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The Interview

Prof. María Josefa Yzuel, president of the Spanish Committee of the International Year of Light 2015

Cover main image: Among inclusions present in liver, several are made of diacylglycerol. Thus identifying the nature of lipids and their cellular localisation during the progression of the disease (i.e. lipids that will trigger inflammation) are key elements in the identification of patients that will need treatment to avoid progression into a severe form of obesity-related liver injury or to fibrosis / This is imaged using synchrotron infrared microspectroscopy.

Reference : Le Naour F.*, Bralet M.P., Debois D., Sandt C., Guettier C., Dumas P., Brunelle A., Laprévote O: Chemical imaging on liver steatosis using synchrotron infrared and Tof-SIMS microspectroscopies. *PLoS ONE*, 2009, 4:e7408.

Courtesy of Paul Dumas

Dear reader

We have chosen to highlight in this first 2015 newsletter the eighth ALBA Beamline, MIRAS, dedicated to Infrared Spectroscopy. A first sign of MIRAS infrastructure is visible in the experimental hall: the hole in the shielding wall of the accelerator. It may seem a minor detail, but it is the starting point of ALBA Instruments Phase II, which include also the ninth beamline dedicated to angle resolved photoemission, LOREA. MIRAS scientific team is being consolidated, the beamline design is finished, and we expect to receive the microscope in few months. Our plan is to offer MIRAS photons to official users in 2017, and LOREA will come thereafter.

2015 is the International Year of Light and Light-based Technologies (IYL2015), as proclaimed by the United Nations. Synchrotron light is starring in events around the world, and ALBA is profiting this opportunity for reaching forums and parts of the society usually not aware of the potentiality of our instruments. Prof. María Josefa Yzuel from UAB is chairing the IYL2015 Spanish Committee, in which ALBA is actively participating. In this issue you'll find an interview to her, where the reasons and usefulness of this initiative are nicely described.

Scientific highlights on bioscience, material science and magnetism, together with technical developments and examples of technological transfer complete My best wishes on behalf of the ALBA team,

Caterina Biscari

ALBA Director



Opening ceremonies of the International Year of Light 2015

• The International Year of Light (IYL2015) is a world-wide initiative endorsed by UNESCO with the aim of communicating to society as a whole the importance of light and lightbased technologies in today's world, in such important areas as energy, health, communication, education and agriculture.

More than 1,000 delegates attended the Opening Ceremony of the International Year of Light and Lightbased Technologies 2015 on 19th and 20th January in Paris. The event gathered decision-makers, industry leaders and renowned researchers from a broad range of scientific disciplines (including five Nobel plenary lectures). Caterina Biscari, director of the ALBA Synchrotron, also took part in the thematic session "Light at the limits" standing in for the light source community with a talk on "Frontiers of synchrotron science". See complete video at this link: https://youtu.be/

Spain also organised a national opening ceremony on 16th February at the Royal Academy of Sciences and Arts of Barcelona (RACAB) with the participation of 500 attendees. Prof. María Josefa Yzuel, president of the Spanish Committee for the celebration of the International Year of Light, announced the activities to be developed in Spain in 2015. Three renowned lecturers offered their different viewpoints on the role and impact of light in our lives: Ignacio Cirac. director of the Theory Division of the Max-Planck Institut für Quantenoptik (Germany), Caterina Biscari, director

of the ALBA Synchrotron (Spain) and Jeroni Nadal, coordinator of the Retina Department and the Macula Unit at the Clínica Barraquer (Spain).



INTERNATIONAL YEAR OF LIGHT 2015

Results of the 2nd call for 2015 experiments

• The second call for experiments in 2015 was open from 26th January to 23rd February. A total of 139 proposals were received during this period that will cover the experiments from July till December 2015.

CIRCE, devoted to photoemission spectroscopy and microscopy, was the most demanded beamline with a total of 43 proposals and 864 shifts. The main research areas of the received proposals were materials science, followed by hard condensed matter, electronic and magnetic properties and chemistry. It is worth mentioning that macromolecular crystallography proposals were not accepted in this call because the XALOC beamline had already covered access for all 2015. This second 2015 call has been the most international, with 45% of the proposals coming from other countries like Germany, Italy and France but also from non-European countries such as the United States, Brazil or Taiwan.

The interest of the scientific community in ALBA's beamlines has raised again as it has reached its maximum number of proposals in a year with a total of 337 proposals (covering the two calls in 2015).



Universitat Rovira i Virgili at ALBA

• Last 29th January 2015, Gemma García and Xavier Farriol from the Health & Safety Office of University Rovira i Virgili (URV) visited ALBA to get information about the business coordination with ALBA users. URV, after having had users doing experiments at ALBA, got in touch with Health & Safety Office in order to share experiences in this field. They focused on the documents that we require to the users and, specially, they were very interested in the online training they must do before starting their experiments. Finally, they also highlighted the proposal document as a good way to carry out the experiment risk assessment.



Members of the URV with some members of the Health & Safety Office and Caterina Biscari at the ALBA experimental hall.© ALBA

MIRAS: infrared lights the community



Gary Ellis Institute of Polymer Science and Technology CSIC

Infrared radiation was discovered by Fredrick William Herschel in 1800 by a simple experiment now popular in schools where, on measuring the temperature of the rainbow spectrum produced by dispersing sunlight through a glass prism, he observed that it not only increased from the violet to the red part of the visible spectrum, but it continued increasing just below (infra-) the red. Subsequently, he showed that infrared light was absorbed, transmitted, reflected and refracted, much in the same way as visible light. This fundamental discovery is the basis of many advanced technologies that we take for granted today: from security cameras and night view goggles, heat dissipation measurements in buildings. engines or electronic systems and medical imaging, to weather satellites and beyond, to our understanding of the universe through infrared astronomical telescopes such as that named after the father of infrared light, Herschel. Arguably it was his son, John, that recorded the first infrared (IR) "spectrum" photographically in 1840, but it was not until IR detectors were developed and combined with prism spectrographs that infrared spectroscopy was born. In 1905, the American physicist William Weber Coblenz published hundreds of IR spectra and tables showing the wavelengths at which many substances absorbed radiation, and is credited for establishing the relationship between these absorption "bands" and specific molecular groupings or "functional groups", and that every molecular substance has a specific molecular "fingerprint", demonstrating the enormous potential of IR spectroscopy.

When a molecule absorbs radiation in the IR region - between 0.77 μm

(1.61 eV) (near-IR) to 1000 µm (1.24 meV) (far-IR), or in spectroscopic wavenumber units; 13,000 - 10 cm⁻¹ - transitions can be excited in vibrational, rotational and translational energy levels. An IR absorption band appears when the energy of an incident photon is equal to that of a vibrational transition, and a change in dipole moment exists during the course of the vibration. a basic selection rule. The nature of molecular vibrations is complex comprising fundamental stretching and deformation modes (bending, twisting, rocking, wagging). For most organic materials, for example, these appear in the mid-IR (between 4000-400 cm⁻¹). Their energy (or frequency) is determined by the mass of the atoms involved in the motion and the forces between them (bond strength). and their intensity corresponds to the magnitude of the dipole moment change for the particular vibration. Generally, molecular groups with large dipoles, such as C=O or O-H will give strong bands in the IR spectrum. Many other factors intervene in the unique nature of the IR spectrum, including molecular symmetry, the appearance of overtones and additive or subtractive combinations of the fundamental modes (many in the near-IR), or cooperative modes or lattice (optical and acoustic) modes (many in the far-IR). Finally, and probably the most powerful feature of IR spectroscopy, band positions and intensities are influenced by internal (structural) factors - such as electronic effects, hybridization (sp, sp², sp³), conjugation, isomerization (configuration, conformation) - or external (environmental) factors - such as crystal-field effects, temperature, pressure, intermolecular interactions (dipole-dipole, van der Waals, hydrogen

bonds), etc. This unique capability of IR to unequivocally describe the molecular environment is one of the keys to the success of the technique.

