ICAR

GenT2025

1st International Conference of AccenT Researchers – GenT

BOOK OF ABSTRACTS

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GENERALITAT VALENCIANA
Conselleria de Educación, Universidades y Empleo

AccenT
L'Associació de Científiques i Científics d'Excel·lència del Pla GenT

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1st International Conference of AccenT Researchers – GenT 2025 (ICARGenT2025)

Castelló de la Plana, Spain, 2025 December 22nd - 23rd
Conference organizers: José J. Baldoví and Teresa S. Ripolles

Conference Program

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Welcome!

As President of the Association of Scientists of Excellence of the Plan GenT (**AccenT**), and on behalf of our organising committee, it is a true pleasure to welcome you to ICAR-GenT 2025: the **1st International Conference of AccenT Researchers** (**ICAR-GenT 2025**), taking place at Hotel Luz in Castelló de la Plana on 22–23 December 2025.

This conference is much more than a scientific meeting; it is *your* space. A place to share ideas, meet colleagues with similar interests, and spark collaborations that can grow into long-term scientific partnerships –and friendships–. Over two intensive days in Castelló, we are here together with a clear purpose: to strengthen the network of GenT researchers, showcase the main results of our work and create real synergies across disciplines.

ICAR-GenT 2025 has been designed as a forum where AccenT members can present the key insights and ambitions of their projects, identify complementary expertise, and explore joint opportunities. The program includes 25 invited talks highlighting outstanding research developed across the three provinces of the Valencian Community by GenT researchers, along with transversal plenary lectures by internationally renowned scientists, who will also bring an external perspective that enriches our discussions and inspires new directions. Beyond the scientific sessions, **ICAR-GenT 2025** will also offer a valuable space to discuss funding and career development pathways.

On behalf of AccenT, I would like to express my sincere gratitude to the **Generalitat Valenciana** for its support to this conference and commitment to scientific talent, and to everyone who has made this first edition possible: our plenary and invited speakers, the full organizing team and ScitoEvents. My warmest thanks.

I encourage you to make the most of these days: ask questions, connect, share your results, propose ideas, and start new conversations. I also hope you can enjoy Castelló de la Plana: its atmosphere, its people and the chance to slow down for a moment between sessions.

From AccenT, we wish you an inspiring, enriching experience that strengthens our community and helps propel your research towards new goals.

Welcome to ICAR-GenT 2025!

José Jaime Baldoví
President of AccenT

Conference Organizers

Dr. José J. Baldoví

Institute of Molecular Science (ICMol), Universidad de Valencia - ICMol (Institute of Molecular Science)

Dr. Teresa S. Ripolles

Instituto de Ciencia de Materiales (ICMUV), Universidad de Valencia

Dr. Anselm Morell Garcia

Desarrollo y acción hormonal de plantas, Instituto de Biología Molecular y Celular de Plantas (IBMCP-CSIC-UPV)

Dr. Arnau Montagud Aquino

Institute for Integrative Systems Biology (I2SysBio), CSIC-UV

Dr. Carlos Doñate Buendia

Institute of New Imaging Technologies, Universitat Jaume I

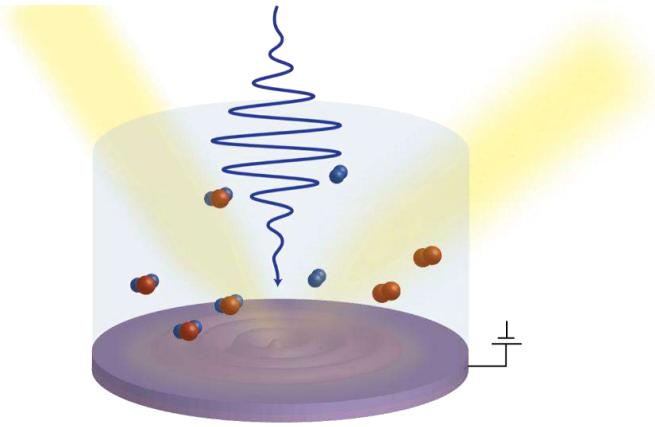
Abstracts of Keynote Speakers

Controlling catalysis with light

Ernest Pastor [*a]

[a]*CNRS, Univ Rennes, Institut de Physique de Rennes, Rennes, France*

Sunlight-to-chemical conversion requires systems that generate long-lived excited states upon illumination. However, this comes with a big energy penalty. For example, the natural photosynthetic system sacrifices a large part of its energy input to gain the excited-state lifetimes necessary to drive chemical reactions. Similarly, in artificial photosynthetic devices, lifetime gain is often achieved through the application of external electrical biases or the use of sacrificial reagents. Currently, there is no blueprint for designing semiconductors with intrinsically long lifetimes. In this talk, I will present recent experimental tools that use ultrafast optical and X-ray lasers to monitor the electronic and atomic dynamics that govern the excited state of photoactive solids. I will compare how transition metal oxide semiconductors, molecules and proteins respond to light excitation, highlighting the similarities between these systems. Finally, I will discuss possible strategies to control the response of photocatalytic materials to try to influence their reactivity on demand.



