possible the accurate structure determination of ZEO-1”, says Camblor.

“The extremely good instrumental resolution offered by the Multi Analyzer Detection setup of the MSPD diffractometer allows resolving high density Bragg peaks. This instrumental condition is necessary for accurately determining big unit cell parameters as exhibited by ZEO-1 and to precisely localize the atoms in the unit cell”, adds François Fauth, scientist in charge of the MSPD beamline at ALBA.





**Figure 11:** Video of ZEO-1



**Figure 12:** Left: ZEO-1 possesses a 3D system of extra-large pores plus a 3D system of large pores, all of them interconnected. In this figure, the structure is viewed along (100). The large circular pores are opened through rings of 16 tetrahedra (around 10 Å, the new “extra-large” pores), while the smaller, ovoid pores are made of 12 tetrahedra (around 7x6 Å, the traditional “large” pores). Right: A perspective view of the extra-large pore of ZEO-1 along (100).

This research is the result of an international collaboration between eight research centers in China, the USA, Sweden and Spain. The team was led by Fei-Jian Chen (Bengbu Medical College, China), Xiaobo Chen (China University of Petroleum), Jian Li (Stockholm University) and Miguel A. Cambor (Instituto de Ciencia de Materiales de Madrid, CSIC).

**REFERENCE:** Qing-Fang Lin, Zihao Rei Gao, Cong Lin, Siyao Zhang, Junfeng Chen, Zhiqiang, Xiaolong Liu, Wei Fan, Jian Li, Xiaobo Chen, Miguel A. Cambor, Fei-Jian Chen. *Science* (2021). DOI: [www.science.org/doi/10.1126/science.abk3258](https://www.science.org/doi/10.1126/science.abk3258)

# Electronic and Magnetic Structure of Matter

Manuel Valvidares, Head of the Electronic and Magnetic Structure of Matter Section (Experiments Division)

The year 2021 was marked by an overall normalization of activities after the impact of the Covid restrictions. The beamlines and instruments at the Electronic and Magnetic Structure Matter Section hosted planned user experiments with full-team visits. Interestingly, the developed protocols for remote experiments have enabled a hybrid format that remains of interest for many user groups, on which a team member follows or operates remotely part of the time some of the instruments (i.e. BOREAS XMCD and XRMS end-stations).

Productivity was again very good this year: 12 publications at CIRCE PEEM branch (recall 50% of the full beamline operation), 26 publications at BOREAS, plus other 2 publication on magnetism at MISTRAL for a total of 40 publications, of which almost half (17) of very high quality at high impact peer-review journals (Science, Nature Nanotechnology or ACS nano).

Year 2021 was also special for becoming the time for the conception of our future facility, ALBA II. To this respect, the section was deeply involved in several activities in close interaction with our user community. As mentioned in previous pages, the section organised ALBA II Workshops on spintronics, 2D materials and coherence and time-resolved soft X-ray science. The series of on-line workshops counted with renamed national and international speakers, included beamline overviews and an open discussion round table to collect the voice and need of the target community. These were completed with other activities on new techniques and opportunities for upgrades for core instruments of the section, such as a X-PEEM workshop (discussing among others new detectors, Aberration Corrected instruments), a colloquia

on XMCD at ultra-low temperatures for XMCD experiments, or the direct imaging of orbitals in quantum materials using Inelastic Scattering. The section staff was also active in preparing together with the user community proposals to the 2021 open call for new beamlines at ALBA. Furthermore, in October a transversal review of the section was conducted, in which the performance of the instruments operation, their present status and future strategy and upgrade was examined by a panel of external national and international experts.

Besides all those activities, relevant improvements of the sample environments and instruments were accomplished along this year. At the PEEM, a novel high frequency stage was implemented, enabling experiments with excitations above 3 GHz; also, improvements of sample holders (advanced protocols) allowing a vectorial control of the in-plane applied magnetic fields. In MISTRAL, several functionalities were added to the sample environments for magnetic experiments: PCB-based sample holders for the application of ns current pulses, and a setup based on permanent magnets for in-situ application of magnetic fields ( $\leq 100$  mT) in different directions without breaking the TXM vacuum. In BOREAS, a large radial distribution chamber (RDC) was installed, allowing fast and secure automatized UHV sample transfer between the ancillary surface science chambers (STM, MBE), vacuum suitcases and the XMCD and XRMS end-stations; furthermore, a full-size Argon atmosphere glove box has been installed, that permanently attached to the RDC enables a broad range of trouble-free experiments on air sensitive samples such as 2D vdW materials or spin crossover molecules.

# 180° magnetic switching using a solid-state hydrogen pump

Manipulating magnetism by electrical means is central to spin-based data storage and manipulation. Achieving voltage driven 180° magnetic switching is desirable for spintronic device applications because of the potential low power consumption. A study lead by researchers from Massachusetts Institute of Technology (US) with collaborators from University of Minnesota (US), Chemnitz University of Technology (DE), Korea Institute of Science and Technology (KR) and the ALBA Synchrotron demonstrates 180° magnetization reversal in the absence of external magnetic fields by voltage induced hydrogen loading into ferrimagnets in an all-solid-state structure. The reversal is realized by changing the relative magnitude of sublattice magnetizations through hydrogen loading into a rare earth-transition metal ferrimagnet, which was revealed using XMCD measurements at the BOREAS beamline in the ALBA Synchrotron.

The rapid increase of data generated nowadays requires denser data storage and more efficient data processing. Controlling the magnetic state of a material by electrical means enables spin-based data storage and data manipulation. One key technological challenge is to achieve 180° magnetic switching efficiently by electrical means, which has the potential to dramatically reduce the global power consumption of data storage.

Ferrimagnets present unique opportunities for achieving 180° switching because of a multi-sublattice configuration with sublattice magnetizations of different magnitudes opposing each other. In the study, researchers showed that the dominant sublattice of GdCo ferrimagnetic film can be reversibly toggled by hydrogen loading/unloading using a solid-state hydrogen pump structure as shown in Figure 13, where a proton-conducting solid-state electrolyte is placed between two electrodes. By applying a gate voltage across the structure, the moisture from the ambient can be dissociated at the top electrode to form protons and oxygen gas. The protons are driven to the bottom electrode and get loaded into the bottom electrode (GdCo). Figure 1 shows that the hydrogen loading switched the dominant sublattice at room temperature, and the hydrogen loading induced a > 100K drop in the compensation temperature of GdCo.

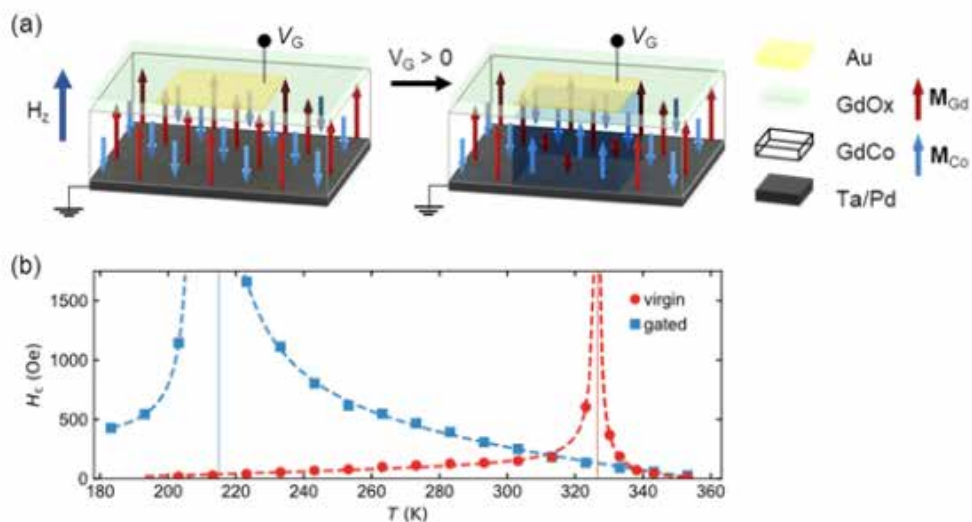
Voltage control of the dominant sublattice and compensation of GdCo. (top) Schematic illustration

of the device structure. (bottom) Coercivity of GdCo versus temperature before and after gate voltage application. The temperature where coercivity diverges corresponds to the compensation temperature, which is reduced by > 100K after applying a gate voltage.

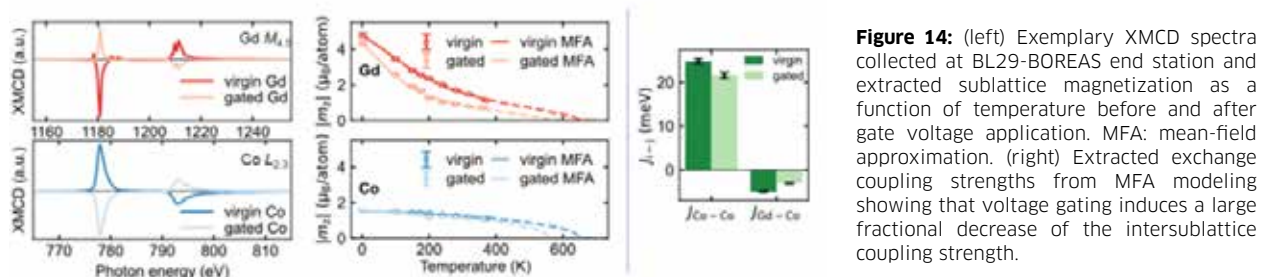
To study the mechanism of the observed compensation temperature change induced by voltage gating, element-specific XMCD spectroscopy was carried out at the BOREAS beamline for devices before and after voltage-induced hydrogen loading into GdCo. As shown in Figure 14, high-quality XMCD spectra were collected for both the Gd and Co elements. Measurements were carried out at different temperatures and the sublattice magnetizations were calculated using the sum rules. The results reveal that hydrogenation substantially reduces the sublattice magnetization of Gd, but only modestly reduces that of Co at finite temperatures. Using mean-field approximation modeling, the study further shows that the effect of the hydrogen loading into GdCo involves a reduction of the strength of the antiferromagnetic coupling between the Gd and Co sublattices.

Using appropriately-designed heterostructures, the study demonstrated gate voltage induced external-field-free deterministic 180° reversal of either the sublattice magnetizations or the net magnetization. Figure 15 shows the 180° switching of sublattice magnetizations, where the integration of a hard nanomagnet into the device provides a





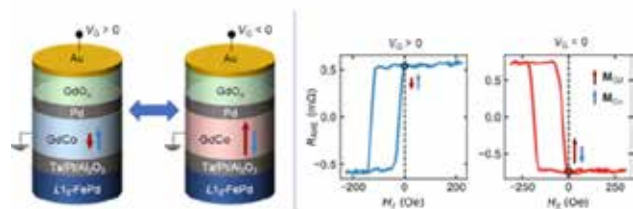
**Figure 13:** Voltage control of the dominant sublattice and compensation of GdCo. (top) Schematic illustration of the device structure. (bottom) Coercivity of GdCo versus temperature before and after gate voltage application. The temperature where coercivity diverges corresponds to the compensation temperature, which is reduced by > 100K after applying a gate voltage.



**Figure 14:** (left) Exemplary XMCD spectra collected at BL29-BOREAS end station and extracted sublattice magnetization as a function of temperature before and after gate voltage application. MFA: mean-field approximation. (right) Extracted exchange coupling strengths from MFA modeling showing that voltage gating induces a large fractional decrease of the intersublattice coupling strength.

bias stray field that is enough to fix the direction of the net magnetization, so that the sublattice magnetizations are flipped by  $180^\circ$  when the dominance sublattice is switched.

In addition to  $180^\circ$  magnetic reversals, the study also covered the switching speed ( $< 50\mu\text{s}$ ), and cyclability ( $> 10,000$  cycles without degradation) of the mechanism. In addition, because the gating effect is localized under the gate region, it also allows for the generation of spin textures such as reversed domains and skyrmion bubbles on a racetrack device. The mechanism may also apply to a wide range of rare-earth transition-metal ferrimagnets for tuning a wide range of properties



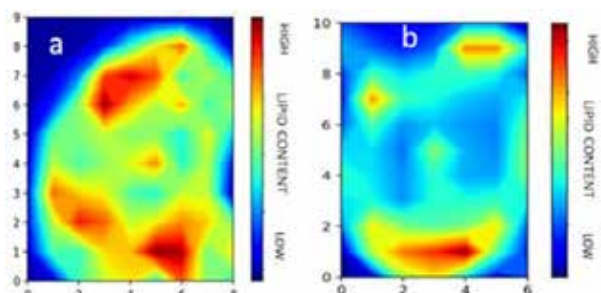
**Figure 15:** (left) Device structure for external-field-free  $180^\circ$  switching of the sublattice magnetizations. (right) Anomalous Hall effect hysteresis loops of GdCo showing switched sublattice magnetizations with voltage gating.

and phenomena such as spin dynamics and spin texture characteristics and may find application in data storage and neuromorphic computing.