Modern IR spectroscopy employs Fourier transform Infrared (FTIR) spectrometers, where dispersive spectrographs are replaced by an interferometer, providing higher throughput, wavelength precision and multiplex advantages. Another strength of FTIR is sampling versatility, and a wide range of sampling arrangements have been developed giving access not only to materials in almost every state, form and size: gases, liquids, and solids in many forms, but also special sampling chambers allowing studies under different conditions (temperature, pressure, flow, reactions, etc.), surface spectroscopies (ATR, RAIRS), depth profiling (PAS) and, of course, microspectroscopy.

IR microscopes with high numerical aperture reflective objectives combined with FTIR spectrometers allow us to focus IR radiation onto very small areas of the sample and the transmitted or reflected light is collected using a highly sensitive IR detector. The region of interest is defined using variable apertures, and precise sample translation and advanced instrument software provides the analyst with not only the possibility to examine specific points on the sample, but also to raster scan and generate chemical and structural images. However, for high spatial resolution, low aperture sizes are required, the IR light produced by the spectrometers thermal (globar) source incident on the sample is very low, poor signal quality is obtained and the mapping time for high spatial discrimination becomes prohibitive.

magnified image plane. However, synchrotron radiation obtained from a bending magnet in a storage ring provides an almost linear broadband source covering the whole IR region that is up to 3 orders of magnitude brighter than globar sources. Consequently, diffraction-limited ($\lambda/2$) measurements can be made routinely with confocal IR microscopes. This opened up enormous possibilities in diverse scientific disciplines, including materials science, geology, astrophysics, cultural heritage, forensics, biological sciences and medicine.

Advances in 2D focal plane array

(FPA) detectors have improved this

situation as the detector pixel size

to defines the spatial contrast at the

The MIRAS Community

Recognition of the extraordinary potential of synchrotron IR microspectroscopy (SIRMS) and the imminent call for Phase II beamline proposals for ALBA. led to the celebration in Madrid in April 2008 of the 1st Spanish Workshop on Synchrotron IR Microspectroscopy (miras2008), where initial ideas for the beamline were presented to over 100 delegates from both academia and industry. The results of a detailed questionnaire sent a very strong message: the MIRAS community was born! Work began immediately on the beamline conceptual design with the assistance and close collaboration of Dr. Paul Dumas from Synchrotron SOLEIL, and in January 2009 a website was set up to network the community, and by March, 39 scientific cases and 70 expressions of interest had been received. The MIRAS Proposal, representing the interests of over 180 scientists from 56 research groups/ departments in 15 Universities, 10 CSIC Institutes and 7 Mixed Centres/ **Research Centres, summarized**

here, was presented to the Scientific Advisory Committee (SAC) at ALBA in April 2009. In September of the same year, Dr. Trinitat Pradell of the Polytechnic University of Catalonia organised the MIRAS2009 Workshop, one of the first to be held at ALBA Light Source, where lectures from international speakers and the SAC Proposal were presented to more than 60 delegates. On the 21st December 2009, the ALBA Council approved the construction of MIRAS. Unfortunately, funding was delayed and finally frozen until further notice in 2012 due to the economic situation. Undeterred. the MIRAS community celebrated the 3rd Workshop at the University of Valencia in April 2012, organised by Prof. Alfredo Segura. Both national and international speakers presented the advances in the field and its applications to over 70 delegates. Subsequently, several important decisions were taken by ALBA and



Figure 1: (a) SIRMS of a graphene/BN heterostructure. Top: Experimental setup of FET. Bottom: 2D plot of transmission difference spectra $T-T_{CNP}$ at different Fermi energies E_{F} , where T_{CNP} is the transmission spectrum for graphene at the charge neutral point (CNP). Feature marked by dotted line originates from the moiré superlattice. Inset: Moiré-superlattice-induced optical conductivity change σ^{M} at different gate voltages (Ref. Nature Physics, 10, 743 (2014), courtesy of Dr Mike Martin, ALS). (b) Hydrogen at high pressure. Top: pressure dependant spectrum of vibronic bands of H₂ (IR inactive at room temperature) in different phases, and image of the tiny diamond anvil window. Bottom: IR signals are still observed at lower frequency confirming that there is no gap, thus no evidence for metallicity. Arrows indicate H₂ vibrons (Ref. Phys. Rev. B 87, 134101 (2013), courtesy of Dr Paul Dumas, SOLEIL).

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its external collaborators at SOLEIL and CSIC to keep the project alive. ALBA decided to build the beamline using internal resources. A survey by ALBA and AUSE of the interests of the Scientific Community revalidated the MIRAS Project, and the roadmap was outlined in the Strategic Plan 2013-2016. The MIRAS beamline is now under construction.

The range and type of user interests for each synchrotron facility vary and it is the community, bringing its specific problems and challenges, which will continue to provide fundamental input for the growth of MIRAS. At present, several Spanish user groups are active with projects in facilities around the world on high pressure, cultural heritage, catalysis, life sciences and polymer materials science. I am convinced that at the 4th MIRAS Workshop the community will continue to grow, especially now that a Spanish synchrotron beam will soon be available.

Opportunities and challenges for MIRAS

IR microspectroscopy is now present in more than 20 synchrotron facilities worldwide and has already made an enormous impact, reflected in a publication rate of 2 to 3 articles/week. Examples are too many to mention, but the largest area is undoubtedly life sciences, with particularly important impact on the study of disease states, including Cancer, Alzheimer, Parkinson, osteoporosis, Malaria, and their remedial strategies. However, SIRMS does not only answer questions, it can also provide solutions to society. An excellent example is the recent implementation in a French general hospital of a routine IR method for early stage diagnosis of liver disease that was the result of careful SIRMS experiments at SOLEIL Synchrotron.

Here, some selected areas where future advances in the technique may provide new opportunities to the Spanish scientific community are highlighted.

Graphene is a key area in Europe, as the Graphene Flagship attests, and many Spanish teams are working to understand and harness its unique properties and to transfer this knowledge into technology. MIRAS will be valuable for the study of electronic properties. Notable advances have already been made using IR in the study of graphene plasmonics, Landau levels, Dirac charge dynamics, tunable bandgaps in bilayer graphene in FET transistors, electron doping in graphene heterostructures (Fig.1a), phonon anomalies, conductivity, collective hybrid phonon-plasmon substrate modes and IR-THz spectroscopy of graphene-based metamaterials.

Very high-pressure studies are fundamental in geological, environmental sciences and astrophysics. One exciting area is the formation of metallic states in rare gases. In the search for hydrogen metallicity, expected > 300 GPa, SIRMS is mandatory since the gaskets required for diamond anvils must be tiny (around 6 μ m). H₂ gas has no dipole moment and thus its vibrations are inactive in the infrared, but at over 150 GPa vibrons appear that vary in shape and number as pressure increases (Fig.1b). Several hydrogen phases have been identified up to 290

GPa but, as no gap appears in the IR region, there is still no evidence of the elusive hydrogen metal. However, if it is there SIRMS is the method to prove it!

Whilst SIRMS is a powerful tool in many areas, particularly biomedicine for tissue and sub-cellular analysis, its spatial resolution is often just not enough. The push beyond the diffraction limit has led to the exploitation of near-field techniques. combining scanning probe microscopy (s-SNOM) with FTIR and broadband synchrotron IR sources (Fig.2a), dubbed as SINS (synchrotron infrared nano-spectroscopy). FTIR spectra can be obtained from domains as small as 20 nm (Fig.2b). Many areas can benefit. Spatial contrast can also be improved using a synchrotron source with FPA detectors for fast IR imaging. The use of carefully designed optical systems coupled with suitable sampling environments (such as microfluidics cells) gives access to powerful experimental approaches, such as real-time live cell 2D-IR imaging (Fig.2c) or 3D-IR spectral microtomography (Fig.2d).



Figure 2: (a) SINS. Top: experimental setup. Bottom: High-sensitivity measurements from fingerprint region of peptides and proteins; left, SINS topography image of peptoid nanosheet on Au, right, γ-globulin SINS spectra at different thicknesses (Ref. PNAS, 111, 7191 (2014), courtesy of Dr Mike Martin, ALS). (b) Top: Live SIRMS 2D imaging of biochemical processes in live fibroblast cells (Ref. Biophys. Chem, 189, 40 (2014), courtesy of Dr Gianfelice Cinque, Diamond Light Source). Bottom: 2D and 3D tomography chemical images of protein (red) and phospholipid (blue-green) distributions in human hair. (Ref. Nature Methods, 10, 861 (2013), courtesy of Dr Mike Martin, ALS).



INDUSTRIAL WORKSHOP

Applications of the ALBA Synchrotron to the biomedical sector



7 May 2015

The workshop is addressed to pharmaceutical companies willing to use synchrotron light in their experiments.

It will include **conferences**, **a poster session**, **case studies and a visit** to ALBA's facilities to promote information exchange and discussion among the attendees.

FREE Registration

Open till 4th May https://indico.cells.es/indico/event/28

ALBA Synchrotron Ctra. BP 1413, km. 3,3 Cerdanyola del Vallès

Some of the available techniques at ALBA will be presented: powder diffraction, absorption, SAXS, WAXS, macromolecular crystallography and X-ray microscopy.









APRIL 2015 - No. 39 ALBA Trews

MIRAS status

Igors Šics - ALBA Synchrotron, Experiments division

MIRAS is one of phase II beamlines, currently in the construction stage at the ALBA synchrotron light facility. Once completed, it will provide ALBA facility users with a modern infrared microspectroscopy facility optimized for work in mid-IR region.

MIRAS' project at ALBA was launched in 2009. Experimental options in both the far-IR and mid-IR regions were projected with the capacity to address the present and future requirements of the scientific community not only in Spain but also in Europe as a whole. The project was formally approved for funding in 2010, but was frozen due to the difficult economic situation in the country. However, by the end of 2013 the project was reactivated again, thanks to a close collaboration between staff from ALBA. SOLEIL and the CSIC.

This project is being developed together with the mechanical engineering group led by Carles Colldelram and the optics group led by Josep Nicolas in close collaboration with the rest of ALBA's divisions. Very recently, in March 2015, Ibraheem Yousef has joined ALBA as the person responsible for the beamline.

Bending Magnet 04 of the ALBA Storage Ring was selected, after careful analysis, to become the IR radiation source for the MIRAS beamline. A modified dipole chamber enabling collection angles of 43 x 25.17 mrad² was installed during the summer shutdown of 2014. The dipole chamber design implements horizontal IR beam extraction geometry using a laterally inserted flat mirror. The mirror is provided with a horizontal transverse slot in order to avoid interaction with the central high energy core of the dipole emissions and thus avoid thermal loading. Only the IR and visible light fraction of the dipole radiation emissions is collected by the mirror and redirected towards the emission port. A high stability XYZ positioning system for M1 mirror, designed by ALBA engineers in collaboration with colleagues from the SOLEIL SMIS beamline, allows for a crucially important accurate positioning of M1 mirror with respect to the dipole emission fan and electron beam (see Fig.3).

During the winter shutdown (in December 2014), a tunnel wall drilling was performed by the Infrastructure section of the Engineering division to accommodate the emission port of MIRAS (see sequence of pictures in Fig. 4). At the time of publication of this article, all hardware parts of M1 Extraction are being manufactured. It is planned to have them delivered and tested during the first half of the 2015 summer with subsequent installation in the dipole chamber during summer shutdown period.

After the extraction, IR beam is transported through an optical train of 1:1 symmetrical imaging scheme to the first endstation inside the MIRAS experimental hutch in the hall. It is scheduled to have the MIRAS experimental hutch erected and functional by the end of the first half of 2015. The design of the experimental hutch foresees two more downstream endstations as a near future upgrade of the MIRAS beamline. One of them is projected as a customizable platform for experiments with user-supplied equipment under the BYOD (Bring Your Own Device) policy.

The optical design of MIRAS includes the option for splitting IR beam in two parts, separating the dipole emission and edge radiation fractions of the IR beam. This enables to use them either separately at different endstations or to deliver both fractions to the same endstation. At the end of the transport chain, a confocal scanning system will deliver a beam of approximately1000x the brightness of a conventional infrared source into a spot of 5-10 um diameter in a commercial FTIR microscope endstation.

Ray-tracing and optical simulations have been carried out using SRW, RAY, SpotX and ART codes in order to simulate IR beam propagation and verify the optical layout. Specifications for the mechanics of the main optical elements comprising the beam transport system as well as mechanical designs have been completed and are about to be manufactured. They are planned to be delivered by the end of 2015. After appropriate commissioning, MIRAS is expected to carry out measurements in Autumn 2016.



stage

Extraction mirror

XYZ Positioning Vacuum interface with dipole chamber

Figure 3: 3D model of the IR extraction mirror assembly for the MIRAS beamline. © ALBA Engineering division











Figure 4: Sequence of images of the tunnel wall drilling done in December 2014. © ALBA Engineering division

What is MIRAS and what are its scientific applications?

IR + MS = IRMS

Infrared Spectroscopy Microscopy

Infrared Microspectroscopy MIRAS (Spanish acronym for "microespectroscopia infrarroja con radiación de sincrotrón") A big community - 42 scientific cases presented with the MIRAS proposal - 182 people from 56 research groups/departments in 15 universities, 11 CSIC institutes and 5 mixed and other research centres

IRMS has a great impact =

2–3 scientific articles per week

27 IR beamlines worldwide

LIFE SCIENCES AND BIOSCIENCES

Biomolecular information from cells and tissues:

- cancer
- neurological diseases
- skin and bone diseases
- diabetes
- tropical diseases
- novel treatment strategies
- biomaterials design
- tissue engineering
- biodegradables for drug delivery
- etc.

Polymeric material science:

 processes like crystalline polymorphism, additive migration, cross-linking, phase-separation and surface structuring
 2D imaging of microscopic chain

orientation phenomena in fibres and composite films • etc.

High Pressure sciences using DAC:

- Synthesis of new materials
- Characterization of materials
- Planetary sciences
- etc.

Food and agriculture:

chemical imaging of plants, seeds, grains, seaweed, etc.
monitorization processes of plant growth, degradation, cooking, etc.

- monitorization of organic
- contaminants in plants
- nutrition and feed science
- etc.

Cultural heritage:

• non-destructive analytical techniques

information about the techniques used in the manufacture, the origin of the materials used, trade, ...
etc.

Environment and geology:

biomineralization studies
in situ and real-time variations in biogeochemical environments
toxicological effects of chemicals, corrosion and pollution
etc.

Surface and catalysis:

- quality control and contaminant identification
- surface corrosion
- solid-state and semiconducting materials
- nanoelectronic devices
- etc.