Designing (bio)materials for 3D/4D printing: towards "living" and more sustainable systems.

Eva Blasco [*a]

[a]*University of Heidelberg (DE)*

3D printing (and more recently 4D printing) has become a promising tool for the fabrication of dynamic and adaptive structures. During the last years, promising examples of defined 4D microstructures employing stimuli-responsive materials have been shown using two-photon 3D laser printing. Herein, I will present our recent work on the field with emphasis on new responsive materials enabling the preparation of adaptive and structures. In particular, shape memory polymers as well as liquid crystal elastomers have been explored. In the first case, a simple and versatile formulation has been developed enabling complex microstructures with remarkable shape memory properties. Also, multi-responsive structures using photo responsive liquid crystal elastomers, are demonstrated. Furthermore, we have exploited the inclusion of dynamic and living bonds in a printable formulation enabling the creation of microstructures with „life-like" characteristics such as adaptability by tunable shape and mechanical properties. In addition, we demonstrated at the macromolecular sequence, specifically the positioning of the crosslinkable group, plays a critical role in both the printability and final properties of the printed material. Last, development of more sustainable materials and approaches will be discussed. We envision that the careful and precise design of new printable materials will open new opportunities for the additive manufacturing of functional and sustainable devices in the near future.

From Alicante to Arabia: lessons from a journey in global dryland research

Fernando T. Maestre [*a]

[a]*Biological and Environmental Science and Engineering Division, King Abdullah University of Science and Technology, Thuwal, Kingdom of Saudi Arabia*

This plenary lecture traces my scientific journey from a PhD student at the University of Alicante to my current role as Professor at KAUST, highlighting the lessons learned while establishing research groups across three universities and two countries. Along the way, I have collaborated with ~400 colleagues from ~50 nations to investigate the ecology, functioning, and resilience of global drylands. This talk will showcase how these international partnerships have enabled us to uncover global patterns in soil and vegetation processes, evaluate the impacts of climate change and human pressures, and identify pathways for sustaining drylands in an era of rapid environmental change. By weaving together personal experience, scientific advances, and the value of diverse global networks, I will reflect on the challenges and opportunities of conducting large-scale, collaborative research—and how such collective efforts are essential to securing a sustainable future.

Abstract of Contributed Talks

Funding and Talent Attraction Programmes of the Generalitat Valenciana

Rafael Sebastián Aguilar [*a]

[a]GVA - Conselleria de Educación, Cultura, Universidades y Ocupación

The Valencian Community has made talent attraction and consolidation a central pillar of its public research and innovation policy. This talk presents the GenT2 Programme, a comprehensive framework designed to attract, retain, and stabilize research talent across the public R&D system through six complementary sub-programmes, covering the full academic and research career path.

The presentation will outline the strategic rationale of GenT2, its structure and objectives, and how it aligns with regional, national, and European research priorities. In addition, it will provide an overview of key figures of the public R&D system in the Valencian Community, including institutions involved, human capital, funding volumes, and research capacity, offering a systemic perspective on how talent policies contribute to strengthening scientific excellence, competitiveness, and societal impact.

The talk aims to situate GenT2 within a broader long-term vision for research and innovation, highlighting lessons learned, current challenges, and future directions in talent-driven science policy.

ValER Program for Attracting Scientific Talent to the Valencian System of Science and Research

Rosa Llusar [*a]

[a]*Universitat Jaume I, Institute of Advanced Materials (INAM) - (ValER)*

The Valencian Foundation for Excellence in Research (ValER) was created by the Generalitat Valenciana in 2021 with the aim of strengthening the Valencian System of Science and Research (SVCI) by attracting and consolidating distinguished research personnel. ValER offers permanent contracts to researchers from around the world so they can develop their professional careers at Universities and Research Centers in the Valencian Community. The main evaluation criteria are scientific excellence and leadership, thus attracting top-level scientific and academic personnel to compete with research systems in other regions and countries. With the creation of ValER, the Generalitat Valenciana complements the talent-attraction policies already in place through programs such as the GenT Plan, by hiring researchers with a recognized international career trajectory.

Global Talent Networks: The role of RAICEX and ECUSA in bridging science between Spain and the World

David Peris [*a, b, c, d], María Badal [d], Araceli Valverde [c], Rodrigo García-Valiente [d]

[a]*Institute of Agrochemistry and Food Technology*

[b]*University of Oslo*

[c]*Spanish Researchers in USA (ECUSA)*

[d]*Network of Associations of Spanish Researchers and Scientists Abroad (RAICEX)*

Following the 2008 economic crisis, Spain experienced an unprecedented scientific diaspora. Thousands of researchers moved abroad, training in internationally renowned research centers. Far from dispersing, this talent organized itself into communities such as SRUK/CERU (Society of Spanish Researchers in the UK) and ECUSA1 (Spanish Scientists in the USA), pioneers in building mutual support networks, promoting Spanish science abroad, and establishing bridges with national institutions.