**REFERENCE:** Mantao Huang, Muhammad Usama Hasan, Konstantin Klyukin, Delin Zhang, Deyuan Lyu, Pierluigi Gargiani, Manuel Valvidares, Sara Sheffels, Alexandra Churikova, Felix Büttner, Jonas Zehner, Lucas Caretta, Ki-Young Lee, Joonyeon Chang, Jian-Ping Wang, Karin Leistner, Bilge Yildiz and Geoffrey S. D. Beach. Voltage control of ferrimagnetic order and voltage-assisted writing of ferrimagnetic spin textures. Nature Nanotechnology (2021). DOI: <https://doi.org/10.1038/s41565-021-00940-1>

# SUMMARY OF SELECTED HIGHLIGHTS

## LIFE SCIENCES AND SOFT CONDENSED MATTER



Clara Barba, Marc Adrià Oliver, Meritxell Martí, Martin Kreuzer, Luisa Coderch. *Skin Research and Technology* 2021. DOI:10.1111/srt.13093

### BL01-MIRAS

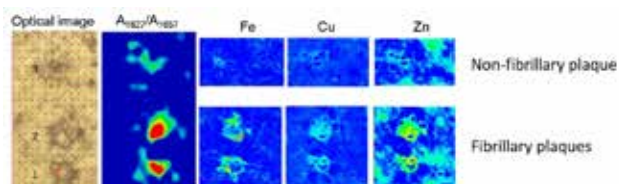
#### THE DIFFERENCES BETWEEN AFRICAN, CAUCASIAN AND ASIAN HAIR ARE DETERMINED BY THEIR LIPID DISTRIBUTION

Researchers of IQAC-CSIC, in collaboration with the ALBA Synchrotron, demonstrated that African hair has more lipids that are highly disordered. This distinction with Caucasian and Asian hair might be relevant to develop new ethnic hair-care products.

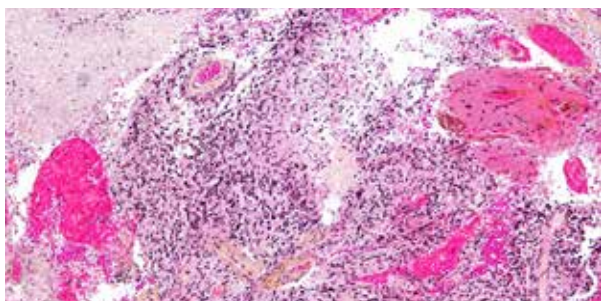
### BL01-MIRAS

#### CHARACTERISING AMYLOID PLAQUES IN ALZHEIMER'S DISEASE

Researchers from the UAB and IDIBELL analysed Alzheimer's disease brain samples at the ESRF and ALBA to characterise two types of amyloid plaques with differences in metal ion composition and in their levels of oxidised lipids. The results could lead to new insights into the development of the pathology.



E. Álvarez-Marimón, H. Castillo-Michel, J. Reyes-Herrera, J. Seira, E. Aso, M. Carmona, I. Ferrer, J. Cladera, N. Benseny-Cases. *ACS Chem. Neurosci.* (2021). DOI: 10.1021/acscchemneuro.1c00048.



### BL01-MIRAS

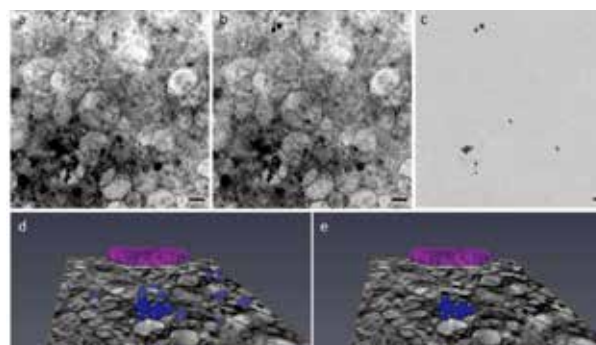
#### POTENTIAL BIOMARKERS FOR THE MOST AGGRESSIVE TYPE OF BRAIN CANCER CELLS

An experiment led by Tanja Ducic, scientist at the MIRAS beamline of ALBA, is analyzing live cells with synchrotron-based Fourier Transformed Infrared (FTIR) spectroscopy to identify crucial potential biomarkers in order to target them and to help develop new therapeutic strategies.

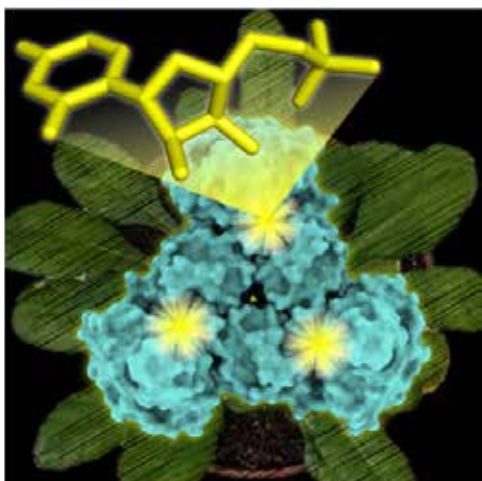
### BL09-MISTRAL

#### RESEARCHERS DISCOVER THE ORIGIN OF CALCIUM IN HUMAN BONES

A study from several Italian institutions and the ALBA Synchrotron suggest crystalline calcium carbonate as a precursor of hydroxyapatite in the process of bone formation. Since hydroxyapatite is a mineral constituting 70% of the mass of bone, these findings may have potential applications in the development of new therapeutic approaches in bone cancer. Thanks to the MISTRAL beamline at ALBA, researchers were able to create a 3D tomogram of human cells and visualize calcium depositions inside them.



Andrea Sorrentino, Emil Malucelli, Francesca Rossi, Concettina Cappadone, Giovanna Farruggia, Claudia Moscheni, Ana J. Perez-Berna, Jose Javier Conesa, Chiara Colletti, Norberto Roveri, Eva Pereiro and Stefano Iotti. *Int. J. Mol. Sci.* (2021). DOI: 10.3390/ijms22094939



Leo Bellin, Francisco Del Caño-Ochoa, Adrián Velázquez-Campoy, Torsten Möhlmann and Santiago Ramón-Maiques. *Nat Commun* (2021). DOI: 10.1038/s41467-021-21165-9

### BL13-XALOC

#### THE FIRST STRUCTURE OF AN ATC PROTEIN FROM PLANTS REVEALS ITS MECHANISM OF INHIBITION

A research team from the Biomedicine Institute of Valencia (IBV-CSIC) and from the CIBER of Rare Diseases (CIBERER), in collaboration with the Universität Kaiserslautern in Germany, has studied the ATC protein, an essential enzyme for the biosynthesis of pyrimidines, the building blocks of the genetic material. The structural determination was carried out at the ESRF synchrotron and at the XALOC beamline of ALBA. The structural data, combined with other analysis, has allowed researchers to describe the functioning mechanism of the enzyme, opening the venue for new strategies to design herbicides and antitumoral compounds.

### BL13-XALOC

#### IDENTIFIED A DRUG TARGET THAT COULD INHIBIT THE TRANSPORT OF VIRUSES IN CELLS

A CSIC project reveals a new pharmacological site of the protein that is part of the roads that carry viruses and spread them in infected cells. The XALOC beamline of the ALBA Synchrotron contributed in determining the structure of this protein. Its discovery, thanks to the use of a new natural compound from cyanobacteria, opens the door to new drugs against viral infections or cancer.



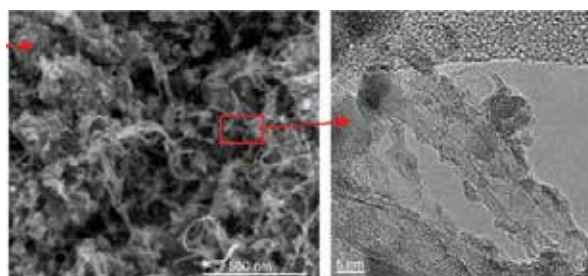
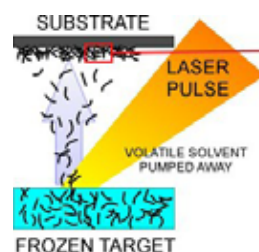
Susan Matthew, Qi-Yin Chen, Ranjala Ratnayake, Charles S Fermaintt, Daniel Lucena-Agell, Francesca Bonato, Andrea E Prota, Seok Ting Lim, Xiaomeng Wnag, J. Fernando Díaz, April L Risinger, Valerie J. Paul, María A. Oliva and Hendrik Luesch. *PNAS* (2021) DOI: 10.1073/pnas.2021847118.

## CHEMISTRY AND MATERIALS SCIENCE

### BL01-MIRAS

#### NEW APPROACH IN LASER FABRICATED ELECTRODES FOR SUPERCAPACITIVE ENERGY STORAGE

Researchers have used, for the first time, a combination of cerium oxide nanoparticles and manganese metal organic precursor in the laser targets for the synthesis of a hybrid material. The used laser deposition technique allowed the versatile fabrication of high-performance supercapacitor electrodes. Supercapacitors are important for their fast and reversible use of energy, high power density, long cycle life, low maintenance cost, and environment-friendly nature. Measurements at MIRAS allowed the identification of the organic part of the composite, especially the chemical groups present at the structure of graphene and carbon nanotubes, which highly influence the functional properties of the material.



Pablo García Lebière, Ángel Pérez del Pino, Guillem Domènech Domingo, Constantin Logofatu, Immaculada Martínez-Rovira, Ibraheem Yousef and Enikő György. *J. Mater. Chem. A* (2021), DOI: 10.1039/DOA06756C

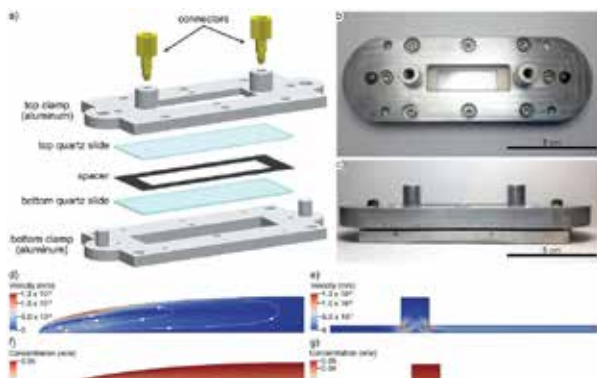
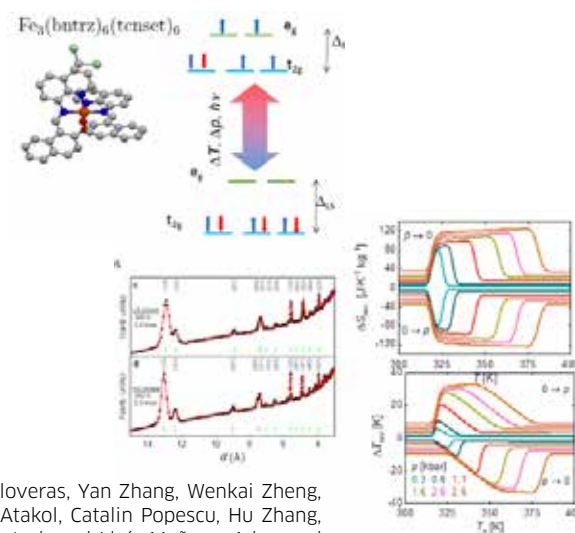


## BL04-MSPD

### NEW MATERIAL WITH REVERSIBLE PRESSURE-INDUCED COOLING EFFECT PROPERTIES

A research studied the barocaloric properties of  $\text{Fe}_3(\text{bntz})_6(\text{tcnset})_6$ , a molecular material that contains a metal complex that undergoes an abrupt spin-state switching close to room temperature. This kind of materials, with giant calorific effect, are the best candidates to develop new efficient and environmentally friendly refrigerators that must replace current devices, which feature low efficiency and use hazardous fluids.

Michela Romanini, YiXu Wang, Kübra Gürpınar, Gladys Ornelas, Pol Lloveras, Yan Zhang, Wenkai Zheng, Maria Barrio, Araceli Aznar, Adrià Gràcia-Condal, Baris Emre, Orhan Atakol, Catalin Popescu, Hu Zhang, Yi Long, Luis Balicas, Josep Lluís Tamarit, Antoni Planes, Michael Shatruk and Lluís Mañosa. *Advanced Materials* (2021). DOI: 10.1002/adma.202008076



Noemí Contreras-Pereda, David Rodríguez-San-Miguel, Carlos Franco, Semih Sevim, João Pedro Vale, Eduardo Solano, Wye-Khay Fong, Alessandra Del Giudice, Luciano Galantini, Raphael Pfattner, Salvador Pané, Tiago Sotto Mayor, Daniel Ruiz-Molina, Josep Puigmartí-Luis. *Adv. Materials* (2021). DOI: 10.1002/adma.202170231

## BL11-NCD-SWEET

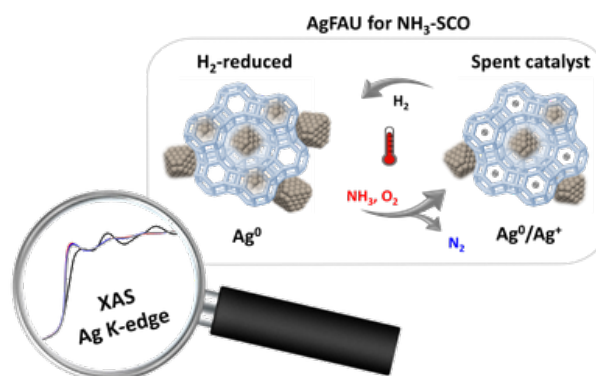
### SPACE LABORATORIES CONDITIONS SIMULATED ON EARTH TO EXPERIMENT WITH MATERIALS

A team of researchers demonstrated that 2D porous crystalline molecular frameworks can be grown with excellent control over their morphology and homogeneity by using a custom-made microfluidic device. This approach recreates on Earth the microgravity environment of laboratories on the International Space Stations. Measurements at the NCD-SWEET beamline allowed studying crystallinity, structure and orientation of the created 2D material.

## BL22-CLAESS

### SILVER NANOPARTICLES FOR THE ELIMINATION OF AMMONIA RELEASED TO THE ATMOSPHERE

Researchers from the ITQ-UPV-CSIC, in collaboration with ALBA, have explored the use of silver nanoparticles as catalysts for the selective catalytic oxidation of ammonia, one of the main atmospheric pollutants. Thanks to the CLÆSS beamline at ALBA, researchers proved that the active catalyst for the reaction of ammonia to nitrogen and water is metallic silver, instead of silver cations. These findings will contribute to developing new methods for the elimination of ammonia released to the atmosphere in industry and in diesel vehicles.

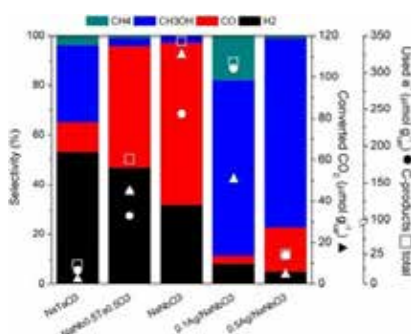


Joaquín Martínez-Ortigosa, Christian W. Lopes, Giovanni Agostini, A. Eduardo Palomares, Teresa Blasco and Fernando Rey. *Microporous and Mesoporous Materials* (2021). DOI: 10.1016/j.micromeso.2021.111230

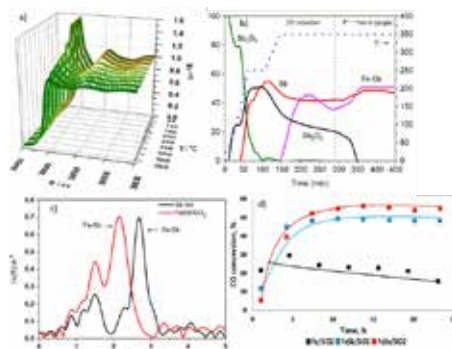
## BL22-CLAESS

### STUDY OF IRON CATALYSTS PROMOTION FOR FISCHER-TROPSCH SYNTHESIS OPTIMIZATION

Researchers have developed a new procedure for light olefins synthesis using Fischer-Tropsch reaction. They added tin and antimony to the iron catalysts, to increase their activity. This process, called promotion, resulted in a major increase in the reaction rate. Fischer-Tropsch synthesis provides an important opportunity for utilization of biomass and plastic waste for fuels and chemicals production. The studies performed in this work enable a clear understanding of the catalytic phenomena and open perspectives for the catalyst improvements.



Fresno, F., Galdón, S., Barawi, M., Alfonso-González, E., Escudero, C., Pérez-Dieste, V., Huck-Iriarte, C., de la Peña O'Shea, V.A., Catalysis Today (2021) DOI: 10.1016/j.cattod.2020.01.013



Deizi V. Peron a, Alan J. Barrios, Alan Taschin, Iulian Dugulan, Carlo Marini, Giulio Gorni, Simona Moldovan, Siddardha Koneti, Robert Wojcieszak, Joris W. Thybaut, Mirella Virginie, Andrei Y. Khodakov. Applied Catalysis B: Environmental (2021). DOI: 10.1016/j.apcatb.2021.120141

## BL24-CIRCE-NAPP

### TOWARDS PRODUCT CONTROL IN ARTIFICIAL PHOTOSYNTHESIS

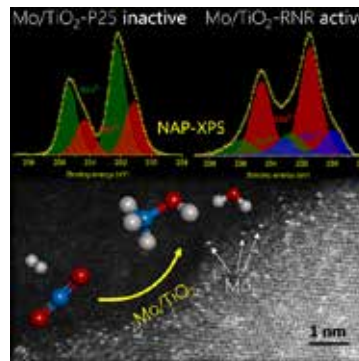
Researchers from the IMDEA Energy Institute in Madrid have used the CIRCE-NAPP beamline of ALBA to study the artificial photosynthesis process, that is, the chemical reaction that plants and other photosynthetic organisms use to transform the Sun's energy into chemical energy. The goal of their research is to selectively control the products of the chemical reaction to obtain those that have industrial and energetic interest.

## BL24-CIRCE-NAPP

### RESEARCHERS HAVE DISCOVERED A NEW CATALYST FOR THE CONVERSION OF CARBON DIOXIDE TO METHANOL

They proved that a system based on molybdenum-on-titania does efficiently catalyze this reaction and represents a promising alternative to current industrial catalysts. This helps eliminating carbon dioxide and producing methanol, which can serve as a "green fuel" or as building blocks for the production of plastics, pharmaceuticals, textiles, etc.

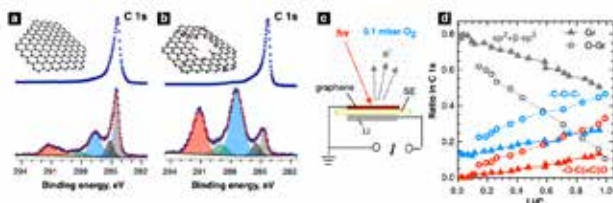
Thomas Len, Mounib Bahri, Ovidiu Ersen, Yaya Lefkir, Luis Cardenas, Ignacio J. Villar-Garcia, Virginia Pérez Dieste, Jordi Llorca, Noémie Perret, Ruben Checa, Eric Puzenat, Pavel Afanasiev, Franck Morfina and Laurent Piccolo. Green Chem. (2021). DOI: 10.1039/d1gc01761f



## BL24-CIRCE-NAPP

### NEW INSIGHTS ABOUT THE CATALYTIC ROLE OF OXYGEN-CONTAINING GROUPS ON CARBON ELECTRODES

For the first time, it has been demonstrated that oxygen functionalities (epoxy, carbonyl, and lactone) on the carbon electrode surface do not affect the kinetics of one-electron oxygen reduction in aprotic media, but enhance both the rate of electrochemical lithium peroxide ( $\text{Li}_2\text{O}_2$ ) formation and carbon degradation in  $\text{Li}^+$ -containing electrolytes. The research has included analysis using synchrotron light at Elettra and ALBA facilities.



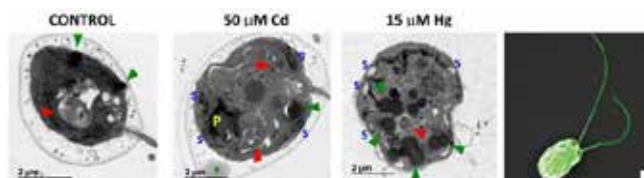
Alina I. Inozemtseva, Elmar Yu. Kataev, Alexander S. Frolov, Matteo Amati, Luca Gregoratti, Klara Beranova, Virginia Perez Dieste, Carlos Escudero, Alexander Fedorov, Artem V. Tarasov, Dmitry Yu. Usachov, Denis V. Vyalykh, Yang Shao-Horn, Daniil M. Itkis, Lada V. Yashina. Carbon (2021) DOI: 10.1016/j.carbon.2020.12.008

# ENVIRONMENT AND ENERGY-RELATED MATERIALS

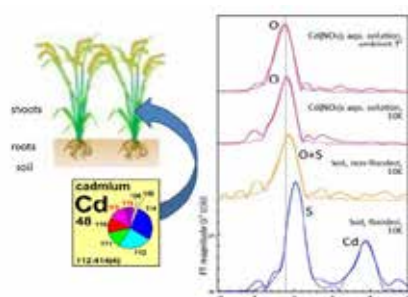
## BL01-MIRAS

### METAL POLLUTANTS CAUSE METABOLIC ALTERATIONS IN ALGAE

Cadmium and mercury are toxic metals that accumulate in the environment and represent a threat to photosynthetic organisms of polluted ecosystems. A research team from the UAM has studied the effects of these harmful metals in the microalga *Chlamydomonas reinhardtii*, a soil-isolated unicellular photosynthetic microorganism. Researchers have identified multiple metabolic alterations in the main types of biomolecules (carbohydrates, proteins and lipids) of the microalga caused by cadmium and mercury. These insights help to optimize approaches for metal decontamination.



Ángel Barón-Sola, Margarita Toledo-Basantes, María Arana-Gandía, Flor Martínez, Cristina Ortega-Villasante, Tanja Dučić, Ibraheem Yousef, Luis E. Hernández. *Journal of Hazardous Materials* (2021). DOI: 10.1016/j.jhazmat.2021.126502.



Matthias Wiggerhauser, Anne-Marie Aucour, Sarah Bureau, Sylvain Campillo, Philippe Telouk, Marco Romani, Jian Feng Ma, Gautier Landrot, Géraldine Sarret. *Environmental Pollution* (2021). DOI: 10.1016/j.envpol.2020.115934

## BL22-CLAESS

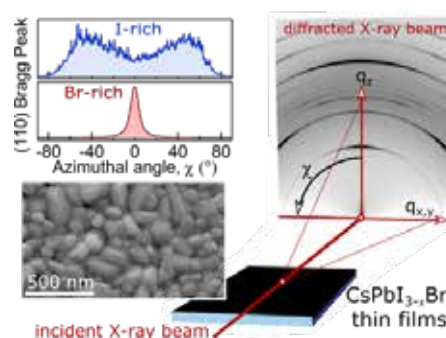
### CADMIUM CONTAMINATION IN RICE CROPS: NEW INSIGHTS ON THE MOBILITY PROCESSES OF THIS POLLUTANT

Cadmium is a heavy metal considered one of the most toxic elements to which humans can be exposed. The present study identified the processes that control the mobility of cadmium in soil-rice system, by means of isotope and X-rays absorption spectroscopy speciation analyses performed at Soleil and ALBA synchrotrons, at the CLAESS beamline.

## BL11-NCD-SWEET

### CONTROL OF TEXTURE FORMATION IN PEROVSKITE-BASED MATERIALS FOR MORE EFFICIENT SOLAR CELLS

A team of scientists shown that Bromine (Br) incorporation in polycrystalline cesium lead triiodide ( $\text{CsPbI}_3$ ) thin films, with composition  $\text{CsPbI}_{3-x}\text{Br}_x$ , modifies the crystal structure by changing the symmetry of the lattice. This change, in turn, governs the formation of the different, energetically favored textures within the thin film. Controlling grain orientations within polycrystalline all-inorganic halide perovskite solar cells can help increase conversion efficiencies, which would represent great progress in the field of renewable energies.



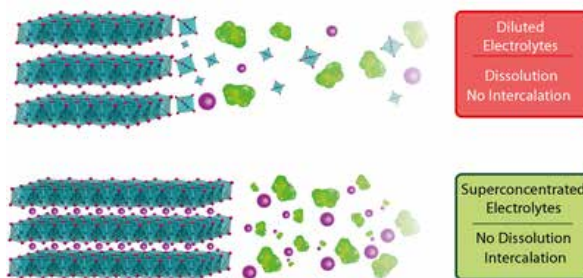
Julian A. Steele, Eduardo Solano, Handong Jin, Vittal Prakasam, Tom Braeckvelt, Haifeng Yuan, Zhenni Lin, René de Kloe, Qiong Wang, Sven M. J. Rogge, Veronique Van Speybroeck, Dmitry Chernyshov, Johan Hofkens, and Maarten B. J. Roeffaers. *Adv. Mater.* (2021). DOI: 10.1002/adma.202007224



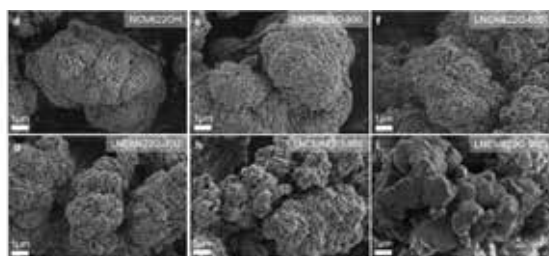
## BL04-MSPD

### NOVEL CLASS OF MATERIALS FOR LI-ION BATTERIES ELECTRODES

A work demonstrated that a novel class of materials, namely transition metal halides, can be employed as Li-ion batteries electrodes by using superconcentrated electrolytes instead of regular diluted electrolytes in which they dissolve. The study was led by the Collège de France and used the MSPD beamline of ALBA to monitor the evolution of the metal halides structures upon cycling in a battery, which was crucial for the study.