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Main issue

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Using synchrotron X-rays to defeat the HIV

Ana Cámara-Artigas Almería University



In the novel written by H. G. Wells in 1898 "The war of the worlds", the Martians that exterminate the humanity with their bright ray were finally defeated by the smallest of organisms: microbes. At the beginning of the 21st century, in spite of the many advances achieved in medicine, the destructive power of some viruses is still a major concern to humanity. Nowadays this is evident with epidemics like the recent Ebola outbreak in West Africa. The most amazing thing is how this virus with less than ten encoded proteins can kill one of the more complex beings on the planet, which requires more than a hundred thousand proteins to function. However, although the Ebola has made headlines for several months, it's a virus whose effects are short term and the disease symptoms are very apparent when it is developed and can be infectious. The virus that causes AIDS, the HIV, is different. It is a lentivirus that can show up many years after infection and its transmission is possible even before the disease symptoms become evident. Statistics indicate that a high percentage of AIDS patients may remain asymptomatic for several years after exposure. Dealing with a virus as HIV, which could remain hidden for both the patient and those around him/her, makes the containment of the virus more difficult. As a result AIDS is currently the most widespread lethal viral disease, with a balance of more than 60 million human beings infected since the disease was diagnosed for the first time at the beginning of the 80s.



Figure 5: This human T cell (blue) is under attack by HIV (yellow), the virus that causes AIDS. © Seth Pincus, Elizabeth Fischer and Austin Athman, National Institute of Allergy and Infectious Diseases, National Institutes of Health.

To date, all attempts to develop an effective AIDS vaccine have been fruitless. Current treatments are only able to control the progress of the virus, but not to heal the disease. For many years, a glycoprotein from the surface of the virus, gp41, has become target for vaccine development. This protein, along with gp120, is the "key" of the virus to enter into the CD4 cells and infect them. Once in the cell, the virus remains hidden for years as a Trojan horse, its DNA being inserted into one of the host cells until it wakes up and starts to destroy the immune system.

At the beginning of the 90s, proof was provided of the inhibitory effect of some peptides on the development of AIDS. Just about ten vears later. the first drug based on this strategy was commercialized, Fuzeon (Roche), which works by impairing the viral and cell-membrane fusion. Although the drug was promising, several problems associated with the peptidenature of the drug have greatly limited its application: high cost of peptide synthesis, low stability and easy degradation by proteases. Today, this drug is used as an alternative therapy for those patients for whom other more widespread therapies do not work.

Within the framework of the EURONEUT-41 (2008-2014) European Community project, and with the participation of more than 15 laboratories, more than 30 variants of the amino-terminal region of the gp41 glycoprotein have been designed. Each of these molecules has been thoroughly characterized and tests have been conducted to verify its effectiveness as a vaccine or to stop **Science and society**

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AIDS continues to be a global public health issue, having claimed more than 39 million lives so far, according to the World Health Organization (WHO). © Auntie P_Flickr

the virus infection. These results have recently been published in PNAS and one of these molecules has been shown have a strong inhibition effect on the HIV-1 infection. Besides, this molecule has several advantages over other drugs already in the market: i) it is easy to produce, since the protein is expressed in EColi; ii) the protein fold is composed by three alpha helices tightly packed, which is very stable and resistant to proteases degradation, and finally; iii) a greater inhibitory power of the virus cell entry step.

During eight years, researchers from the Granada University, in collaboration with several European laboratories, have been working on the design and characterization of these molecules. The protein with better results, covNHR3-ABC, has been crystallized at the Almeria University and its structure has been solved from data collected at the ALBA Synchrotron. This information will afford us the chance to study the molecular basis of the enhanced interaction of this new protein with the gp41 glycoprotein. It would help in the future design of new molecules with improved interaction and more inhibitory power. We hope that the bright rays of the ALBA Synchrotron may contribute to the eradication of one of the deadliest microorganisms for humanity, the HIV.





Figure 6: Crystallographic structure of the protein construct. Representation of the superposition of the protein construct onto the theoretical model of the gp41 ectodomain. © Ana Cámara-Artigas, Almería University

Figure 7: View of the crystals where proteins were grown. These crystals were analysed with ALBA X-rays at the XALOC beamline. © Ana Cámara-Artigas, Almería University

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"Single-chain protein mimetics of the N-terminal heptad-repeat region of gp41 with potential as anti-HIV-1 drugs" Sara Crespillo¹, Ana Cámara-Artigas², Salvador Casares¹, Bertrand Morel¹, Eva S. Cobos¹, Pedro L. Mateo¹, Nicolas Mouz³, Christophe E. Martin³, Marie G. Roger³, Raphaelle El Habib⁴, Bin Su⁵, Christiane Moog⁵, Francisco Conejero-Lara¹. *PNAS* **111(51)** 18207-18212 (2014)

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Measuring SESAME magnets

ALBA is testing the bending magnets to be installed at the storage ring of SESAME, the first synchrotron facility that is being built in the Middle East.

• Bending magnets are used in synchrotron light facilities to guide the trajectories of electrons. They are also used as photon sources, since electrons, when submitted to centripetal acceleration, emit synchrotron light.

The ALBA Synchrotron collaborates with the European Organisation for Nuclear Research (CERN) in the construction of the SESAME dipoles. The ALBA Magnetic Measurements lab is responsible for characterizing the magnetic field map of these magnets, that is, for measuring in detail the intensity of the magnetic field in a flat grid containing the trajectory of the electrons. This process is the final step in the production of the magnets, and it ensures that the needed strict tolerances, which are set according to beam dynamics considerations, are met.

To this end, ALBA experts use a measurement bench with a 3D robotic arm with a high accuracy magnetic sensor and a specific methodology –developed during the construction of ALBA Synchrotron– to measure the magnetic field inside the magnets, checking their uniformity and their gradient with an error margin of maximum 0,05%.

This activity is part of the CESSAMag FP7 project, led by the CERN, whose objective is to support the construction of the SESAME light source. Tests have started at the end of 2014 with the validation of the prototype and they will last until the end of 2015 when the last of the 16 bending magnets will be measured.

The ALBA's Magnetic Measurements laboratory is the only laboratory in Spain specialized in measuring big magnetic structures. Apart from ALBA's magnets and insertion devices, it has also been contracted for testing magnets for a number of national and international companies and research centres.



Members of the ALBA Synchrotron involved in the measurement of SESAME's bending magnets. © ALBA

High power RF lab is fully operational

The RF lab, in the ALBA Warehouse, is fully operational since spring 2014, when it obtained the approval to operate by the CSN (Consejo de Seguridad Nuclear).

• The purpose of the RF lab is dual, on one side it is the test bench lab for testing RF equipment before installation into the accelerators, and on the other side, since it is a unique installation in Spain, it is intended to provide support to Spanish institutions and industries performing R&D developments in the RF field. The importance of this last aspect was recognized by the MINECO by giving ALBA a three-year grant to contract a technician (*Personal Técnico de Apoyo*) to operate the RF lab.

Examples of the works being performed at the RF Lab are: the acceptance tests of new IOT tubes for the ALBA Storage Ring and the high power RF conditioning performed on the RF cavity designed and built by CIEMAT (Madrid) for the IFMIF-EVEDA project (Japan).

IOT tests

The ALBA RF system is based on vacuum tube amplifiers, concretely in IOTs (Inductive Output Tubes). Each time one IOT arrives to ALBA, it requires a specific Site Acceptance Test in order to verify compliance with specifications and proper performance before final installation in the ALBA accelerators. This work is done in the RF lab, so that it does not interfere with the normal operation of the accelerators.

High Power RF conditioning of a CIEMAT cavity for IFMIF

Operating the facility is the main objective of ALBA, but secondly, and also of great importance, is to provide support to the Spanish R&D system. One of the several actions in this sense is the collaboration with the CIEMAT institute in Madrid for the development of accelerator technologies.

In this particular aspect we are very proud to have participated in the validation of the first RF cavity fully designed and built in Spain: the buncher cavity for the IFMIF-EVEDA project in Japan, which has been designed by CIEMAT, built by the Spanish industry and tested at ALBA.

Successful high power tests were finished in December last year, when the cavity was powered up to 110% of its nominal operating power at the ALBA RF lab.



