



GE3C
XXXI Simposio
ICIQ Tarragona
16-19 de enero 2024

**Avanzando hacia el Futuro a través de la
Cristalografía**



Real
Sociedad
Española de
Física

Programa Científico Detallado

Martes 16 de enero

13:30 – 14:30 Registro ICIQ
Avinguda dels Països Catalans, 16, 43007 Tarragona

14:30 – 15:00 Acto Bienvenida
Organizadores XXXI Simposio GE3C:
Jordi Benet-Buchholz y Eduardo C. Escudero Adán

Santiago García Granda (Presidente de la Unión Internacional de Cristalografía)
Luis Viña (Presidente de la Real Sociedad Española de Física)
Antonio M. Echavarren (Presidente de la Real Sociedad Española de Química)
Armando Albert de la Cruz (Presidente del Grupo Especializado de Cristalografía y Crecimiento Cristalino)
Emilio Palomares (Director del Institut Català d'Investigació Química)

Entrega de Premios
Moderadores: Jordi Benet-Buchholz y Sol López Andrés

Premio Xavier Solans Bruker 2023

15:00 – 15:30 Conferencia premiada: **Álvaro Vílchez-Cózar**
Tuning the activity of cobalt 2-hydroxyphosphonoacetates-derived electrocatalysts for water splitting and oxygen reduction: Insights into the local order by pair distribution function analysis

Presentación de Empresas Patrocinadoras de la reunión

15:30 – 15:45 Empresa: Bruker • Conferenciante: **Carsten Lenczyk**
Bridging the gap between Electron and X-ray Diffraction

15:45 – 16:00 Empresa: Rigaku • Conferenciante: **Khai-Nghi Truong**
XtaLAB Synergy-ED: 3D ED/MicroED made easy

16:00 – 16:15 Empresa: Anton Paar • Conferenciante: **Marius Kremer**
Modern non-ambient X-ray diffraction for the investigation of minerals, metals and industrial materials of any type

16:15 – 16:30 Empresa: Malvern Panalytical • Conferenciante: **Javier Bolivar**
Towards automated high-throughput screening in materials chemistry

16:30 – 17:00 Pausa Café

Entrega de premios del GE3C

17:00 – 17:15 Insignia de Oro GE3C

17:15 – 17:30 Premio Sagrario Martínez Carrera 2023

Conferencia a cargo de los Premios Sagrario Martínez Carrera 2022

17:30 – 18:00 Guillermo Mínguez: Solvent-free synthesis of Metal-Organic Frameworks: a route towards elusive materials

18:00 – 18:30 Felipe Gándara: Desentrañando la Red: El Papel Crucial de la Química Estructural y la Cristalografía en la Química Reticular

Mesa Redonda: Mujeres y Cristalografía.
Moderadoras: María José Sánchez Barrena y Josefina Perles

18:30 - 19:30 Mesa Redonda

19:30 – 21:00 Cena

Miércoles 17 de enero

Sesión 1: Cristalografía de Proteínas y Más Allá
Moderadores: Inés G. Muñoz y José Antonio Gavira

9:00 – 10:00 Ponente invitada: **Aitziber López Cortejarena**
Crystal Assembly Design through Protein Engineering and Contact Modulation Strategies

10:00 – 10:20 **Immaculada Pérez-Dorado:** Pursuing the enzyme N-myristoyl-transferase as drug target in human disease, deciphering its catalytic mechanism and interactome

10:20 – 10:40 **Isabel Uson:** Predictions and experiments in structure determination

10:40 – 11:00 **Alberto Marina:** Un nuevo mecanismo de represión en fagos que se comunican por el sistema arbitrium

11:00 – 11:30 Pausa Café

11:30 – 11:43 **Alice Grieco:** Serial synchrotron crystallography to decipher NQO1 dynamics at the active site during the formation of the NADH-reductive competent interaction

11:43 – 11:55 **Fernando Ceballos-Zúñiga Ulla:** Unraveling the role of the Ecc5DUF domain in the ESX5 secretion in Mycobacterium tuberculosis

11:55 – 12:05 **María Rivera Moreno:** Towards a more resilient agriculture: Re-engineering ABA receptors

12:05 – 12:18 **Miguel Daniel Mozo:** Unveiling a Novel pH Sensing Module in Plant Proteins: Implications for Vacuolar Antiporter Regulation

12:18 – 12:30 **Uxía Pérez De José:** Structural Characterization of PdaA, an N-deacetylase from Clostridium difficile

12:30 – 12:43 **Alejandra Alba:** Crystal optimization and structural characterization of metallo- β -lactamase CAU-1 from Caulobacter crescentus

12:43 – 13:00 **Ángela Fernández García:** Crystallographic analysis of a short unspecific peroxygenase and molecular characterization of the substrate binding site

13:00 – 14:00 Pausa Comida
Reunión Abierta GE3C/Comité Español de Cristalografía

Sesión 2: Grandes Instalaciones para Estudios Estructurales (esponsorizado por AUSE)
Moderadores: Laura Cañadillas Delgado y Guillermo Mínguez Espallargas