Dubouis, N., Marchandier, T., Rousse, G. et al. Nat. Mater. (2021). DOI: 10.1038/s41563-021-01060-w



Suning Wang, Weibo Hua, Alexander Missyul, Mariyam Susana Dewi Darma, Akhil Tayal, Sylvio Indris, Helmut Ehrenberg, Laijun Liu, and Michael Knapp. Adv. Funct. Mater. (2021). DOI: 10.1002/adfm.202009949

## BL04-MSPD

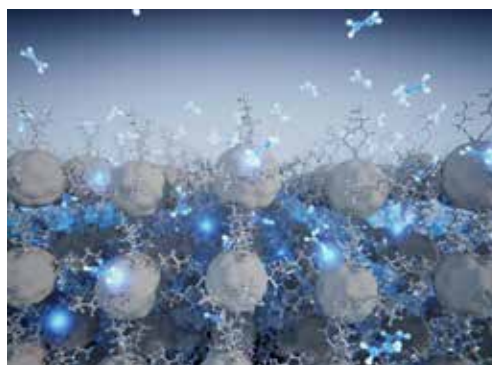
### A STEP FORWARD IN THE OPTIMIZATION OF CATHODE MATERIALS FOR BETTER LI-ION BATTERIES

Researchers showed the synthesis optimization of NCM622 cathode material for Lithium-ion batteries, achieving both lower energy capacity cost and high cyclability. The results can be directly applied to production of better Li-ion batteries for modern electronics. Reaction was investigated using in situ X-Ray Diffraction technique at the MSPD beamline.

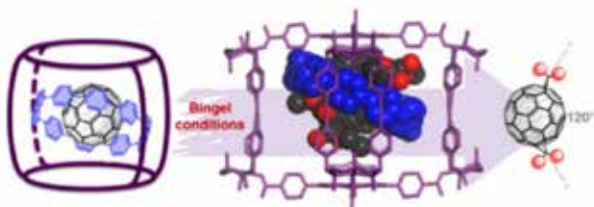
## BL13-XALOC

### PLAYING WITH THE WEAKEST SUPRAMOLECULAR INTERACTIONS IN A FULLERENE COMPOUND

Researchers at IMDEA Nanociencia controlled the weakest van der Waals forces in a fullerene C60 compound by applying an external stimulus. The study represents a landmark achievement in the field of Supramolecular Chemistry, where weak forces can play a crucial role in chemical reactions. This strategy has allowed for the first time to selectively and in a controlled manner hydrogenate the C60 and may have relevant implications for hydrogen storage.



E. Fernandez-Bartolomé, A. Gamonal et al. Chem. Sci. (2021). DOI: 10.1039/D1SC00981H



Ernest Ubasart, Oleg Borodin, Carles Fuertes-Espinosa, Youzhi Xu, Cristina García-Simón, Laura Gómez, Judith Juanhuix, Felipe Gándara, Inhar Imaz, Daniel Maspocho, Max von Delius and Xavi Ribas; Nature Chemistry (2021). DOI: 10.1038/s41557-021-00658-6

## BL13-XALOC

### INNOVATIVE METHODOLOGY FOR SYNTHESIZING FULLERENES

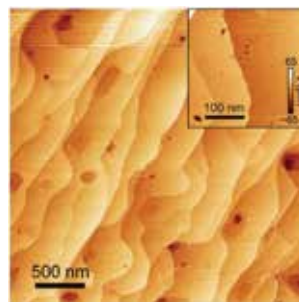
A Catalan-German collaboration has developed an innovative three-shell structure with the aim of improving future organic solar cells. XALOC beamline of the ALBA Synchrotron offered structural insights of this new system.

# ELECTRONIC AND MAGNETIC STRUCTURE OF MATTER

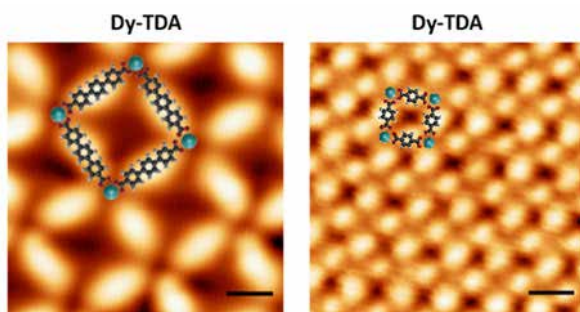
## BL29-BOREAS

### DISCOVERY OF NOVEL CLASS OF 2D MAGNETS: 2D-XY FERROMAGNETISM IN MONOLAYER CrCl<sub>3</sub>

Scientists from the Max Planck Institute for Microstructure Physics, the ALBA Synchrotron and the Helmholtz-Zentrum Berlin have succeeded in creating a two-dimensional ferromagnetic material for the first time exhibiting an easy-plane magnetic anisotropy, i.e. an “XY class” of 2D ferromagnet. This is of fundamental relevance and was elusive so far, without discarding potential application in energy efficient information technologies.



Amilcar Bedoya-Pinto, Jing-Rong Ji, Avanindra Pandeya, Pierluigi Gargiani, Manuel Valvidares, Paolo Sessi, James Taylor, Florin Radu, Kai Chang and Stuart S.P. Parkin. *Science* (2021). DOI: 10.1126/science.abd5146



S. O. Parreiras, D. Moreno, B. Cirera, M. A. Valbuena, J. I. Urgel, M. Paradinas, M. Panighel, F. Ajejas, M. A. Niño, J. M. Gallego, M. Valvidares, P. Gargiani, W. Kuch, J. I. Martínez, A. Mugarza, J. Camarero, R. Miranda, P. Perna, and D. Écija Small (2021). DOI: 10.1002/smll.202102753

## BL29-BOREAS

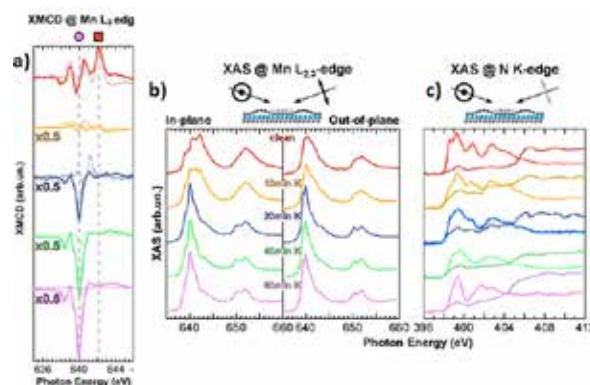
### TUNING THE MAGNETIC ANISOTROPY OF LANTHANIDES ON A METAL SUBSTRATE BY METAL-ORGANIC COORDINATION

The magnetism of lanthanide-directed nanoarchitectures on surfaces can be drastically affected by small structural changes. The study carried out in a collaboration between researchers from IMDEA Nanociencia and BOREAS beamline reports the effect of the coordination environment in the re-orientation of the magnetic easy axis of dysprosium-directed metal-organic networks on Cu(111). The authors show that the magnetic anisotropy of lanthanide elements on surfaces can be tailored by specific coordinative metal-organic protocols.

## BL29-BOREAS

### TURNING THE MOLECULAR MAGNETIC SWITCH: TUNING THE MAGNETIC COUPLING OF A MOLECULAR SPIN INTERFACE VIA ELECTRON DOPING

Researchers from the Sapienza University in Rome, in collaboration with the ALBA Synchrotron, have demonstrated a further pathway to tune the magnetic response of a metal-organic semiconductor molecule interfaced with a graphene-covered cobalt film. Organic molecules with a spin, coupled to a magnetic substrate, can be a key element in the development of future organic-spintronic applications.



Giulia Avvisati, Pierluigi Gargiani, Carlo Mariani, and Maria Grazia Betti. *Nano Letters* (2021) DOI: 10.1021/acs.nanolett.0c04256



Claudia Fernández-González, Jesús C. Guzmán-Mínguez, Alejandra Guedeja-Marrón, Eduardo García-Martín, Michael Foerster, Miguel Ángel Niño, Lucía Aballe, Adrián Quesada, Lucas Pérez and Sandra Ruiz-Gómez. *Nanomaterials* (2021). DOI: <https://doi.org/10.3390/nano11071657>

## BL24-CIRCE-PEEM

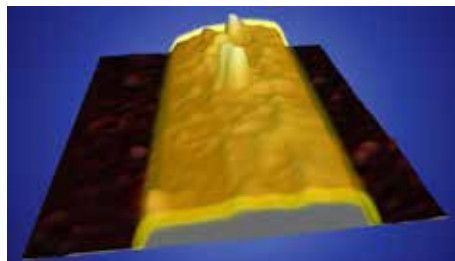
### NOVEL PROTOCOL FOR MASS PRODUCTION OF NANOWIRES

Researchers from the UCM and CSIC, in collaboration with ALBA, have established a novel synthesis protocol to produce a larger number of nanowires than conventional laboratory fabrication processes with considerably reduced production time and cost. The use of recycled aluminium and the fact that the nanowires growth process is performed at room temperature allows the nanowires to be used in industry at lower costs.

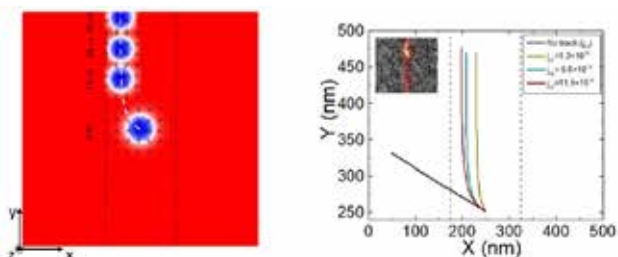
## BL24-CIRCE-PEEM

### EXOTIC ELECTRICAL PROPERTIES OF NANOTHICK ANTIMONEN ARE OBSERVED

An international collaboration, led by the UAM, has studied the electrical properties of a few layers thick sheets of antimonen, a two-dimensional material composed of antimony atoms. The results indicate an electrical transport that occurs mainly on the surface of the material. This, coupled with its stability and simple structure, make it a promising candidate for nanoelectronic and optoelectronic applications.



Ares, P., Pakdel, S., Palacio, I., Paz, WS, Rassekh, M., Rodríguez-San Miguel, D., Aballe, L., Foerster, M., Ruiz del Árbol, N., Martín -Gago, JA, Zamora, F., Gómez-Herrero, J., Palacios, JJ 2021. *Applied Materials Today* (2021) DOI: [10.1016/j.apmt.2021.101132](https://doi.org/10.1016/j.apmt.2021.101132)



Roméo Juge, Kaushik Bairagi, Kumari Gaurav Rana, Jan Vogel, Mamour Sall, Dominique Mailly, Van Tuong Pham, Qiang Zhang, Naveen Sisodia, Michael Foerster, Lucía Aballe, Mohamed Belmeguenai, Yves Roussigné, Stéphane Auffret, Liliana D. Buda-Prejbeanu, Gilles Gaudin, Dafiné Ravelosona, and Olivier Boulle *Nano Letters* (2021) DOI: [10.1021/acs.nanolett.1c00136](https://doi.org/10.1021/acs.nanolett.1c00136)

## BL24-CIRCE-PEEM

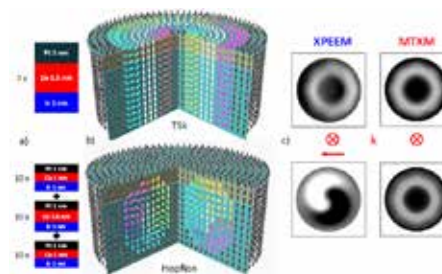
### A NEW WAY OF CONTROLLING SKYRMIONS MOTION

A group of researchers from France has been able to create and guide skyrmions in magnetic tracks. These nanoscale magnetic textures are promising information carriers with great potential in future data storage and processing devices. Experiments at the CIRCE-PEEM beamline of the ALBA Synchrotron enabled to image how skyrmions move along tracks written with helium ions.

## BL09-MISTRAL

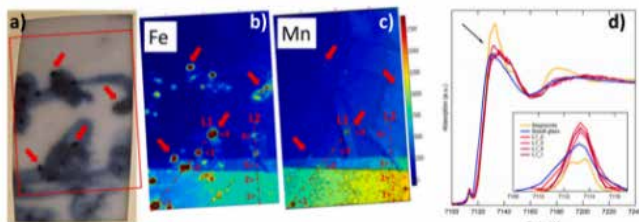
### CREATION AND OBSERVATION OF HOPFIONS IN MAGNETIC MULTILAYER SYSTEMS

The combination of magnetic images from surface sensitive PEEM and bulk sensitive transmission X-ray microscopy supported by micromagnetic simulations, provided experimental evidence of the existence of the stabilization magnetic hopfion quasiparticles in magnetic multilayers.



Kent, N., Reynolds, N., Raffrey, D. et al. *Nat Commun* (2021). <https://doi.org/10.1038/s41467-021-21846-5>





J. Roqué-Rosell, A. Pinto, Carlo Marini, Jose Prieto Burgos, Jesse Groenen, M. Campeny, Ph. Sciau. *Ceramics International* (2021). DOI: <https://doi.org/10.1016/j.ceramint.2020.09.123>

### BL22-CLAESS

#### UNRAVELLING THE HISTORY OF 15<sup>TH</sup> CENTURY CHINESE PORCELAINS WITH SYNCHROTRON LIGHT

Researchers from French and Spanish Institutions used the combination of two synchrotron light characterization techniques to study Chinese blue-and-white Ming porcelains, which are decorated under the glaze with Cobalt-based blue pigments, and produced during a one-step firing at high temperatures. They were able to identify the firing temperature by determining the porcelain's pigments and the reduction-oxidation media conditions during their production. The approach they used can also be applied on a broad range of modern and archaeological ceramics to elucidate their production technology.