Installation at the RF lab of a new IOT, by ALBA personnel under the supervision of a company expert. © ALBA



View of the high power RF lab at the Warehouse. $\ensuremath{\mathbb{C}}$ ALBA



IFMIF Cavity by CIEMAT at the ALBA RF lab. © ALBA

BIOSCIENCES

Visualizing the DNA double-strand break process for the first time

BL-13 XALOC

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Researchers from the Spanish National Cancer Research Centre (CNIO) have been able to observe for the first time DNA double chain breaks. X-ray crystallographic studies were performed at the ALBA Synchrotron and the SLS. Results have been published in Nature Structural & Molecular Biology.

 DNA breaks occur in several natural processes that are vital for life: mutagenesis, synthesis, recombination and repair. In the molecular biology field, they can also be generated synthetically.

Led by Guillermo Montoya from CNIO, a group of scientists have described in detail the mechanism of the DNA double-strand break process. To this end, they developed a method for producing biological crystals to illustrate the chemical process behind this reaction. They also created a computer simulation that makes this process – which lasts a matter of microseconds – visible to the human eye.

Data was collected from about 200 frozen crystals at the macromolecular crystallography XALOC (ALBA) and PXI (Swiss Light Source, SLS, Switzerland) beamlines.

This information can be used in many biotechnological applications: from the correction of mutations to treat rare and genetic diseases, to the development of genetically modified organisms.

The study was carried out in collaboration with Modesto Orozco's computational group at IRB Barcelona, and has been funded by the Ministry of Economy & Competitiveness and the Ramón Areces Foundation.



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 $Biomedicine\ (IRB), Institute\ for\ Research\ in\ Biomedicine\ (IRB\ Barcelona),\ Barcelona,\ Spain.$

4 Departament de Bioquímica, Facultat de Biologia, University of Barcelona, Barcelona, Spain.



Figure 11: The crystal structure of IDmol enzyme in complex with DNA and CA. © Protein Data Bank

Reference: "Visualizing

phosphodiester-bond hydrolysis by an endonuclease" Rafael Molina¹, Stefano Stella^{1,2}, Pilar Redondo¹, Hansel Gomez³, María José Marcaida¹, Modesto Orozco^{3,4}, Jesús Prieto¹ & Guillermo Montoya^{1,2} Nature Structural & Molecular Biology

22, 65-72 (2015), doi: 10.1038/ nsmb.2932 ence Highlic

MATERIALS SCIENCE

First user PDF experiment on Li-ion battery cathode materials at MSPD

BL-04 MSPD

For the first time an international group of researchers from KIT (Germany) and the ALBA Synchrotron performed ex situ total scattering (PDF) experiments at beamline MSPD to complement their in situ powder diffraction investigation of Liion battery cathode materials.

• Pair Distribution Function (PDF) experiments are complementary to traditional crystallographic analysis on powder diffraction data, in which only Bragg reflections are considered. The method utilizes both, Bragg and diffuse scattering, and is a useful technique to investigate short and intermediate range order in materials like glasses, liquids or nanoparticles, as well as amorphous and crystalline materials. PDF measurements require very high momentum transfer, high Q-resolution and good counting statistics at high angles where the intensity of reflections decrease significantly.

PDF measurements on Li-ion battery electrode materials were performed at beamline 04 MSPD at an energy of 30 keV (0.41 Å) using a Mythen II detector. Data was collected using a monochromatic beam in the angular range 0-120° with 0.006° resolution. In order to obtain good counting statistics at high Q values, longer exposure time was used at high scattering angles. Whereas Qmax in the experiment determines the wavelength of the termination ripples in the Fourier Transform G(r), Qdamp is correlated to the (angular) resolution of the setup and leads to a dampening of the peak height in G(r). It is determined by measuring an ideal crystalline material giving the maximum range of coherently diffracting regions that can be investigated with this setup. A measurement with a Ni standard was carried out to find Qdamp and the envelope function for G(r). The fit using a Gaussian envelope function, is shown in Fig. 12. Real space data were processed up to 2000 Å r-value using PDFgetX3 [J. Appl. Cryst. 46, 2013, 560-566] in the range $0 < Q < 26.1 \text{ Å}^{-1}$. The Qdamp value due to limited resolution in Q-space, is 0.005. Fig 12) shows that structural correlations can be detected up to ~600 Å at the MSPD beamline.

The PDF method was then applied on pristine cathode material Li_2VO_2F with space group $Fm\bar{3}m$. Good PDF data was obtained in 3 min. exposure time with excellent beam conditions. The average structure refined by either the Rietveld (Fig 13-a) or PDF method (Fig 13-b) resulted in very similar values (e.g. atomic distances) with a very large atomic displacement parameter (ADP) for Fluorine.

When the atomic fractional coordinates of the F atoms were also refined in the PDF refinement the ADP values of the F sites decreased and the quality of the fit was considerably increased as shown in Fig. 14). This can be explained by a local distortion around the F atoms that cannot be handled with the Rietveld method. For the refinement a 2x2x2 supercell was used with randomly distributed F-atoms according to stoichiometry. The supercell was created using the program DISCUS [J. Appl. Cryst. 30, 1997, 171-175].

Additionally, the PDF method was applied on $Li_{2-x}VO_2F$ at different charge/discharge states showing also distinct differences in local ordering (see Figure 15).



Figure 13: Rietveld refinement (a), and PDF fit (b) of pristine Li₂VO₂F using average structure.



Figure 14: PDF fit of Li₂VO₂F obtained refining scale factor, lattice parameters, isotropic ADPs and atomic fractional coordinates (x, y and z) for Fluorine.

Figure 15: XRD patterns of Li_2VO_2F cathode material at different charge/discharge states.

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ALBA Preced APRIL 2015 - No. 39

MATERIALS SCIENCE

Polymorphic study of alimentary triacylglycerols by SAXS/ WAXS simultaneous measurements: from pure components to end food products

BL-11 NCD

Researchers from the Department of Crystallography and Mineralogy at the Faculty of Geology (University of Barcelona) have analysed the crystallization and polymorphic behaviour of lipid materials from pure triacylglycerol components to end food products.

• Lipids are major nutrients and widely employed as lipophilic materials in the food, cosmetic and pharmaceutical industries. In this large group of compounds, triacylglycerols (TAGs) become the main components of alimentary and industrial fats and oils. The physical properties of the food lipids are primarily influenced by three main factors: crystallization and transformation behaviour, microstructures of lipid crystals and rheological and textural properties exhibited by lipid crystal networks. Lipids exhibit a highly complicated crystallization behaviour, and their physico-chemical properties (e.g. melting, rheology, morphology and texture) are mainly determined by their fatty acid structures and compositions, which are most typically revealed in polymorphism.



We conducted several experiments on different lipid samples at BL11-NCD of ALBA with different objectives: (i) the analysis of triacylglycerol binary mixtures in order to determine their phase behaviour, as a primary approach to more complex systems. (ii) the polymorphic behaviour of fractions of final products, such as cocoa butter under different experimental conditions, and (iii) the analysis of end food products for food authentication (different categories of Iberian ham) and fraud determination (extra virgin olive oil samples). As an example, Figure 16 depicts the SAXS/WAXS patterns obtained when cocoa butter was cooled from 50°C to -50°C and subsequently heated to the initial temperature.

Experiments were based on SAXS and WAXS simultaneous measurements with temperature variation by using a Linkam stage coupled to the beamline, which enable rapid (15 degrees a minute) thermal programs to provide highly accurate structural information. XRD can facilitate fast cooling/heating rate measurements because of its high-intensity X-ray beam and its very high resolution also permits to discriminate between polymorphs of different TAGs, whose characteristic diffraction peaks are almost overlapped. Thus, it is interesting and valuable to examine the polymorphic crystallization of these complex fatty samples, including end food products.