14:00 – 15:00 Ponente invitada: **Judith Juanhuix**

	Review of the crystallography beamlines at the ALBA synchrotron light source and future perspectives within the ALBA-II major upgrade project
15:00 - 15:25	Gastón Gabarino: New opportunities on the studies of condensed matter systems under extreme conditions at the ESRF-EBS
15:25 - 15:50	Iván Da Silva: Crystallographic studies at ISIS Neutron and Muon Source facility
15:50 - 16:05	María José Sánchez Barrena: Exploiting the most from synchrotron fragment-screening data for the discovery of protein-protein interaction regulatory compounds with therapeutic potential in neuronal disease
16:05 – 16.35	Pausa Café
16:35 - 17:00	Pablo Bereciartua: Resonant Elastic X-ray Scattering at beamline P09
17:00 - 17:25	Iurii Kibalin: Elucidating Individual Magnetic Contributions in Bi-Magnetic Fe ₃ O ₄ /Mn ₃ O ₄ Core/Shell Nanoparticles by Polarized Powder Neutron Diffraction
17:25 - 17:40	Stanislav Savvin: XtremeD: new Spanish CRG diffractometer for extreme conditions
17:40 - 17:55	José Manuel Martín García: Towards deciphering the structure and dynamics of biological and non-biological molecules using time-resolved serial crystallography
18:30 – 20:30	Actividad Social: Visita guiada de Tarraco: la Tarragona romana

Jueves 18 de enero

Sesión 3: Cristalografía de Ciencias Químicas y de la Vida

Moderadores: Lourdes Infantes San Mateo y Jordi Benet-Buchholz

9:00 – 9:40	Ponente invitado: Martin Schmidt Nanocrystalline Organic Compounds: Structure Determination by Global PDF Fit
9:40 – 10:05	Sergi Plana: Full structure determination and refinement of an organic dye with triclinic symmetry by means of three-dimensional electron diffraction
10:05 – 10:30	Jordi Cerón-Bertrán: Salt or co-crystal? Monitoring a co-crystal screening with Electron Diffraction
10:30 – 10:45	Mónica Benito: Halogen Bonding in Pharmaceutical Cocrystals
10:45 – 11:00	Sebastián Suárez: Unlocking the Colorful World of Spiro-Rhodamines: rational design and characterization of switchable molecules
11:00 – 11:30	Pausa Café
11:30 – 12:10	Ponente invitada: Carolina Von Essen Absolute Structure Elucidation through the Crystalline Sponge Method: Challenges and Insights
12:10 – 12:35	Elna Pidcock: More than just visualization with Mercury
12:35– 12:48	Jacinto López-Sagaseta: Adaptive structural plasticity in pMHC drives pathogenic T cell recruitment in autoimmune disease
12:48 – 13:00	Javier Merino: A drug discovery approach to drought resistance in crops
13:00 – 14:00	Sesión de Posters
14:00 – 15:00	Pausa Comida

Sesión 4: Ciencias de Materiales para la Sostenibilidad

Moderadores: Inés Puente Orench y Felipe Gándara Barragán

15:00 – 16:00	Ponente invitada: Montserrat Casas Cabanas Advancing Battery Materials through Operando and High Throughput X-ray Diffraction techniques
16:00 – 16:30	María Retuerto: Ru-Mixed Oxides as efficient and durable electrocatalysts for PEMWE anodes
16:30 – 17:00	Víctor de la Peña-O'Shea: New advances in the development of multifunctional catalysts for the Photo(electro) catalytic solar chemistry
17:00 – 17:30	Pausa Café
17:30 – 17:43	Francesc Gispert-Guirado: Application of parametric equations to phase transformation in NiTi shape memory alloys from synchrotron data
17:43 – 17:56	Santiago Garcia-Granda: Pink $\text{MgCo}_x\text{Ni}_{1-x}\text{SiO}_4$ ($0 \leq x \leq 1$) and $\text{CaMg}_{0.5}\text{Co}_x\text{Ni}_{0.5-x}\text{Si}_2\text{O}_6$ ($0 \leq x \leq 0.5$) solid solutions: towards more sustainable pigments
17:56 – 18:09	Clara López-García: MOF-413 and Ga ₇ Ni-TCPP: Two new multimetal MOFs obtained by the use of messenger building units
18:09 – 18:22	Luis León-Alcaide: Clip-Off Chemistry in Heterometallic Iron-Zinc ZIF-8
18:22 – 18:35	Álvaro Vílchez-Cózar: Carbon paper supported cobalt phosphide electrocatalysts for water splitting
18:35 – 18:48	Abraham Sánchez-Caballero: Study of mixed molybdates of lanthanum and praseodymium, $\text{La}_{5.4-x}\text{Pr}_x\text{Mo}_{1-y}\text{Nb}_y\text{O}_{12-\delta}$, for H ₂ separation membranes
18:48 – 19:00	J. M. Vila Fungueiriño: Transmission electron microscopy study of porous metal-organic frameworks (MOFs)
19:00 – 20:00	Asamblea General GE3C
21:00	Cena – Restaurante El Barquet

Viernes 19 de enero

Sesión 5: Cristalografía Inorgánica y Mineralogía

Moderadores: Sol López Andrés y Vicente José Esteve Cano

10:00 – 11:00	Ponente invitada: M^a de los Ángeles Fernández González El polimorfismo del carbonato de calcio precipitado en condiciones ambientales: la influencia de la presencia de aniones tetraédricos en medio acuoso
11:00 – 11.30	Pausa Café
11:30 – 11:50	Gerardo Gil De Cos: Understanding a Ferroelectric Hysteresis cycles in $\text{La}_{2-x}\text{Er}_x(\text{MoO}_4)_3$ solid solutions
11:50 – 12:10	Josefina Perles: ¡No imagines los cristales! Comprender las estructuras con modelos 3D y realidad virtual
12:10 – 12:30	Gwilherm Nénert: Polymorphism and re-entrant phase transition in NaSrPO_4
12:30 – 12:50	Eva Nieto Piñero: Molibdita nano y microcristalina: Estudio y potencial de los materiales 2D.

12:50 – 13:30 Entrega de Premios y Ceremonia de Clausura

13:30 – 15:00 Comida / Comida para llevar

Organizado por:



Patrocinado por:

