



XI AUSE Conference VI ALBA Users Meeting

> Oviedo 2-6 September 2024





















# **WELCOME**

Welcome to the **joint XI AUSE conference and VI ALBA User Meeting at the town of Oviedo**. In a time of new funding opportunities and the need to address the big challenges of our time, the meeting is a platform for celebrating great scientific success, exchange and align within the community and learn more about what is planned to make your X-ray research infrastructures ready for your needs. Perhaps even more important, it will give you a voice to communicate your needs as well as ideas to improve the services.

This conference joins, as usual in the last decade, the **biannual AUSE meetings with the ALBA User meeting**, reflecting a long success story of community growth and community engagement with its X-ray research infrastructures. Alternating between hosting universities and ALBA as venue, the meeting series is a symbol and expression for the great integration of the facility with its user community and the open welcome culture to new communities.

The meeting is connecting three building elements: the first one dedicated to the AUSE activities, including an update on the Spanish ESRF CRG beamline SpLine, the second focused on ALBA and its upgrade ALBA II, and the last session dedicated to the Spanish XFEL Hub activities.



**Network:** AUSE\_2024 WiFi **Password:** Sincrotron 24

# **SPONSORS**





# **SPECS**GROUP



# **COMMITTEES**

### **CONFERENCE CHAIRS**

Caterina Biscari, ALBA Synchrotron Director Inés Muñoz, AUSE President

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Bárbara Calisto, AUSE, ALBA Synchrotron Inmaculada Ramos-Lerate, AUSE, Universidad de Cádiz Juan Rubio, AUSE, ESRF Wojcjech Gawelda, AUSE, IMDEA-UAM

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María Vélez Fraga, Universidad Oviedo
Ramon Pons, IQAC-CSIC
Wojcjech Gawelda, IMDEA-UAM

# **PROGRAM**

# **Monday, 2nd September 2024**

# **Timetable**

11:00 - 13:00	Hall (Edificio del Aulario, Facultad de Geología, Universidad de Oviedo (Oviedo, Spain)) Registration & Sponsors' Exhibition
13:00 - 14:30	Hall (Edificio del Aulario, Facultad de Geología, Universidad de Oviedo (Oviedo, Spain)) Lunch, Poster & Sponsors' exhibition
	Aula E (Edificio del Aulario, Facultad de Geología, Universidad de Oviedo (Oviedo, Spain))
14:30 - 14:45	Chair: Aurelio Hierro (Universidad de Oviedo) Opening Irene Diaz Rodriguez, Vicerector of Research, Univ. de Oviedo
14:45 - 15:30	Plenary Speaker Gianluigi A. Botton (Diamond Light Source) Diamond Light Source: Science and updates on the Diamond-II upgrade

Timetable	Session A   Soft Condensed Matter Aula E, Facultad de Geología, Univ. Oviedo	Session B   Advanced Materials for Energy and Sustainable Applications Aula B, Facultad de Geología, Univ. Oviedo	
15:30 - 16:00	Keynote Speaker Mari Cruz García-Gutiérrez (IEM-CSIC) Synchrotron radiation in polymer science: techniques and sample environments	Keynote Speaker Enrique G. Michel (IFIMAC, UAM) Understanding Li-ion battery materials with synchrotron radiation	
16:00 - 16:20	Esther Rebollar (IQF-Blas Cabrera, CSIC) Structure development during "in-operando"3-D printing using simultaneous Small and Wide Angle X-ray Scattering measurements	Juan J. Velasco (ALBA Synchrotron) Controlling the number of coordinatively unsaturated iridium oxide active centers for optimize the electrocatalytic oxygen evolution reaction	
16:20 - 16:40	Alba Cazorla Moreno (ICMAB-CSIC) Monitoring the structural transformation on thin films of an Asymmetric Benzothieno[3,2-b] [1]-benzothiophene Derivative	Cheng Liu (ICMAB-CSIC) Synchrotron radiation to solve the puzzle of capacity limitation in Aqueous Zn-MnO2 Batteries	
16:40 - 17:00	Fernando Garcia Martinez (DESY) Structure and pressure gap in the NO reduction on Rh studied by ambient-pressure HAXPES Wojciech Olszewski (University of Bialystok) The role of the local structural properties in the electrochemic characteristics of Na1-xFe1- yNiyO2		
17:00 - 17:20	Aula E, Facultad de Geología, Univ. Oviedo Wojciech Gawelda (AUSE) and Barbara Calisto (ALBA Synchrotron) News from ESUO and the NEPHEWS project		
17:20 - 18:00	Aula E, Facultad de Geología, Univ. Oviedo AUSE Assembly		
18:00 - 19:00	Hall, Facultad de Geología, Univ. Ovi Poster Session, Coffee & Sponsor		

# **Tuesday, 3rd September 2024**

Timetable 09:00 - 09:45	Aula E (Edificio del Aulario, Facultad de Geología, Univ. Oviedo) Chair: Judith Juanhuix (ALBA Synchrotron) Plenary Speaker - Blake H. Balcomb (Diamond Light Source) XChem: High throughput crystallographic fragment screening and structure enabled fragment progression			
	Session A   Drug Discovery Aula E, Facultad de Geología, Univ. Oviedo  Session B   In-situ and in- operando processes Aula B, Facultad de Geología, U Oviedo			
09:45 - 10:15	Keynote Speaker Jose Manuel Martin (IQFR-CSIC) Time-resolved Crystallography: A New Frontier in Drug Discovery	Keynote Speaker Manuel Izquierdo (EuXFEL) Femtosecond soft X-ray photoelectron spectroscopy on solids at the European XFEL		
10:15 - 10:35	Ruben Martínez-Buey (Universidad de Salamanca) Structural approaches to identify novel inhibitors of IMP dehydrogenase enzymes	Anna Makarova (Helmholtz-Zentrum Berlin) Catalytic oxidation of CO by step and kink sites of curved Au crystal		
10:35 - 10:55	Stefano Pernigo (ALBA Synchrotron) Fostering innovation in drug discovery by automated data collection and X-ray based fragment screening at ALBA	Alexander Missyul (ALBA Synchrotron) In situ powder diffraction as a key for understanding materials behavior in non-ambient atmosphere		
10:55 - 11:15	Alba Garay Álvarez (IQF Blas Cabrera-CSIC) Combating Friedreich's Ataxia with Nanobodies: Structural Characterization of complexes with Frataxin  Cristina Echevarria Bonet (Universidad de Oviedo) The role of anharmonicity or thermoelectric properties of Heusler alloys			
11:15 - 11:40	Hall, Facultad de Geología, Univ. Oviedo Coffee Break & Sponsor exhibition			
11:40 - 12:25	Plenary Speaker - Carlos Martí-	ultad de Geología, Univ. Oviedo) Gastaldo (ICMol and Universidad de mical complexity in reticular frameworks		

# **Timetable**

	Aula E (Edificio del Aulario, Facultad de Geología, Univ. Oviedo)
12:25 - 12:55	Keynote Speaker - Juan Rubio (SpLine ESRF) BM25-SpLine at the ESRF: Status and perspectives
12:55 - 13:15	AUSE Thesis Award - Shiva Shirani (University of Malaga) Advanced Quantitative Synchrotron X-ray Imaging of Cement Microand Meso-Structures
13:15 - 13:35	AUSE Thesis Award - Daniel Perez Salinas (ALBA Synchrotron) Inhomogeneity and disorder in ultrafast phase transitions
13:35 -15:00	Hall, Facultad de Geología, Univ. Oviedo Lunch, Poster & Sponsor exhibition
15:00 - 15:45	Chair: José Luis García Muñoz (ICMAB-CSIC) Plenary Speaker - Amalio Fernández-Pacheco (TU Wien) Investigations in three-dimensional nanomagnetism using X-ray techniques
15:45 - 16:15	Keynote Speaker - Antonio Urbina (Universidad P. Navarra, SETN) Neutron scattering as a complementary tool for X-Ray Synchrotron Radiation techniques
16:15 - 17:00	Hall, Facultad de Geología, Univ. Oviedo Poster, Coffee & Sponsor exhibition

# **Tuesday, 3rd September 2024**

# **Timetable**

	Session A   Biotechnology & Biological Sciences Aula E, Facultad de Geología, Univ. Oviedo Chair: Tanja Ducic (ALBA)	Session B   Electronic and Magnetic Matter Aula B, Facultad de Geología, Univ. Oviedo Chair: Maria Velez (Universidad de Oviedo)
17:00 - 17:30	Keynote Speaker Montserrat Soler-Lopez (ESRF) Advancements in Biological Sciences at the European Synchrotron	Keynote Speaker Lucas Perez (UCM) Unveiling the magnetic secrets of cylindrical nanowires with X-ray microscopy
17:30 - 17:50	Alessandra Patera (ALBA Synchrotron) Fast X-ray TomogRaphy Beamline for ALBA	Ji Dai (ALBA Synchrotron) Spin polarized bulk bands with large energy splitting due to Dresselhaus effect in ZnTe(110)
17:50 - 18:10	Hector Dejea (ESRF) Synchrotron-based phase contrast tomography for cardiovascular applications: from rodents to humans	José Luis Garrido Álvarez (Universidad de Oviedo) Structural Analysis by High- Resolution X-Ray Diffraction of Ferromagnetic Lu2Fe17 Melt- Spun Ribbons
18:10 - 18:30		Beatriz Muñiz Cano (IMDEA Nanociencia) Experimental observation of a magnetically induced warping transition in a topological insulator mediated by rareearth surface dopants using angle-resolved photoemission spectroscopy

# Wednesday, 4th September 2024

Timetable 09:00 - 09:45	Aula E (Edificio del Aulario, Facultad de Geología, Univ. Oviedo) Chair: Klaus Attenkofer (ALBA Synchrotron) Plenary Speaker - Caterina Biscari (ALBA Synchrotron) ALBA and its future, ALBA II
09:45 - 10:25	Science at ALBA Session Amadeu Llebaria (MCS, IQAC-CSIC) Photopharmacology: light and molecules for dynamic structural crystallography
10:25 - 11:05	Arantzazu Mascaraque (UCM) How ARPES can contribute in advanced materials research?
11:05 - 11:30	Hall, Facultad de Geología, Univ. Oviedo Coffee Break & Sponsor exhibition
11:30 - 12:10	Christian Masquelier (UPJV, LRCS) Crystal Chemistry of Important Polyanionic Materials used as Cathodes in Sodium-Ion Batteries: the decisive impact of Synchrotron X-Ray diffraction
12:10 - 12:50	Gonzalo Abellan (ICMol, UV) Two-dimensional Layered Hydroxides for Energy Applications
12:50 - 13:30	Elzbieta Pach (ICMAB-CSIC) In-situ X-Ray Diffraction revealing the reaction mechanism of ultrafast Transient Liquid Assisted Growth of superconducting thin films
13:30 - 15:00	Hall, Facultad de Geología, Univ. Oviedo Lunch, Poster & Sponsor exhibition
15:00 - 15:25	Chair: Montserrat Soler-Lopez (ESRF) ALBA Beamlines Upgrade Program Session Judith Juanhuix (ALBA Synchrotron) Updates from the Life Sciences Section
15:25 - 15:50	Manuel Valvidares (ALBA Synchrotron) Updates from the Electronic and Magnetic Structure of Matter Section
15:50 - 16:15	Carlo Marini (ALBA Synchrotron) Updates from the CHEMAT Section, The Beamline Upgrade Program
16:15 - 16:40	Lucia Aballe (ALBA Synchrotron) Updates from the IMM Section

# Wednesday, 4th September 2024

Timetable 16:40 - 17:10	Hall, Facultad de Geología, Univ. Oviedo Coffee Break & Sponsor exhibition			
	<b>Session A</b>   Materials Science Aula E, Facultad de Geología, Univ. Oviedo Chair: Alexander Missyul (ALBA)	Session B   Life Sciences Aula B, Facultad de Geología, Univ. Oviedo Chair: Inés Muñoz (CNIO)		
17:10 - 17:30	Iciar Monterrubio (CIC energiGUNE) Building a Materials Acceleration Platform (MAP) for battery materials research: Automated module for the synthesis of inorganic compounds	Marc Corrales (MRC-LMB) Multiscale connectomics for neuroevolution: X-Ray tomography and FIBSEM		
17:30 - 17:50	Frederik Schiller (Centro de Física de Materiales) Near ambient pressure oxidation of silver in the presence of steps: electrophilic oxygen and sulphur impurities	Tanja Ducic (ALBA Synchrotron) Macromolecular and structural changes in glioblastoma cell line after carbon dots and riluzole treatments: Synchrotron-based FTIR and X-ray		
17:50 - 18:10	Miguel Ángel García Aranda (Universidad de Malaga) 4D nanoimaging of Portland cement hydration			
18:10 - 18:30	Gloria Subias-Peruga (INMA, CSIC-Univ. Zaragoza) The barocaloric effect in the Fell(5NO2-pap)2 spin-crossover complex via low-pressure synchrotron powder X-ray diffraction	Round Table on Life Sciences 17:50-18:30		
20:00	Conference dinner at Restau C. Rúa, 15, 33003 Oviedo, Asturias	rant Ruaquince		

# Thursday, 5th September 2024

Timetable	Aula E (Edificio del Aulario, Facultad de Geología, Univ. Oviedo)		
09:00 - 09:45	Chair: Lucía Aballe (ALBA Synchrotron)  Plenary Speaker Santiago Garcia-Granda (CINN-CSIC, U. Oviedo and IUCr President)  Design of processable polymeric carbon nitride materials for catalytic applications		
	Session A   Magnetism Aula E, Facultad de Geología, Univ. Oviedo Chair: Manuel Valvidares (ALBA)	Session B   Multi-modal studies Aula B, Facultad de Geología, Univ. Oviedo Chair: Lucía Aballe (ALBA)	
09:45 - 10:05	Massimo Tallarida (ALBA Synchrotron) Searching for monolayer flakes at LOREA	Iris Henríquez Valido (UAB-IPREM) Multi-scale and multimodal imaging combining NanoSIMS and Synchrotron techniques	
10:05 - 10:25	A. Estela Herguedas-Alonso (Universidad de Oviedo) The transition of magnetic textures from quasi 2D to 3D microstructures	Ignacio José Villar García (CEU San Pablo University) XPS, XAFS, XRD and FTIR Operando Studies of a Vanadium based (H2V3O8) Lithium-ion Battery at ALBA beamlines	
10:25 - 10:45	Sofia de Oliveira Parreiras (IMDEA Nanociencia) Engineering of organolanthanide sandwich complexes by on- surface synthesis	María González Ingelmo (INCAR-CSIC) Ni and Fe Doped Graphene Aerogels Prepared by Freeze-Casting: Investigating the Effect of Fe through In Situ Synchrotron Characterization	
10:45 - 11:05	Kevin Garcia Diez (ICN2-ALBA) Electronic properties of Bismuth monolayers grown on metallic substrates	Laia Pascua Solé (UPC) Impact of Co-doping on Pd/Al2O3 Catalysts for Methane Oxidation: A Characterization Study	
11:05 - 11:30	Hall, Facultad de Geología, Unio Coffee Break & Sponsor exhi		

# Thursday, 5th September 2024

Timetable 11:30 - 11:50	Aula E (Edificio del Aulario, Facultad de Geología, Univ. Oviedo) Chair: Alejandro Sánchez (ALBA) Oscar Matilla (ALBA Synchrotron) More Than Data: Computing Services for Synchrotron Users
11:50 - 12:10	Barbara Calisto (ALBA Synchrotron) ALBA Industrial Program
12:10 - 13:30	Moderator: Klaus Attenkofer (ALBA Synchrotron) Round Table: The Next Generation Light Sources
13:30 - 15:00	Hall, Facultad de Geología, Univ. Oviedo Group Photo, Lunch, Poster & Sponsor exhibition
15:00 - 15:45	Chairs: W. Gawelda (AUSE, IMDEA-UAM), J.M. Martín (IQF-CSIC) Plenary Speaker Roberto Alonso Mori (LCLS-SLAC) Using LCLS to study ultrafast structural and electronic changes in bio and condensed phase chemistry systems
15:45 - 16:05	XFEL session Yifeng Jiang (EuXFEL) Capturing ultrafast molecular motions and lattice dynamic response in a spin crossover thin film using femtosecond electron diffraction and X-ray diffraction
16:05 - 16:25	Rebeca Castillo (MPI Mulheim) Investigation on electronic structure and reactivity in heterometallic proteins using femtosecond X-ray absorption spectroscopy
16:25 - 16:45	Ben van Kuiken (EuXFEL) Ultrafast soft X-ray investigations of solution phase molecular photochemistry and photophysics at EuXFEL
16:45 - 17:10	Hall, Facultad de Geología, Univ. Oviedo Coffee Break & Sponsor exhibition
17:10 - 17:40	Keynote Speaker Filipe Maia (Uppsala University) Ultrafast biological imaging at the European XFEL, without crystals
17:40 - 18:00	Jos Kamps (Diamond Light Source) Expanding drop on fixed target approaches using droplet addition
18:00 - 18:20	Cristian Svetina (IMDEA Nanociencia) The long path to extend transient grating spectroscopy into the X-rays
18:20 - 18:40	Ángel Fernández Rodriguez (EuXFEL) Imaging femtosecond laser-induced lattice distortions inside crystalline semiconductors by Ultrafast Dynamical Diffraction

# Friday, 6th September 2024

Timetable	CoDI workshop Aula E (Edificio del Aulario, Facultad de Geología, Univ. Oviedo) Chairs: M.A. Garcia Aranda (Univ. Malaga), A.Fernández Rodriguez (EuXFEL)
09:00 - 09:30	Irene Calvo (Univ. Zaragoza) Leveraging X-ray coherence to probe the complexity of materials under realistic conditions
09:30 - 10:00	Virginie Chamard (Univ. Marseille) Bragg Coherent Diffraction Imaging: from simple particles to complex crystalline materials
10:00 - 10:30	Pablo Villanueva-Perez (University of Lund) Coherent imaging opportunities at diffraction-limited storage rings (remote talk)
10:30 - 11:00	Hall, Facultad de Geología, Univ. Oviedo Coffee Break
11:00 - 11:30	Angel Rodríguez-Fernández (EuXFEL) CoDI, Coherent Diffraction Imaging BL at ALBA II - technical details
11:30 - 11:50	Ana Diaz (PSI) Non-destructive imaging of computer chips on the nanoscale by X-ray ptychography
11:50 - 12:10	Miguel A. G. Aranda (Universidad de Malaga) X-ray nanoimaging of cement hydration
12:10 - 12:30	Catalin Popescu (ALBA Synchrotron) X-ray nanodiffraction as a probe for structural dynamics in Earth and Planetary sciences ( <i>remote talk</i> )
12:30 - 12:50	Allan Johnson (IMDEA Nanociencia) Imaging phase co-existence in quantum materials (remote talk)
12:50 - 13:10	José Solla (Univ. Alicante), Victor de la Peña (IMDEA Energia) X-ray nanoimaging in photo-electrocatalysis (remote talk)
13:10 - 13:30	Miguel Anaya (Univ. Sevilla) X-ray nanoimaging of optoelectronic materials (remote talk)
13:30 - 13:50	Sandra Ruiz Gómez (ALBA Synchrotron) Unveiling New Frontiers in spintronics through Multi-Length Scale Imaging and Correlative Microscopy
13:50 - 14:30	Round table including future actions