Figure 16: SAXS (up) and WAXS (bottom) patterns for cocoa butter obtained by cooling the sample from the melt (50°C) to -50°C and subsequently heated to 50°C.

MAGNETISM

Researchers determine the surface magnetic moment of magnetite

BL-24 CIRCE

Using the photoelectron microscope at the CIRCE beamline, researchers from the Institute of Physical Chemistry "Rocasolano" (CSIC) and the ALBA Synchrotron have determined the magnetic moment of a well defined magnetite surface. Results of this research have been recently published in Physical Review B.

• Magnetite is the oldest magnetic material known to mankind. With applications in catalysis and magnetic storage of information, it has been proposed for use in spintronics. However, its surface magnetic properties, which can be different from the bulk ones, are still under discussion. Now researchers from the Institute of Physical Chemistry "Rocasolano" of the Spanish National Researcher Council (CSIC) and the ALBA Synchrotron have determined the magnetic properties is crucial for potential applications in interfacing devices, such as spin valves.

The first research work performed uniquely by means of the only low-energy electron and photoelectron microscope in Spain, located at the CIRCE beamline of the ALBA Synchrotron, has just been published in *Physical Review B*. Using the high surface sensitivity and multi-technique capabilities of the microscope, a well-defined magnetite surface has been prepared in-situ and then characterized. The surface magnetic moment, oriented fully in-plane, was found to be crucially affected by the local atomic structure of the surface reconstruction.

"Our next step is to modify in a controlled and reversible way the surface atoms of magnetite to observe the effect on the magnetic moment. By doing this, we will be able to manipulate it", says Juan de la Figuera, CSIC researcher of the Institute of Physical Chemistry "Rocasolano".



Figure 17: Image of the magnetite surface acquired with electrons (left) and its magnetic domains with X rays (right). Field of view: 10 um.

1 Instituto de Química Física "Rocasolano," CSIC, Madrid 28006, Spain 2 ALBA Synchrotron Light Facility, Barcelona, Spain **Reference**: "Spin and orbital magnetic moment of reconstructed $\sqrt{2x}\sqrt{2R45^\circ}$ magnetite(001)" Laura Martín-García¹, Raquel Gargallo-Caballero¹, Matteo Monti¹, Michael Foerster², José F. Marco¹, Lucía Aballe², and Juan de la Figuera¹. *Phys. Rev. B (Rapid Comm)* **91** (2015) 020408(R). DOI: http://dx.doi.org/10.1103/ PhysRevB.91.020408 cience Highlight

MAGNETISM

A (not *that*) soft x-ray magnetic circular dichroism study of ferromagnetic SrRuO,

BL-29 BOREAS

Using the brilliant soft x-rays from the BOREAS beamline, a group of international researchers from Korea, Taiwan, Japan, Germany, Italy, and Spain have studied the magnetic properties of SrRu0,. The results - recently published in Physical Review B - show that the Ru⁴⁺(3d⁴) orbital magnetic moment is close to zero and that the Ru atoms are in the low spin (S=1) state for strained as well as unstrained samples. The BOREAS beamline is one of the few soft x-ray beamlines in the world allowing for magnetic circular dichroism studies well beyond 2 keV photon energies, thus making this rather unique study on 4d transition metal magnetism possible.

SrRuO, is one of the few known 4d transition-metal oxide ferromagnets with a Curie temperature as high as 160 K. Its rare physical properties have raised the interest of the scientific community during the last fifty years and recently also of the applied science sector due to its capacity for being used as an electrically conducting layer within heterostructured magnetic devices as used in storage technologies.

In this study, researchers have grown strained SrRuO, thin layers on (001)- and (111)- oriented SrTiO, substrates and compared them with unstrained SrRuO, single crystals. The technology for

Reference: "Electronic and spin states of SrRuO, thin films: An x-ray magnetic circular dichroism study" S. Agrestini¹, Z. Hu¹, C.-Y. Kuo¹, M. W. Haverkort¹, K.-T. Ko¹, N. Hollmann¹, Q. Liu¹, E. Pellegrin², S. M. Valvidares², J. Herrero-Martin², P. Gargiani², P. Gegenwart³, M. Schneider⁴, S. Esser³, A. Tanaka⁵, A. C. Komarek¹, and L. H. Tjeng¹. Physical Review B 91, 075127 (2015). DOI: http://dx.doi. org/10.1103/PhysRevB.91.075127

growing SrRuO, thin layers on (001) oriented SrTiO, substrates is well known. However, the systematic growth of thin films on (111)-oriented SrTiO, substrates is very recent.

Using synchrotron light from the BOREAS beamline, researchers wanted to determine if the compressive strain from the SrTiO, substrate can indeed induce a spin state transition of the Ru⁴⁺ cations (i.e., from S=1 to S=2) and if the Ru orbital magnetic moment is guenched (i.e., close to zero). Although the latter orbital magnetic moments are usually small, they can have a considerable influence on the anisotropic properties of magnetic systems. To this end, X-ray magnetic circular dichroism (XMCD) studies of the Ru L_{23} absorption edges were performed.

Results show that for the strained as well as the unstrained samples the Ru orbital moment is close to zero and that the Ru spin (and thus the associated spin magnetic moment) is close to the low-spin value of S=1, as could be verified using theoretical calculations on the shape of the Ru L_{23} absorption spectra (see Fig. 18).



Figure 18: Experimental (top) and simulated (bottom) Ru $L_{2,3}$ X-ray absorption (XAS) and x-ray magnetic circular dichroism (XMCD) spectra (the sign of the experimental L_3 XMCD spectrum has been reversed for clarity). The latter theoretical spectra show a transition from the S=2 high spin (HS) to the S=1 low spin (LS) state of the Ru atoms as a function of the ligand crystal field. The best agreement between experiment and theory is obtained for a Ru crystal field strength of 2.62 eV (solid and dotted red lines in bottom part).

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5 Department of Quantum Matter, ADSM, Hiroshima University, Higashi-Hiroshima 739-8530, Japan

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Unique collaboration between Henkel and the University of Malaga towards eco-cement characterization at the ALBA Synchrotron

Working together, scientists from Henkel, ALBA and University of Malaga, using synchrotron-based high-resolution powder X-ray diffraction, have conducted a series of novel experiments to study in real time the setting behavior of new cement formulations.

• The work is an excellent example of a successful collaboration between industry (Henkel), academia (University of Malaga) and a research institution (ALBA), each making their own, unique contribution to the development of new, sustainable technology.

Henkel, under the brand Ceresit, has been in the cement business for over 100 years, ever since the introduction of first cementitious insulation mortar in 1910 (Fig. 19). In recent years, the focus in both construction and consumer cement applications is on eco-friendly technologies, with smaller carbon footprint and reduced CO₂ emissions.

The development of the new eco-cement formulation was performed by Henkel R&D in Dusseldorf, but for advanced real-time characterization the company chose to partner with an external research facility with the necessary expertise in the field of X-ray crystallography, since the knowledge of how crystal phases are developed in novel eco-cement formulation was critical for the performance of the product.

As luck (or perhaps good planning) would have it, the ALBA Synchrotron in Spain had recently commissioned a new MSPD X-ray beamline that was uniquely suited to conduct in-situ studies, thanks to a combination of wide-range, high-energy X-ray beam (8 to 50 keV) and state-of-the-art X-ray detectors. This allowed acquisition of powder X-ray patterns both at high speed to monitor the changes in cement formulations, as well as with high resolution, producing high-quality data, suitable for quantitative analysis (Fig. 20). Thanks to good planning of ALBA staff, and especially the expertise of beamline scientists (Dr. François Fauth, Dr. Inma Peral), the experiments went without a hitch.