### BL04-MSPD

#### SYNCHROTRON LIGHT REVEALS WHY MODERNIST STAINED GLASS DETERIORATE

Scientists from Universitat Politècnica de Catalunya have studied the materials and methods used in the production of modernist (late 19<sup>th</sup> and early 20<sup>th</sup> century) stained glass from the city of Barcelona, with special regards to the degradation mechanisms. The data obtained at MSPD beamline of ALBA was key to deciphering the structure and composition of the glazes used in the stained glass windows, as well as their state of conservation, with the aim of improving the preservation of this cultural heritage.



PhD Thesis from Martí Beltrán González "Analysis and degradation mechanisms of enamels, grisailles and silver stains on Modernist stained glass" (2021).

# INDUSTRY

Marta Ávila, Bárbara Calisto, Alejandro Sánchez, Núria Valls  
Industrial Liaison Office, [industrialoffice@cells.es](mailto:industrialoffice@cells.es)

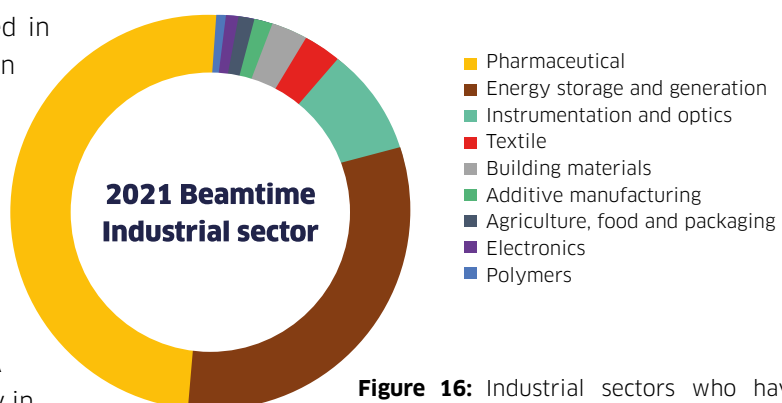
The mission of the ALBA industrial program is to promote and to make available to the industrial sector all the potential of the synchrotron services, technology transfer and developments to boost the competitiveness and innovation of the industry to benefit the society. For this, the Industrial Liaison Office (ILO) promotes the ALBA services, actively looks for external funds and acts as one-entry contact and support industries during the service and the technology transfer, with a dedicated access mode for companies to ensure the property of the results and confidentiality.

## INDUSTRY SERVICES

One of the main activities of the ILO is to engage new companies to use the services available at ALBA. To that end, in 2021, the ILO participated in fairs like Expoquimia and Cosmetorium (both in-person), training courses like the ICTP School on synchrotrons and webinars such as Anticovid day, New Space, Hangar 21 and Advanced Microscopy, managed by the industrial network, Secpho. Also, several on-line workshops have been organised by the ILO: “Industrial Applications of ALBA Synchrotron in cements, pigments and ceramics”, “Webinar on TamaTA” and “Smart Agrifood Industry Expo” (in collaboration again with the industrial cluster Secpho). These events resulted in new contacts and specific discussion meetings with companies interested in using ALBA techniques. All these activities, together with other parallel actions like for example participating in the innovation network HubB30, contacts with Biocat, the Sabadell city council, etc. are crucial to disseminate the ALBA capabilities among industries, not only in the local area but also at an international level.

In 2021, the services related to the metrology lab experienced an enormous increase of activity related to X-ray mirrors characterization with the NOM technique, among others, up to very high levels of precision that were very much appreciated by the companies requesting this kind of service. On the other hand, the industrial beamtime activity showed an increase of the battery industrial sector in line with the high interest shown by the industry for new and more efficient storage systems to address the energy challenges of the society. During this year, ALBA has provided different synchrotron services to a wide range of industrial sectors (Fig. 16). It is worth to mention that, considering both services together, the metrology lab and the industrial beamtime, the ALBA industrial services reached a good global service level.

In addition, European Union competitive funds are being granted with specific tasks and deep involvement of the ILO, which will help to stimulate and promote industrial services at ALBA addressed to SMEs (in LEAPS-INNOV project) or related to circular economy (ReMade@ARI) and nanotechnology (NFFA). Some of these actions started already in 2021, when the first call for SMEs proposals within the project LEAPS-INNOV



**Figure 16:** Industrial sectors who have benefitted from ALBA Synchrotron services in 2021.

was launched. Thus, active participation in European projects such as CALIPSOplus (ended in October 2021), Sylinda, LEAPS-INNOV, ReMade@ARI or NFFA are important tasks carried out at the industrial office which benefit and promote the industrial services, activities and technological transfer foreseen in ALBA.

## TECHNOLOGY TRANSFER AND INNOVATION

The new beamline, MINERVA, funded by the European Space Agency (ESA) and the Spanish Ministry of Science and Innovation is entering into the construction phase. During this year, the detailed design of the beamline has been approved and the optical hutch was built. This new beamline will be used for the characterization of the main mirror components of the space X-ray telescope ATHENA mission (Advanced Telescope for High Energy Astrophysics) and reinforces the metrology measurements and services offered by ALBA.

In addition, there has been one new patent application for the monochromator cooling system of LOREA and one license agreement related with

a sample bender for BOREAS for flexible samples such as flexible chips for electronics (outcome from TNSI-POCTEFA Interreg project).

ALBA is continuously growing and there is an intense requirement for new and advanced technological solutions. In order to address these needs, INEUSTAR, the Spanish Science Industry Association, and ALBA organized a very successful event at ALBA premises with supplier companies to establish new synergies and commercial relationships.

All these industrial activities will be promoted and enhanced within ALBA II project, that opens new opportunities to the scientific and industrial community. In that regards, the ILO participated in the section reviews performed during 2021, providing the industrial program overview developed so far and analysing the future industrial needs that range from having new synchrotron techniques, upgrades and automation of the existing tools and going forward to offering full services to the local and international industrial community. All this sets the basis for the industrial contribution to the ALBA II white paper.



**Figure 17:** New opportunities for SMEs through TamaTA-INNOV call. Above, image of the webinar organized for companies from the cements, pigments and ceramics sectors.



# Altinco company enhanced agrochemicals using synchrotron light



**Figure 18:** Detail of red apples on tree, picture by Tom Swinnen from Pexels.

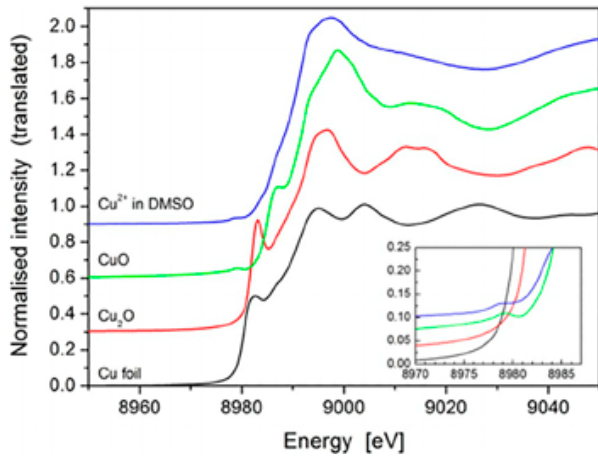
Altinco is a company based in Lleida, specialized in sustainable agrochemical products, that has developed a formula to optimize the pruning process in fields and thus achieve a significant reduction in crop management costs. The product consisted of a complexed copper solution whereby the greater the amount of complex, the more effective the application will be.

After obtaining promising results in the formulation phase and in field trials, Altinco used synchrotron light to determine the content and composition of its product. At the ALBA Synchrotron, the spectral data and analytical information were obtained to verify the identity and composition of the substance. This is one of the most important phases of the project since the characterization tests are necessary to register the product under the ECHA (European Chemicals Agency).

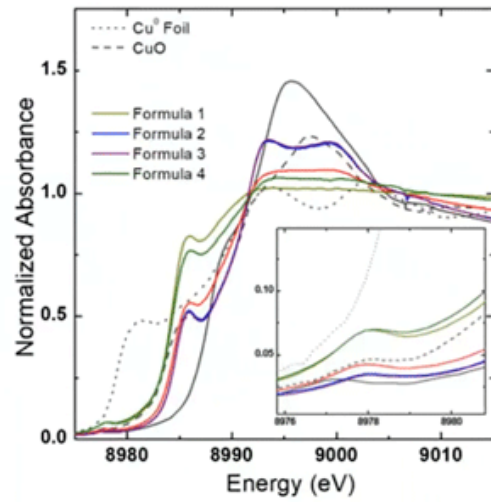
Using the X-ray absorption spectroscopy technique at the CLAESS beamline, the composition and amount of copper complex in four different

formulations of the agricultural product could be verified. It was concluded that the variability in the amount of complexed copper was due to slight differences in the pH of the solutions and the concentration of copper and ligand. It was also observed that the four formulations contained only copper complexed or bound to ligands or compounds, with an oxidation state of +2. No reduced copper, Cu(I) ions or Cu(0) metallic copper were detected in any sample.

These measures were funded by the TamaTA program, which is part of the European CALIPSOplus project in which ALBA participates. This program provides small and medium-sized companies access to European synchrotron facilities for the improvement of their research and industrial developments. This project has received funding from the European Union's Horizon 2020 Research and Innovation program under Grant Agreement No. 730872.



**Figure 19:** X-ray absorption spectra of different copper standards.



**Figure 20:** X-ray absorption spectra of the different analyzed formulations

# ACCELERATORS

Francis Pérez, Head of the Accelerator Division

Year after year, and 2021 has not been an exception, the Accelerators' team has progressed in several fronts, in the installation and commissioning of equipment for the new beamlines, in improvements for the day to day operation, and in new developments for the future.

About the future, in June 2021, the basic conceptual design of the new Storage Ring for the upgrade ALBA II was presented to the Spanish and the ALBA User's community. This was an important milestone for the future of the ALBA facility.

Talking about the present, and after the successfully commissioning of the LOREA and NOTOS beamlines' equipment the previous years, in 2021, the commissioning of the in-vacuum undulator (IVU) for XAIRA, and its front-end, has been successfully accomplished. By September, the IVU was fully commissioned with beam, the front-end conditioned, and the XBPM calibrated, all ready for its full operation for the beamline commissioning.

Also, in December, as scheduled, the front-end for the MINERVA beamline was installed in the tunnel. Its commissioning foreseen to start after Easter 2022.

With respect the FAXTOR beamline, the contracts of the front-end, and of the novel in-vacuum (2.5T, 5-pole, 5mm gap) wiggler (IVW) did progress, but with some delays due to the global situation of saturation of the production and logistics chains.

On the other hand, there has been no stop to the continuous day-to-day work for maintaining, operating, development and improving the complex of the three ALBA accelerators: the Linac, the Booster and the Storage Ring.

One of these developments, which is a major improvement for the polarization experiments on

the MISTRAL beamline, is the implementation of the so-called Fast Polarization Switching (FaPS). With this new set-up, the change of the polarization on the sample is done by moving the electron beam in the Storage Ring, and so, maintaining all the beamline optical elements fixed, which improve the synchrotron light intensity on the sample, and the speed of the experiment. Details of the system are given in the technical note that follows.

Also, in order to improve our diagnostics of the electron beam, two new systems were installed in the Storage Ring in 2020, and have been commissioned along 2021. A novel Integrating Current Transformer (ICT) installed for the first time in a Storage Ring, which has been implemented at ALBA in close collaboration with the company which has developed it. And a new synchrotron radiation pin-hole diagnostics system, in order to have a second and more precise measurement of the transversal beam size.

In terms of development for the future, as mentioned earlier, the upgrade of ALBA towards a 4<sup>th</sup> generation light source, ALBA II, has maintained us extra busy along the year. All the groups have been involved in the design of the new Storage Ring, resulting in the definition of the baseline lattice design; the proposal of the layout scheme for the new ring, maintaining the existing beamlines and the accommodation for the new ones; and the basic considerations for the required magnets, vacuum, RF and diagnostics systems. All these contributions are ready for the White Paper document.

As part of the ALBA II upgrade, but also of use for the present ALBA, we are developing an active 3<sup>rd</sup> harmonic RF system which shall improve the beam lifetime of the Storage Ring by a factor of around three. During this year, the prototype of the RF cavity and of the Low Level Radio Frequency (LLRF) system were finished, and has



passed successfully the acceptance tests. And so, at the end of the year, both systems were sent to Berlin, to the HZB institute, to perform operational test during 2022 in the BESSY II Storage Ring. In addition, the fabrication of a solid-state power amplifier's prototype, at 1.5GHz, has started.

On top of that, we have been actively involved in several international collaborations in accelerator's R&D, including several H2020 projects, as the Compact Light Source XLS collaboration, and the ARIES collaboration for new accelerator's technologies development. We have also participated in research activities related to the FCC, the Future Circular Collider project from CERN, with the study of high-temperature superconductors for the vacuum beam screen, and the development of the Speckle technique for beam size measurements. Also, we are involved in the project BEATS, which is an European contribution of a hard X-ray imaging beamline for the Middle East Synchrotron SESAME, located in Jordan. And with the Canadian Light Source, to implement the ALBA LLRF digital system in their accelerators, starting with the LLRF of the Booster, which shall be commissioned in May 2022. Finally, in October, we did organize the international Workshop on Accelerator Operation (WAO'21, <https://www.wao2021.com>).

All of these still under the pandemic restrictions, meaning that the collaborations mentioned earlier have been conducted without travelling, using videoconference tools to perform the meetings and, even, to share experimental results; that installations have been conducted with the minimum people required on-site; and that operation has been performed with extra



**Figure 21:** 3rd Harmonic Cavity Prototype at the ALBA lab with part of the RF team.

safety procedures to ensure the health of the staff. The commitment of the operators and floor coordinators, of the rest of the Accelerator division, and of the support division personnel has, despite the difficulties, made possible this successful year.

# Switching Photons Polarization with the Electron Beam at MISTRAL

L. Aballe, S. Ferrer, U. Iriso, Z. Marti, J. Moldes, E. Pereiro, A. Sorrentino, L. Torino, D. Yepez  
Experiments division, Accelerator division

In 2013, a long-term research program devoted to imaging magnetic domains with the X-ray microscope was launched at MISTRAL beamline. It was based on circular magnetic dichroism which requires the subtraction of two images with opposite circular polarizations.

The X-rays emitted at a bending magnet have three polarizations: linear in the plane of the orbit, circular clockwise above the orbit plane and circular counter clockwise below the orbit plane as represented in Fig. 22.

During the first six years of MISTRAL operation,, circular polarization was selected by blocking the unwanted polarizations with a movable slit. This method had some inconveniences related to the inequivalent optical paths of the X-rays, which requires realigning the beamline optics. A more convenient method, already used in other synchrotrons, consists in modifying the angle of emission of the X-rays by introducing a displacement of the electron orbit in a way that only one polarization, selected at will, reaches the beamline optics.

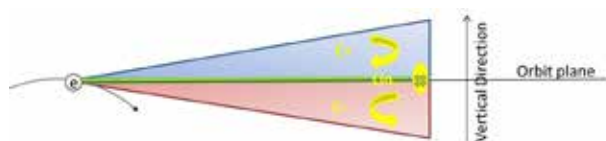
In September 2019 the first tests were carried on and today the project has reached a point where the MISTRAL users can select the desired circular and linear polarization while operating. At present, changing the polarization takes about 40 seconds and an update of the system behind the switching mechanism is foreseen in the frame of ALBA II. This could further reduce the switching time down to the one second scale.

The success of this project is a big step forward in the magnetism research at MISTRAL. It has been the result of a close collaboration among MISTRAL scientists and staff from the Accelerators and Computing Divisions. As illustrated in Fig. 20, different polarizations are emitted at different angles with respect to the electron beam orbit plane.

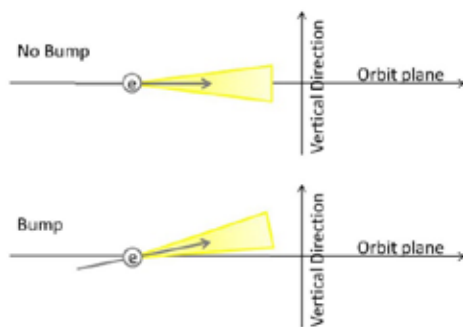
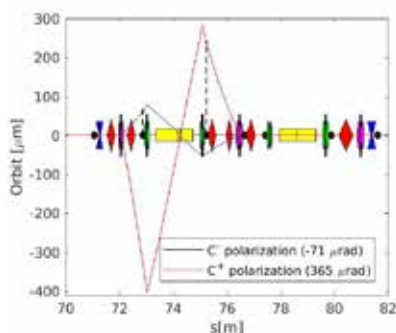
The idea behind the Fast Polarization Switch operation mode is to create a local bump with the electron beam in order to modify the direction of the orbit plane at the MISTRAL source point, located in the first bending magnet of sector 5. In order to change the polarization, the bump is changed and the electron beam crosses the MISTRAL source point at a fixed position but with a different angle. Thanks to this, the photon beam impinges on the beamline optics with a different angle, enabling the selection of the desired polarization by cutting out the others. In this way, the angular portion of the photon beam with the desired polarization propagates always along the same optical path. Figure 23 illustrates the trajectory of the beam when no bump is created and the change of angle of the production of synchrotron radiation when the bump is active.

The Fast Orbit FeedBack (FOFB) system is used to perform this orbit modification as fast as possible. In general, the FOFB takes care of keeping the electron beam orbit stable in the order of 50 nm RMS. This is achieved thanks to 176 Correctors Magnets (88 in horizontal and 88 in the vertical plane) which steer the beam towards the so called “golden-orbit”, representing the ideal trajectory. The actual beam position (horizontal and vertical) is measured by 88 Beam Position Monitors (BPMs) and the measurement-correction loop is performed at a 5 kHz rate (5000 times/second).

In order to perform the electron bump, the FOFB has been upgraded to include the possibility to modify the offsets of the BPMs surrounding MISTRAL. The idea is to “trick” the BPM measurement, subtracting



**Figure 22:** Polarization distribution of synchrotron radiation produced by a bending magnet. C+ stands for Circular Positive, C- for Circular Negative and Lin. for Linear



**Figure 23:** Bump at MISTRAL location for positive (red) and negative (blue) circular polarization, dashed lines represent BPMs position. Red and blue line represents the trajectory of the electron beam. The source point of MISTRAL, at the center of the first dipole, is crossed with a certain angle when performing the bump.

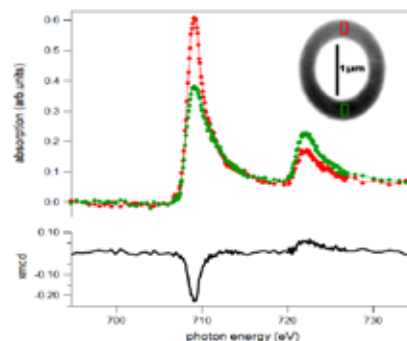
an offset corresponding to the one selected for the desired polarization. In this way the FOFB system notices a discrepancy with respect to the golden-orbit and compensates it using corrector magnets.

In addition, to avoid affecting the rest of the beamlines when switching polarization, two new magnets were put into operation in the Storage Ring: a “corrector magnet” to steer the beam for the bump, and a “skew magnet” to control the beam size changes produced when the electron beam traverses off-center the sextupole magnets surrounding the source point in MISTRAL.

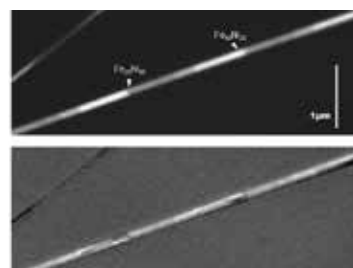
The modification of the BPMs offset has to be performed gradually to minimize the perturbation of the beam. Thanks to the performances of the FOFB, this disturbance is at the same level than the ones produced when an Insertion Device from another beamline moves its setting. Moreover, the repeatability of the polarization switch using the FOFB is guaranteed at nm scale and the time to switch polarization is reduced to roughly 40 seconds.

Magnetic imaging using the fast polarization switch has already proved to be of much higher quality than the methods previously used. While fine-tuning of all the details of this operation mode are still ongoing, we have already demonstrated a polarization degree above 88%, illustrated in Figure 24.

This method for switching polarization is particularly relevant for imaging nanostructures, where inequivalent illumination causes strong



**Figure 24:** Top: Fe L edge absorption spectra from oppositely magnetized regions of a thin permalloy micro-ring, marked in the inset by red/green boxes. The magnetization is in the sample plane and the measurements were done at 45° beam incidence. Bottom: The obtained X-ray circular magnetic dichroism, corrected by the incidence angle and using known values for the Fe polarization, reveals 88.5% of circular polarization. Sample by A. Hierro-Rodríguez et al., Universidad de Oviedo.



**Figure 25:** Images of cylindrical magnetic nanowires with modulated composition, comparing the absorption (top) and magnetic (bottom) contrast. Subtle details of the magnetization configuration are revealed thanks to the use of the bump. Sample by C. Fernández-González et al., IMDEA Nanociencia.

edge artifacts. Figure 25 shows magnetic domain images of nanowires that are only 110 nm in diameter. In addition, they have variable composition, preventing reliable magnetic imaging by comparing two different photon energies, a method sometimes used for nanostructures to avoid edge effects.

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# ENGINEERING

**Joan Casas, Head of the Engineering Division**

The Engineering Division comprises a team of 37 multidisciplinary engineers and technicians, giving support to the other divisions in ALBA, and maintaining and upgrading the general infrastructures and services of the facility.

One of our two sections is devoted to civil engineering projects (construction and technical services/supplies like electric power supply, compressed air, technical gases, de-ionized water) and maintenance of facility related assets and processes (electrical maintenance and mechanical maintenance including HVAC, compressed air, and dynamic UPS among others).

The other section offers transversal engineering services to the beamlines and to the accelerator, as well as support to the operation on vacuum, survey & alignment and cryogenics. This section went to important organizational changes during 2021. The former vacuum group was splitted into the new “vacuum engineering” group fully focused on the design of the vacuum systems, while the vacuum technicians joined the workshop & logistics group. A new “Simulations and fluid mechanics” group was formalized, including all the calculator operators and the cryogenics engineer. The already existing technical office group got a new group head. This group includes all the beamline engineers, but no longer the draftsman, which will be managed directly by the section head, providing support to all the groups of the section (and also to the rest of the division). On an operational phase, the beamline engineers from the technical office are supporting the beamlines with plenty of projects for small or medium upgrades. On a new beamlines design phase, they play a key role not only developing specific synchrotron instrumentation but also giving technical management support to the beamline scientist.

Finally, the workshop and logistics group is a key element in all manufacturing and installation operations, including most of the technical

installations upgrades hereafter pointed out. After the organizational changes above introduced, this group was complemented with the vacuum technicians from the former vacuum group, and will take full responsibility of the support to operations related to the vacuum system.

Worth to mention is the continuation of the cooling de-ionized water system erosion/corrosion project during all the year. This project has completed the first phase (instrumentation) during 2021, and it is now ready to face the second phase along 2022 and 2023 (oxygen removal plant). The criticality of the outcome of this project has been reviewed, because the new Storage Ring for ALBA II is being already planned and the erosion/corrosion problems in the existing ring are no longer a threat for the operation of the synchrotron.

## **FACILITY UPGRADES**

Some of the facility upgrades planned and designed during 2020 have led to the implementation phase at different levels. The conditioning of PO-L1 to host the new Microscopy Center has evolved up to the completion. This means that the works were finished by end 2021 and the first microscope (Glacios cryo-TEM 200 Kv from Thermofisher) was already installed to start commissioning. Another important project was the completion of the compressed air system upgrade, with the installation of a third oil-free compressor and the required control system to recover the redundancy on this technical supply.

Finally, among decens of little upgrade projects, it is worth to mention that we already started with the construction of ALBA's Battery Lab. This laboratory is a joint facility with CSIC. During 2021 the design phase has been completed. The former “archiving” room has been split in two identical 80m<sup>2</sup> spaces. One of these spaces will be devoted to the new battery lab.

## PROJECTS FOR THE NEW BEAMLINES

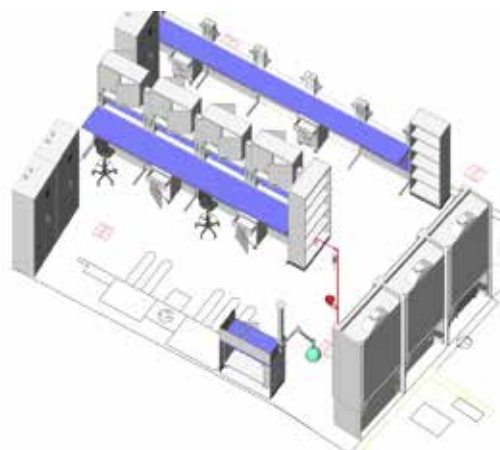
During 2021, a lot of activity has been deployed for the new beamlines in construction. For NOTOS all the components inside the optical hutch and almost all at the end station have been installed, both M1 & M2 mirrors, the diffractometer, the sample stages and the in-house developed metrology table.

For LOREA, the installation of the end station has been finished.

At XAIRA most of the beamline components have been already received. The mirrors mechanics and benders have arrived and have been installed, the Horizontal Focusing Mirror & the Kirkpatrick-Baez mirrors have been installed as well. The monochromator has been installed with the cryo-cooler, together with a number of auxiliary components like the Fluorescence Screen Monitor or the slits. This will allow to complete the part of the backbone included in the optical hutch by beginning 2022. The in-house design for the end station has advanced during 2021.

For FAXTOR, the call for tenders for the main optical components have been launched and awarded. The synchrotron radiation absorber required at the source, in the Storage Ring has been designed and ordered as well as the vacuum chambers surrounding the Insertion Device. The call for tender for the lead hutches has been also published and awarded. The front-end and the multi-pole wiggler insertion device evolved from the design up to the manufacturing. Following the completion of the call for tender for the optical components, the design of the end-station has already started during 2022.

MINERVA beamline has completed the Conceptual Design and almost the full detailed design. The project team successfully held a full ESA-standard Critical Design Review, CDR, and the Radiation



**Figure 26:** Simulation of the already finished battery lab, and location next to the archiving room.

Shielding Acceptance review. The front end has been installed and the absorber (with the window) was ready for installation by beginning early 2022. Also the radiation shielding optical hutch has been constructed and commissioned. Moreover, the installation of the clean room for the sample chamber has been done. The mirror for the monochromator has been ordered and its manufacturing has started. In the same way, most of the long lead items as well as the gross batch of mechanical parts have been ordered for production like the detector tower granites and its mechanics. In addition the call for tender for the laser tracker and the sample chamber hexapod have been completed and published.