# **POSTERS**

# #110 Javier Ignacio Diaz Fernández

Large segregation to the surface of the rare earth in NdCo5 amorphous thin films with perpendicular magnetic anisotropy probed by hard X ray photoemission

# **#111 Alicia Estela Herguedas Alonso**

X-ray transmission microscopy of dipolar-coupled bilayers with crossed anisotropies for reconfigurable spin wave transport

# **#116 Angel Rodriguez Fernandez**

Materials Imaging and Dynamics Instrument at the European XFEL Facility

### #127 Beatriz Muñiz Cano

Effects on the topological surface state induced by Er magnetic doping in the prototypical topological insulator Bi2Te3 studied by photoemission spectroscopy

## #131 Mariam Barawi Moran

The potential of in situ XAS to reveal the role of aliovalent dopants in TiO2 nanocrystals for advanced energy storage and smart windows

### #139 Lucia Aballe Aramburu

RIANA - Research Infrastructure Access in NAnoscience & nanotechnology

#### #140 Inmaculada Ramos Lerate

Preliminary Studies for the Use of Sludges from the Petroleum Industry as Agricultural Fertilizers. Characterization by XANES

#### #144 Julia Herrero Albillos

Morphology and dynamics of domains and domain walls through asymmetric hole densitygraduated 2D-arrays

# #145 Alicia Estela Herquedas Alonso

GUI for magnetic imaging and tomography in MISTRAL

## #147 Alicia Estela Herguedas Alonso

Normalization for visualization of weak magnetic signals at MISTRAL beamline

# **#148 Antonio Urbina**

In operando XRD study of Bi2O3, h-MoO3 and MnO2 electrodes during charge/discharge processes of Zn batteries

## #150 Jose Luis García-Muñoz; Marti Gich

Tuning the magnetic properties of epsilon-Fe2O3 nanoparticles by Cr-doping

### #154 Nicolas Soler

Bridging Science and IT: ALBA's Scientific Data Management Section

# #168 Juan Francisco Hidalgo Lopez

Dynamic re-shaping of single Au NRs in colloidal suspension observed with ultrafast coherent diffractive imaging

### #173 Camilo Andrés Jaramillo Hernández

Influence of Crystallographic Structure on the OER Performance of Co & Ni-based Layered Hydroxides

## #176 Josep Roqué Rosell

Applying X-ray Absorption Spectroscopy (XAS) at ALBA to the Study of Heavy Metal Pollution in Marine Sediments

### #179 Wojciech Gawelda

NEXT - An international network for Nonlinear Extreme ultraviolet to hard X-ray Techniques

#### #180 José Manuel Martín García

Spain XFEL Hub: A bridge between the Spanish research community and XFEL facilities

## **#181 Elizabeth Vergara**

Electron transfer-induced structural changes in prion proteins studied by ultrafast X-ray absorption spectroscopy

### **#186 Carlos Quirós**

In-situ micro-Laue x-ray diffraction strain mapping of piezoelectric actuators

## #193 Seyedeh Leila Panahi

The Methodology Group at ALBA: Bridging Disciplines to Innovate Analysis in Science and Industry

### #194 Juan J. Velasco

3Sbar: The new HAXPES/SXRD ALBA synchrotron beamline