The Rietveld refinement, a complex mathematical process of quantitative analyzing X-ray diffraction data, also required a unique set of skills. Here, the expertise of the Head of the ALBA Experiments Division, Dr. Miguel Ángel García Aranda, and his connection with experts from the University of Malaga was leveraged to conduct detailed analysis of experimental data.

As a result of this collaboration, a clear picture of evolution of crystalline phases in cement formulation was obtained, at the extremely wide time scale (15 min - 3 months). But perhaps more importantly, the experience of scientists from Henkel, ALBA and University of Malaga working shoulder-toshoulder has built a good foundation for future collaborations. This work serves as a good example of successful industryacademia-government partnerships.



SER-PAVILION DER WUNNER SCHEN BITUMEN WERKE UNNA LW. WELTAUSSTELLUNG BRÜSSEL. 1910

Figure 19: Advertising poster, showing Ceresit navillion at 1910 World's Fair in Brussel. © Henkel

Henkel



ALBA 7200000 APRIL 2015 - No. 39

New viewport design compatible with high vacuum

A team of ALBA engineers in collaboration with the Centro de Láseres Pulsados Ultracortos Ultraintensos (CLPU) have developed a new design of viewport compatible with high vacuum that can be adapted to a laser compressor chamber.

• At the first step of laser amplification, the laser beam can be transported under normal environmental conditions but compression of beam has to be done under vacuum conditions to avoid scattering. For this reason, it is necessary to introduce a system to allow the laser beam entrance to the vacuum chamber. The system used is a viewport of 126 mm diameter of free space that contains a BK7 glass with a suitable coating that does not disturb the beam. The glass is independent of the viewport structure and a mandatory requirement is that it must be replaceable.

The design of the viewport provides important improvements compared with the classic equipment in the laser field. The design is done in such a way that it does not introduce any local deformation or punctual stress which may deviate the optical properties including a friendly self-centering easy and repeatable way to assemble different glasses on the viewport reducing time and costs.

This technology is the result of the innovation activities within the ALBA Synchrotron and the CPLU. It has been protected via an utility model that has been successfully approved paving the way to its future commercialization.





Fig. 21: Top, 3D model of the viewport. Bottom, viewport test assembly. © ALBA

ALBA and Alibava sign a license agreement for commercialising an X-ray detector

ALBA, Alibava Systems and the Institute of Microelectronics of Barcelona (IMB-CNM CSIC) have developed a radiation detector aimed at measuring the intensity of the beam with high precision when performing an experiment at a synchrotron facility. This new detector enables a correct development of the experiment, ensuring the quality of the obtained data and reducing the time of the experiment.

• The developed device is based on thin transmissive photodiodes (about 10 microns versus 300 microns of the current devices) which are able to detect and characterize X-rays absorbing only a small part of the intensity. The collaboration between the ALBA Synchrotron and Alibava Systems, a spin-off company of the Spanish National Research Council (CSIC) located at the UAB Research Park, has been complemented with a license agreement that lets Alibava commercialise a product originated from research results of the synchrotron facility and the CSIC.

As of today, the device has been successfully tested at the ALBA Synchrotron and other synchrotron facilities, such as the European Synchrotron Radiation Facility (ESRF). It is expected to sell the first detectors in the following months to universities and synchrotron facilities and the person responsible for the project estimates that about 50 devices will be sold per year.

This project is part of the Innovation Team Program (EDI), led by the Catalan Government, whose aim is to improve knowledge transfer from research institutions to companies.





Top, photograph of the X-ray detector. Bottom, view of the detector being placed at the NCD beamline. © ALBA

What's on? Agenda of events

2015 APRIL 21 st -24 th	EuCARD-2 2 nd Annual Meeting
2015 MAY 7 th	Industrial workshop: applications of the ALBA Synchrotron to the pharmaceutical sector
2015 JUNE 15 th - 16 th	DEELS workshop: Diagnostics Experts of European Light Sources
2015 JUNE 16 th - 19 th	VII AUSE Congress and II ALBA User's Meeting
2015 JUNE 22 nd - 23 rd	20 th ALBA Scientific Advisory Committee Meeting

Specialization course on Pair Distribution Analysis

• From 12th to 14th November 2014, former ALBA scientist Inma Peral organised a course for learning the Pair Distribution Function (PDF) method, a very useful tool to study the local structure of glasses, liquids and amorphous materials, crystalline or partly crystalline (e.g. disordered) materials.

The course gathered more than 30 scientists working in the structural characterization of materials from national and international research institutions. The course was addressed to present and future users of the Materials Science and Powder Diffraction beamline (MSPD) at ALBA who were interested in getting experience with the Pair Distribution Function method at all stages: from sample preparation and measurement to the data analysis of the experimental Pair Distribution Function.

Lectures and practical sessions were given by the MSPD beamline staff Inma Peral and Oriol Vallcorba and Mauro Coduri, researcher of the Istituto per la Energetica e le Interfasi (Lecco, Italy). The companies PANalytical and Bruker also took active part in the course explaining how to use Pair Distribution Function at laboratory sources.



Group of participants in the specialization course on Pair Distribution Function (PDF). © ALBA

ALBA celebrates light in 2015

During 2015, the ALBA Synchrotron is organising different activities to make the society aware of the important role of light in our everyday life and, specially, the great advantages of synchrotron light as an analytical tool for performing research of excellence.

• On February 16th the Institute of Photonics Sciences (ICFO), the Spanish Society of Optics (SEDOPTICA), the Royal Academy of Sciences and Arts of Barcelona (RACAB) and ALBA organised the Spanish Opening Ceremony of the International Year of Light.

The participation of ALBA in the Science Festival of Barcelona to be held on April 25th and 26th is focused on light with two demonstrations to show children and their families what the electromagnetic spectrum is and how we use synchrotron light to perform experiments.

The European Researchers' Night at the end of September will let young and adult people from Cerdanyola del Vallès know a bit more about synchrotron light and its properties with games, shows, demonstrations and chats with scientists.

The ALBA Synchrotron will open its doors again in its Open Day planned for the end of 2015 with new activities and contents enhancing the importance of synchrotron light.

Images of the conferences of Ignacio Cirac and Caterina Biscari during the Spanish Opening Ceremony of the International Year of Light 2015. © ICFO / R. Josa







New exhibition in Cosmocaixa

On May a new exhibition about the ALBA Synchrotron will be released at Cosmocaixa, the science museum of Barcelona managed by La Caixa Foundation. In the last months, ALBA has been collaborating with members of La Caixa Foundation to prepare ALBA's presence at the "Top Ciencia" section which is aimed at promoting scientific careers and showing Spanish cutting-edge research. This exhibition will be available during one complete year.

Cosmocaixa receives an average of 7.5 million visitors every year and offers interactive, enjoyable science and an open door for anyone who is eager to learn and understand and who never stops wondering why things are the way they are.



Audiovisual game inside the exhibition. © La Caixa Foundation

Welcome on board!

• From December 2014, nine new members have joined the ALBA Synchrotron. Massimo Tallarida and Ibraheem Yousef have assumed the coordination of phase II beamlines LOREA and MIRAS, respectively. Artur Gevorgyan is a project engineer, specialised in vacuum technologies. Zahra Hazami is performing her PhD on RF systems. Pedro de la Rubia, Antonello Rizzo, Iván García and Iñaki de Diego have started working as floor coordinators, inside the Experiments division. Isidro Crespo has also started working at the XALOC beamline as young researcher hired from CSN grant.