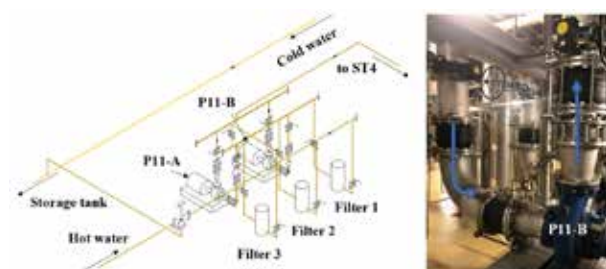
# CFD predictions of water flow through impellers of the ALBA centrifugal pumps and their aspiration zone

An investigation of fluid dynamics effects on cavitation problems

Marcos Quispe. Head of Simulations, Cryogenics and Fluid Mechanics Group (Engineering Division)

During the last years, ALBA's operation has been affected by general thermal stability problems that prevent the correct performance of the system. The cooling capacity of the facilities, which depends on the cold water supply from an external cogeneration plant (ST4), is affected by irregularities in the supplier's operation. The ST4 changes its operating mode for a few hours each weekend, producing losses in the stability of the cold water supply. Moreover, from the ALBA side, the thermohydraulic system cannot move the required design flow in the heat exchange zone due to cavitation problems, which arise when the pump system (called P11) operates on design conditions. For this reason, the operating flow was reduced by 33% to protect the pumps from such phenomenon, worsening the heat transfer efficiency between ALBA and ST4.

Seeking to solve the local problem, this study focuses on investigating whether the cause of cavitation in P11 pumps is a bad configuration of the distribution panel in the suction zone or a bad dimensioning of the aspiration zone. For this research, CFD (Computational Fluid Dynamics) systematic studies, are applied. The simulations have been carried out with the ANSYS-FLUENT software.



**Figure 27:** Schematic of the overall circuit studied (left) and photograph of the P11 pumps (right).

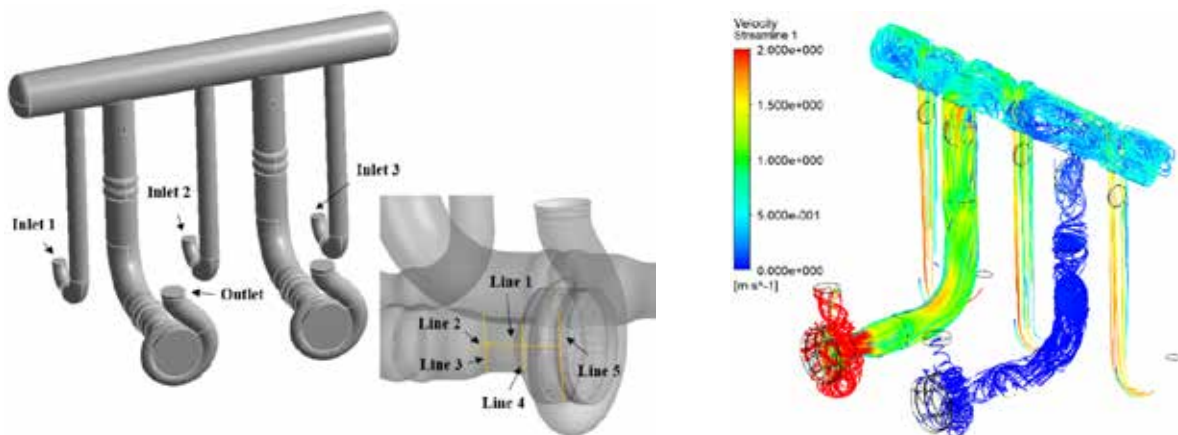
**P11 Operation.** P11 is the main pumping system of ALBA, composed by a couple of pumps. They are fed by the hot water from the accelerator, after passing through filters and the three pipes connected to them (see Fig. 27). The flow is then redirected towards a group of heat exchangers before reaching the storage tank, where the water is cooled with the incoming flow from ST4.

Different problems have been detected in the P11 system during its operation in recent years: (i) Reduced flow rate to avoid cavitation problems at nominal value, (ii) Non-uniform geometry of the suction zone and distribution panel, which produces a flow imbalance detected with ultrasound reading, and (iii) Flow oscillatory behavior measured with ultrasound in the suction branches, which could be due the pump or the geometry of the suction zone.

The NPSH (Net Positive Suction Head) required by the manufacturer is 2.42 m for 645 m<sup>3</sup>/h. Under current operating conditions at 430 m<sup>3</sup>/h, the pressure gauge reading in the suction zone is 1.6 bar, value over the NPSH limit taking 23 °C water conditions. However, there are still exploding bubbles noises which indicate cavitation. Therefore, the conclusion that the NPSH complies may be questioned by a possible malfunction of the pressure gauge, and/or a high-pressure gradient in the suction zone. On the other hand, a poorly designed aspiration zone could promote high speeds and/or a complex, unstable distribution, which is also a source of cavitation. A situation expected to worsen with flow rate increases from 430 to the nominal value of 645 m<sup>3</sup>/h.

**CFD Model.** The geometry used includes the general manifold in the aspiration zone and a





**Figure 28:** Boundary conditions and lines set to extract data from the 3D model of the system (left). CFD streamlines in the manifold and pumps at 430 m<sup>3</sup>/h (right)

simplified model of the pump impeller (see Fig. 28), as confidentiality prevents access to its drawings. Moreover, an ideal setup of the pump together with a 6 m straight pipe was simulated. For both cases, the lines depicted at Fig. 26 have been used to extract the data, being lines 2 and 3 at the current pressure gauge location.

At the inlets, the velocities obtained from uniformly distributing the current and nominal flow rates (430 and 645 m<sup>3</sup>/h, respectively) and the current non-uniform distribution (36.441, 33.377 and 30.182% for inlet 1, inlet 2 and inlet 3, respectively) as measured by ultrasound were applied. A zero value has been set as the reference pressure at the pump outlet. Water at 23 °C is considered, together with steady, isothermal and no-slip walls conditions.

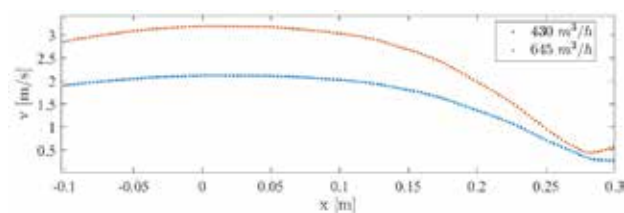
**Results and Discussion.** As part of the research, a hydraulic test on the system was performed, forcing a flow increment on the P11 from 430 to 585 m<sup>3</sup>/h. It is observed that the aspiration pressure tends to decrease from 1.59 up to 1.24 bar, a value which would leave the system far below the NPSH limitation given by the manufacturer.

Based on CFD studies, an approximately constant distribution of pressure is obtained in all directions of the inlet suction tube. This uniformity allows to conclude that the readings of the pressure gauge installed in the area of lines 2 and 3 is

representative of the suction pump. The results also conclude that at nominal flow the pressure value in the suction zone should increase to comply with the NPSH limit.

The main difference between regimes is given in the order of magnitude of the velocity as it can be observed in Fig. 29, going from a maximum of 2.12 to 3.2 m/s. However, such values fall above the limits established by the literature regarding adequate velocities in the suction zone of centrifugal pumps, becoming a problem to be solved.

On the other hand, it is recommended to implement a modification of the existing rigid tubes to avoid vibrations transmission. Moreover, the manifold must be redesigned and the pumps must be changed or a third must be added to distribute the flow between two and keep another one as backup. Finally, this research has been dedicated to the aspiration zone, but the impulsion zone immediately after the pump remains to be investigated.



**Figure 29:** Velocity distributions at line 1 for both flow regimes. Case with uniform inlet distribution.

# COMPUTING

**Óscar Matilla, Head of the Computing Division**

The 2021 year has allowed the Computing Division to reach cruising speed again. Hopefully, the times when the focus had to be on the short-term response to the pandemic slowly faded into our memory. An example is the ALBA II Computing Preliminary Study project which will be shown later. In general, major changes are bouncing into the Computing field, providing crucial advances for the years to come. On one hand, the progress in the new beamlines projects brings the scenario of having high throughput beamlines at ALBA looming on the horizon. But before that, different challenges will need to be tackled to allow efficient data handling during its processing and storage. On the other side, new policies for the management of scientific data must be drawn up to ensure the scientific success of our users. They will necessarily expand our current role as data custodians towards delivering comprehensive computing services to our users. Some definitive steps are already here. In 2021, ALBA began to provide unique DOIs (Digital Object Identifiers) to datasets in the experiments. But many of these new functionalities discernible from the surface require far-reaching architectural transformations. For example, in 2021, the deployment of containers was extended in the Computing Division, requiring intensive coordination between the section which provides the IT infrastructure and those who exploit it. One case is the migration of the Management Information Systems (MIS) applications, which started tailoring the IT infrastructure to ensure the required performance is served. Another example is the spread of cloud computing use. In 2021, different proofs of concepts started to take the first steps on the long way until successful applications will be delivered.

But all the above must be done without removing our view from the road. Our primary mission is to support the organization in every process. For example, automating internal processes to save staff time, as with the Digital Annual Evaluation application deployed this year. Another example was developing the tools to implement our internal safety prevention service to comply with

national regulations. Similarly, the accelerator and the beamlines continuously operate, generating endless needs. ALBA is a non-stop train. For example, in 2021, implementing the fast polarization switching in the MISTRAL beamline required extensive work in the accelerator's control software. And in parallel, we have had four beamlines under construction. Each with its own pace and tight deadlines. None of them would be fulfilled without the Computing Division's support: building the electronics infrastructure, providing support during the instrumentation validation, designing control electronics, deploying control software and graphical user interfaces, implementing the equipment and personnel safety systems, developing the data processing pipelines, or providing IT infrastructure as servers or network, among others. In addition, the JEMCA (Joint Electron Microscopy Center at ALBA) is a new facility supported by the Division. The first Electron Microscope was installed in 2021, and all previous work for the second was also completed. Besides, there is the work done out of sight from the surface. For example, the Controls Section made a big effort to migrate aged code from Python 2 to Python 3 in 2021. Another example is the huge work to strengthen the institution's IT security: the implementation of two-factor authentication in external users' access or the migration of our old operating systems that are no longer maintained.

In parallel important changes in the division were established in 2021. One was the creation of the ALBA Scientific Data Management Section. Four new members were on-boarded in 2021 and already had their first successes in supporting beamlines data processing while also working towards FAIR data transition. Second, the IT first-level support service was implemented. Two experienced technicians are already relieving IT system administrators of this day-to-day support, allowing them to specialize further in their fields.

2021, in closing, has been a busy year, but we'll be surprised to have less fun in 2022.

# Building the backstage of the ALBA II

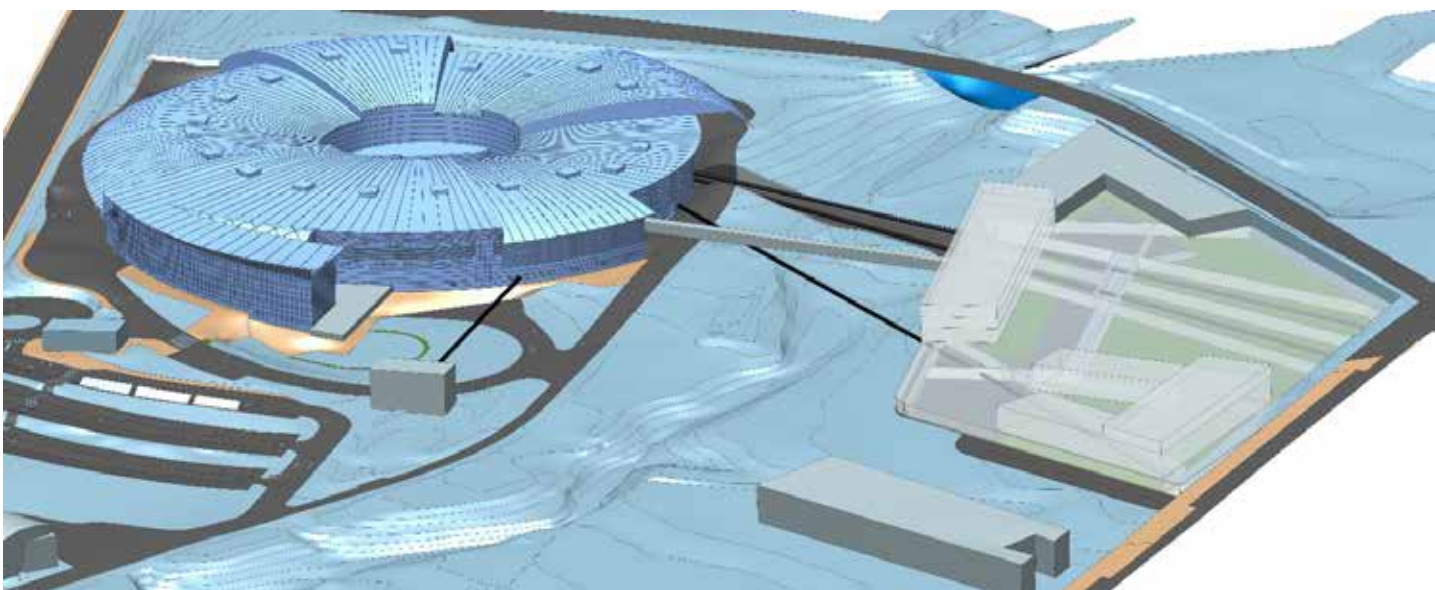
Óscar Matilla, Head of the Computing Division

In 2021, the ALBA Synchrotron started the works for upgrading the accelerator and beamlines towards a 4th generation source, the future ALBA II (Figure 29). The goal is to upgrade the accelerator in 2029, increasing its photon brilliance by 40 times. The accelerator will require a new lattice design that reaches the boundaries of what is technologically possible. In addition, it will be necessary to master other technologies, such as nanoscale positioning, to exploit the new beam enhancements in the experimental stations. In fact, the success of ALBA II will depend on many other factors. Most of the subsystems of the current accelerator must be overhauled. Over the last years, advances have improved many technologies' performance and reliability. These evolutions are not just a choice factor: using the latest developments will also prevent obsolescence in the medium term. In light of this, the ALBA II Computing Preliminary Study started in 2021. First, eleven different fields were identified. The extensive list went from using standards to specific tailored solutions designs in hardware and software. Second, a group of experts were appointed to each one with the mission to analyze the different challenges and needs for the future accelerator.