IÑAKI DE DIEGO, floor coordinator, Experiments division





ANTONELLO RIZZO, floor coordinator, Experiments division



IVÁN GARCÍA,

floor coordinator,

Experiments division



ARTUR GEVORGYAN, vacuum engineer. Engineering division



MASSIMO TALLARIDA beamline responsible of LORFA Experiments division



IBRAHEEM YOUSEF, beamline responsible of MIRAS Experiments division

Adela Muñoz awarded recognition for highlighting women's role in science

ALBA collaborator Adela Muñoz, from the University of Sevilla, has been awarded the Meridiana recognition by the regional government of Andalusia. Meridiana awards have the aim of highlighting the work done by institutions, associations or individual persons to defend gender equality rights and



Adela Muñoz next to the president of the regional government of Andalucía, Susanna Díaz, during the Meridiana awards ceremony. © Adela Muñoz

opportunities. Adela Muñoz was selected by the jury because of her personal and professional career, promoting an active role of women in science. She has given many talks about this topic and has written more than 40 articles. She is also taking part in the Association for Human Rights in Afghanistan (ASDHA) to improve women situation in this country.

Beamline responsible for MIRAS and LOREA

Massimo Tallarida is the beamline responsible of LOREA (ARPES phase-II beamline under construction). He received his M.S. degree in Physics at the University of Rome "La Sapienza" and a Ph.D. in Physics at FU in Berlin. working at Fritz Haber Institut. Since 2004, he has been working at the Chair of Applied Physics-Sensors at BTU-Cottbus. His research concerns photoemission (PES) and X-ray absorption spectroscopy (XAS) with synchrotron radiation.

Ibraheem Yousef is the beamline responsible of MIRAS (infrared microspectroscopy phase-II beamline under construction). He received his M.S. degree in Physics at the Hashemite University (Jordan), Then, he performed his Ph.D. at SOLEIL synchrotron entitled "Simulation and design of an infrared beamline for SESAME: applications in microspectroscopy and imaging" (certified by the University Pierre and Marie Curie in Paris). Since 2012, he has been working as a responsible of the Infrared beamline EMIRA at the SESAME synchrotron. His research concerns synchrotron-based Fourier-transform infrared microspectroscopy and imaging.

Francis Pérez, appointed member of the ESRF MAC

Francis Pérez, head of the Accelerators division, has been appointed member of the Machine Advisory Committee (MAC) for the second phase of the European Synchrotron Radiation Facility (ESRF) upgrade. Members of the MAC are selected to advise on all issues related to accelerators research, construction and operation. Congratulations!!







Prof. María Josefa Yzuel, president of the Spanish committee of the International Year of Light 2015

Emeritus professor at the Universitat Autònoma de Barcelona (UAB) and member of the Royal Academy of Sciences and Arts of Barcelona (RACAB), María Josefa Yzuel has developed her professional career in the area of Optics at a national and international level. She has been president of the International Society for Optics and Photonics (SPIE) and recently and she has recently been awarded the Medal of Physics by the Royal Spanish Physics Society (RSEF). This year 2015 she is chairing the Spanish committee for the celebration of the International Year of Light and Lightbased Technologies.

• Why did the United Nations dedicate one year to light and light-based technologies? What is the purpose of the IYL2015?

In December 2013 the United Nations proclaimed 2015 as the International Year of Light and Light-based Technologies to raise awareness of how optical technologies promote "Photonics was designated by the European Commission in 2009 as one of the five key enabling technologies"

development at the same time that provide solutions to worldwide challenges in energy, education, agriculture, communications and health.

2015 was also an appropriate moment because there were noteworthy scientific anniversaries: from the first studies of Optics in 1015 by Ibn Al Haythem to the optical fibre technology discovered by Charles Kao in 1965 or the celebration of 100 years of the general relativity theory by Einstein.

Professor John Dudley led this initiative to ensure that society is aware of the problem-solving potential of light and light-based technologies.

• Which scientific disciplines relate to light?

Optics, Photonics, Physics, Synchrotron-based science, Communications and many other relate to light. Fundamental properties of light can be found in different science disciplines and technologies. Just to mention some of them: the origin of life thanks to the photosynthesis, the study of stars and planets' movements and the Big Bang, the use of X-ray, infrared or lasers in medicine or the spectroscopy technique for studying the structure of matter.

• Light and light-based technologies are in almost every aspect of our everyday life. Which are the main challenges of the field?

Light is everywhere. Many photonic devices are replacing electronic devices in areas like medicine, communications or energy but there is still a long way to go. For example, more efficient photovoltaic instruments are needed to transform solar energy into electricity winning energy independence for future generations. It is also necessary to widen the use of optic and photonic techniques to detect and measure environmental indicators such as the pollution levels or the ozone hole status. Light-based technologies with applications in biology and medicine have already improved disease diagnosis and therapies - for example endoscopy advances or the use of laser in ophthalmology – but they will also make progress in other fields. Our society has to better define the uses of artificial lighting and try to balance the equilibrium between nature and city life. Light and light-based technologies will play an important role in culture and art integrating light in architecture, art restoration and conservation or artistic performances. The use of light in research will also evolve: synchrotron light facilities will be able to produce an even brighter light to perform new experiments in the future.

PRIL 2015 - No. 39 ALBA Decus

These challenges highlight why Photonics was designated by the European Commission in 2009 as one of the five key enabling technologies to allow the development of new goods and services and the restructuring of industrial processes needed to modernise EU industry and make the transition to a knowledge-based and low-carbon resourceefficient economy.

• Which kind of events and activities will be organized in Spain during this year?

In Spain, there are many planned activities to enhance the role of light during 2015. This project has three main objectives. The first one is to improve the science culture about light by organizing public festivals, street activities, exhibitions, seminars, publications, etc. Another goal of this celebration is to improve science teaching and to encourage scientific careers preparing educational materials, workshops at museums and primary and secondary schools, universities and research centres. Collaboration shall also be strengthened between the public and private sectors by organising meetings, trade fairs, scientific forums. etc.

• Is the Spanish society aware of the relevance of light and light-based technologies?

The Spanish society is fully familiarized with light and light-based technologies regarding aspects such as communications, health, art, energy or industrial processes. However, they do not know or understand the science behind them. This is why it is necessary to profit from this unique occasion to explain the society the importance of light and the progresses made in light-based research to improve our well-being.

• When did your interest in understanding light begin?

When I finished my degree in Physics, I had two options: doing my PhD in Theoretical Physics or in Optics, Finally, I chose Optics, under the guidance of Prof. Justiniano Casas. That was a right decision because I extremely enjoyed the experimental work that I performed during my thesis about the quality of photographic image in relation to residual aberrations.

My professional career has continued linked to the understanding of light in different ways: from the evaluation of the image in optical systems to the establishment of quality criteria in medical images or the study of spatial light modulators. During all these years, I've seen how photonics technologies have been introduced in our everyday objects: mobile phones, GPS, television screens, etc. to improve our quality of life.

Further information about IYL2015 activities: International website - www.light2015.org Spanish website - www.luz2015.es

"The Spanish society is fully familiarized with light and light-based technologies. However, they do not know the science behind it."

VII AUSE Congress II ALBA User's Meeting

16-19 June 2015

ALBA Synchrotron Cerdanyola del Vallès (Barcelona)

AUSE Congress

Plenary lectures

- Tilo Baumbach (ANKA)
- Gianfelice Cinque (DIAMOND)
- Klaus Lips (BESSY)

Key-note contributions

- Germán Castro (ESRF)
- Winner of the PhD thesis AUSE award

Oral contributions

ALBA Updates

- Beamline status presentations
- ALBA phases II and III
- Users oral contributions

Satellite workshops

- Photoemission Electron Microscopy (PEEM) at ALBA: Practical user guide and data analysis
- High pressure powder diffraction at ALBA

Awards

- **AUSE Best PhD thesis**
- **AUSE Best oral contribution**
- **ALBA Best oral contribution**
- **AUSE Best poster contribution**
- **ALBA Best poster contribution**

CALL FOR ABSTRACTS OPEN till May 8th





For further information and registration http://indico.cells.es/indico/event/AUSE-ALBA-2015

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