The first task of the different groups was to conduct a risk analysis to identify the need for replacement due to obsolescence or expected lifespan. One identified case, for example, was the Personnel Safety System, which ensures secured access to the personnel to areas with radiation levels hazards.

Another case was the Timing System, which provides the most constrained synchronization signals to multiple accelerator's subsystems. Different architectural designs that were unavailable ten years ago are now possible, and a horizon for generalizing deterministic event systems to experimental stations is conceivable nowadays.

The Input/Output Controller used at ALBA has proven to be performant and reliable, but it dates from the 90s. The renewal possibilities are many and will undoubtedly increase the current processing capabilities. But, actually, here, the decision is not straightforward. First, because of its impact on the budget. And second, even more critical, because of the implications in the software layers that must be run on top. Hardware obsolescence is readily noticeable to everybody.



**Figure 30:** The ALBA II will upgrade the existing accelerator to a 4th generation source.



But, in fact, software ageing has also the deepest impact on the performance of the systems. For this purpose, a comprehensive analysis of the Control System Stack was carried out. The conclusion is that an in-depth redesign is a priority and that different aspects require critical design choices. For example, nowadays, IT infrastructure allows isolating processes seamlessly in containers. The benefits are huge as it enables dynamically increasing the allocated computing capabilities, implementing high availability in critical processes and facilitating the systems' upgrade, maintenance and recovery. Of course, the virtualization of the Controls System's stack has clear boundary lines since, in practice, it controls "real" hardware. Other cases, such as archiving or alarm systems, are well-suited candidates for implementing such architectures.

The study also raised other self-evident changes, such as the need to replace all the power converters that will drive the new ALBA II magnets. The design of the new lattice is in the early stages, but we already have some insights from the scientists working on it. Certainly, the number of independent power converters is going to increase dramatically. Over 600 power supplies are expected to drive the

Storage Ring main magnets. In addition, many of them will be mission-critical. That is, if there is a single failure in any of them, it will produce a beam loss. This increase may make the overall system less reliable. Architectural changes in the power converters must be considered to mitigate it.

Finally, all the IT infrastructure and security policies must be adapted to the new requirements. The study also raised the need to study emerging technologies further. For example, the growing use of AI algorithms, especially machine learning, is palpable in many domains, and the inertia present in other fields could bring good opportunities for successful implementations. We must keep an eye on it and move slowly toward the first study cases.

In 2021, eleven groups of highly experienced engineers had the mission of raising our sight, looking beyond our daily operations, and planning for the future of the ALBA II accelerator. The outcome has been excellent. After their work, we now have a clear vision of the first required developments toward making the most of the ALBA II accelerator. This will be a long way, but the journey has already begun in the Computing Division.

# PROJECTS & COLLABORATIONS

## PROJECTS CO-FUNDED BY THE EUROPEAN REGIONAL DEVELOPMENT FUNDS (ERDF)

Spain Multi-Regional Operational Program 2014-2020



Fondo Europeo de Desarrollo Regional  
Una manera de hacer Europa



PROJECT	BUDGET	FUNDS	DATES
Update of the data management infrastructure	1,915,466.00 €	957,733.00 €	2015 - 2021
Design and construction of the phase-III beamline XAIRA	6,900,000.00 €	3,450,000.00 €	2015 - 2023
Improvement of phase-I infrastructures (NCD beamline and Booster)	445,000.00 €	222,500.00 €	2015 - 2022
Design and construction of the phase-III beamline NOTOS	3,294,370.00 €	1,647,185.00 €	2015 - 2022
1.5 GHz radiofrequency (RF) systems prototype for ALBA - 3HCprot	390,000.00 €	195,000.00 €	2015 - 2023

ERDF Catalonia 2014-2020 for the Strengthening of the Large Scientific and Technological Infrastructures with the participation of the Catalan Government



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Generalitat de Catalunya  
Departament de Recerca i Universitats

PROJECT	BUDGET	FUNDS	DATES
Improvements in the reliability of the radiofrequency (RF) transmitters used by the ALBA accelerator rings	2,055,112.00 €	1,027,556.00 €	2015 - 2019
Transversal electronics equipment and cabling systems for new and operational beamlines	1,466,000.00 €	733,000.00 €	2015 - 2023
Transversal standard vacuum technology and equipment for new and operational beamlines	1,861,000.00 €	930,500.00 €	2015 - 2023
Construction of phase-II beamline LOREA	4,267,000.00 €	2,133,500.00 €	2015 - 2022
Construction of the phase-III beamline FAXTOR	5,104,550.00 €	2,552,275.00 €	2015 - 2023
Implementing upgrades at different beamlines and subsystems of ALBA	1,246,180.00 €	623,090.00 €	2015 - 2023

ERDF Catalonia 2014-2020 for cooperative projects for the construction, acquisition and improvement of research equipment and facilities



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Generalitat de Catalunya  
Departament de Recerca i Universitats

PROJECT	BUDGET	FUNDS	DATES
EM01-Cryo-TEM for biological applications	1,700,000.00 €	850,000.00 €	2020 - 2023



EM02-METCAM-FIB for materials applications	4,098,000.00 €	2,049,000.00 €	2020 - 2023
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PROJECT CO-FUNDED BY NEXTGenerationEU



Financiado por la Unión Europea  
NextGenerationEU



PROJECT	FUNDS	DATES
ALBA01 - Prototyping accelerators and Nano-positioning laboratory for ALBA II	7,527,360.00 €	2021 - 2025

## EUROPEAN PROJECTS IN WHICH ALBA PARTICIPATES



Project for designing, building and starting a beamline for X-ray tomography at SESAME synchrotron lightsource in Jordan.



Project for putting together small and medium enterprises (SMEs) and research centres in the border regions of Spain and France to promote cooperation in R&D&I and technology transfer.



Sylinda (Synchrotron Light Industry Applications) aims at boosting R&D capabilities of the National Synchrotron Radiation Centre SOLARIS, located in Kraków (Poland), through the cooperation with experienced project partners: ALBA Synchrotron, Hochschule Niederrhein and University of Bonn.



EU-funded ExPaNDS project to enable photon and neutron research infrastructures at national levels by making the majority of their data 'open', following FAIR principles, and harmonising their data catalogues and data analysis services through the European Open Science Cloud (EOSC).



With the goal of removing barriers for access to world-class accelerator-based light sources in Europe and in the Middle East. More than 82,500 hours of trans-national access are provided to these research infrastructures and specific programmes are in place to teach new users how to successfully use synchrotrons and FELs.



Integrating Activity project that aims to develop European particle accelerator infrastructures, improving the performance, availability, and sustainability of particle accelerators, transferring the benefits and applications of accelerator technology to both science and society, and enlarging and integrating the European accelerator community.



Project for designing a hard X-ray FEL facility beyond today's state of the art, using the latest concepts for bright electron photo injectors, very high-gradient X-band structures at 12 GHz, and innovative compact short-period undulators.



The iNEXT-Discovery project aims to facilitate the access to advanced technological instrumentation for the development of new drugs, advanced vaccines, novel biomaterials, engineered enzymes for food production, efficient biofuels, and other benefits. ALBA participates with MISTRAL beamline for cryo soft X-ray imaging of cells, which includes tomography and spectroscopy.



4-year pan-European research and innovation project. CoCID is focused on the development of a soft X-ray-based methodology that enables fast and inexpensive three-dimensional imaging of whole internal structure of intact biological cells.



The LEAPS-INNOV pilot project will contribute to solving key technological challenges for the European light sources. It will also enhance partnership with industry through open innovation by offering joint technological developments and advanced research capabilities for industry as collaborators, suppliers and users.



Doctoral training programme in Functional Advanced Materials.

# EDUCATION & OUTREACH

ALBA successfully promotes synchrotron-based education and knowledge to wider audiences.

## EDUCATING YOUNGER GENERATIONS

ALBA's commitment towards training and education affects different levels and areas of specialization. Since 2014, students from different backgrounds have had the possibility to be trained at our facilities.

In 2021, 31 students could widen their knowledge about synchrotron facilities. 15 of them were vocational training students who learn a technical job while they are studying. 16 students were undergraduates from areas like Physics, Electronics, Computer engineering, Communications or Industrial Engineering.

Besides, two PhD students finished their thesis. Nithyapriya Manivannan studied the selenium plant uptake mechanisms and its interaction with pollutants using synchrotron analytical techniques at CLÆSS beamline. Johannes Groen's experiments at MISTRAL beamline enabled to visualise for the first time in 3D the exact location and how a nanomaterial drug behaves in whole cells. This drug is a therapeutic protein-nanomaterial hybrid specifically designed to inhibit the collagen overproduction after a myocardial fibrosis event.

As in previous years, some members of the ALBA staff have also been involved in teaching activities

## EVENTS TO KEEP IN TOUCH WITH OUR USERS

Still in 2021, most of the organized events have been held in remote mode, as the effects of the pandemic have been present with difficulties for gathering in-person and travelling abroad.

The ALBA II Colloquium series (already described at the beginning of this document) has attracted



Figure 31: Thesis defense of Nithyapriya Manivannan.

(degree of Physics at the Universitat Autònoma de Barcelona and two master studies at Universitat Politècnica de Catalunya).

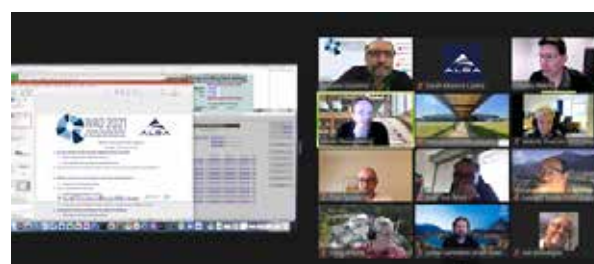


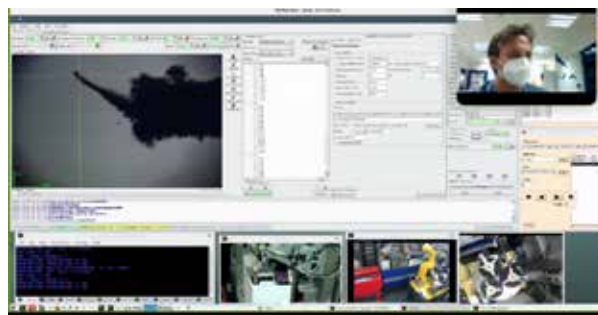
Figure 32: Snapshot of the WAO Conference, organized by the Accelerator division.



the interest of many of our users. The workshops on different research areas were also followed by a large number of participants. In total, more than 1,500 attendants were present in these events.

The 12th edition of the workshop on Accelerator Operations was celebrated in October 2021, becoming an excellent forum where to exchange ideas and best practices among worldwide experts in accelerators.

In March, ALBA hosted virtually the European Hercules school, where 19 young researchers



**Figure 33:** Snapshot of the HERCULES School, organized by the Experiments division.

could delve into a wide variety of synchrotron techniques with the help of ALBA scientists.

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### **CONSOLIDATED OUTREACH AND EFFECTIVE COMMUNICATIONS TO ATTRACT NEW TALENT**

The communications and outreach activities have continued developing their yearly program to disseminate the scientific results obtained at the facility as well as to promote scientific vocations among the youngest audiences.

In 2021, the visits' program was fully adapted to a virtual environment, offering new products such as the live virtual tours or the video in 360°.

The educational project Misión ALBA, addressed to 10-12 years-old students, reached its highest number of participants in its 3<sup>rd</sup> edition. More than 15,000 students from all Spain were enrolled in this project. It is worth to mention that the project was recognized by the Catalan Association of Science Communication as the best outreach initiative in 2021.

Finally, as part of the services provided to different divisions of ALBA, it is of particular relevance to highlight the series of communication campaigns launched in social media to promote specific job offers. These campaigns were very helpful to attract new talent to our facilities in areas like Computer Engineering.



**Figure 34:** A live virtual tour at ALBA's premises.



**Figure 35:** The Catalan Association of Science Communication awarding the Misión ALBA project.





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