In 2018, fourteen Spanish science diaspora associations came together to form RAICEX2,3 (Network of Associations of Spanish Researchers and Scientists Abroad), which today represents 22 associations across 38 countries and five continents, bringing together over 4,500 researchers and serves as a direct interlocutor with public institutions, advocating for return policies, international collaboration, and both science diplomacy and policy.

In this talk, as a RAICEX Ambassador and member of the ECUSA Retorno working group, I will present the main lines of action of these networks: from supporting researchers in their return and professional reintegration, to creating collaborative spaces between those who have returned and those still abroad. Initiatives such as the Return Mentoring Program, scientific mobility reports, and potential collaborations with entities like the Generalitat Valenciana under the GenT Plan will be highlighted.

The goal is twofold: on one hand, to inspire GenT researchers to connect with these networks and strengthen their international ties; on the other, to invite institutional stakeholders to actively collaborate in initiatives that leverage Spain's global scientific capital. Because returning is not just about coming back - it's about building lasting bridges between science, society, and policy.

References:

1Spanish Scientists in USA (ECUSA). (2025). Official website. https://ecusa.es/

2Network of Associations of Spanish Researchers and Scientists Abroad (RAICEX). (2025). Official website. https://raicex.org/

3Ortega-Paino E, Oliver E. RAICEX: A Successful Story of the Spanish Scientific Diaspora. Front Res Metr Anal. 2022 Jul 13;7:905765. doi: 10.3389/frma.2022.905765. PMID: 35910708; PMCID: PMC9326310.

Acknowledgements:

I am particularly thankful to the boards of ECUSA and RAICEX for their leadership in shaping strategic guidelines and actively fostering the return of Spanish researchers to Spain.

An introduction to the ERC

Yolanda Álvarez [*a]

[a]*European Research Council*

The European Research Council (ERC) plays a pivotal role within Horizon Europe, offering up to five years of financial backing for independent frontier research to researchers around the globe, irrespective of their research topic or host institution. Prioritising excellence, the ERC provides a range of grant opportunities for researchers at various career stages while maintaining flexibility regarding research subjects. Its grants are intended to support significant advancements in global science and can include additional resources for major research needs. By embracing an interdisciplinary strategy, the ERC seeks to promote groundbreaking research, enhance infrastructure, and propel both economic and societal development across Europe and beyond. The influence of the ERC is demonstrated through its support for more than 14,000 researchers and the generation of substantial research outputs such as numerous scientific papers and patents.

The presentation will cover key facts and figures about the ERC, provide an overview of its various funding schemes with a spotlight on Starting and Consolidator Grants along with their specific eligibility requirements, and describe the ERC's evaluation process, including helpful tips and common pitfalls.

Abstract of Invited Speakers talks

Engineering semiconductor materials for next-generation optoelectronic Devices

Teresa S. Ripolles *[a]

[a] *ICMUV*

Our research focuses on engineering semiconductor materials, particularly hybrid organic-inorganic halide perovskites, to enable next-generation optoelectronic technologies. We design and synthesize perovskite nanocrystals, polycrystalline and single crystals, with controlled crystallization, tunable optical properties, and enhanced stability. In parallel, we develop advanced charge-transport layers, including BiEDOT-based conducting polymers and optimized SnO_2 electrontransport materials, which significantly improve interfacial quality and reduce recombination losses in devices. Using impedance spectroscopy, we unravel the individual physical processes governing device operation, allowing accurate j–V curve reconstruction and guiding the optimization of high-e=iciency perovskite solar cells. To support scalable manufacturing, we implement slot-die coating combined with rapid photonic annealing (FIRA), achieving uniform large-area films compatible with rigid and flexible substrates. Additionally, we explore emerging perovskite-based technologies such as multistate memristors and amplified spontaneous emission (ASE) in nanocomposite waveguides. Overall, our research integrates materials innovation with device engineering to advance perovskite solar cells alongside a broader portfolio of optoelectronic applications.

Acknowledgments

T. S. R. acknowledges financial support from Generalitat Valenciana through

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Metal Halide Perovskites as Building Blocks Towards More Sustainable Photovoltaics

Pablo P Boix [*a]

[a]*Instituto de Tecnología Química (ITQ), Universitat Politècnica de València- Consejo Superior de Investigaciones Científicas (UPV-CSIC), València, Spain*

The urgent need for climate action demands the rapid expansion of carbon-free energy sources. Therefore, we cannot rely on a single technology, especially if it faces sustainability challenges such as limited reparability and recyclability, which pose risks of growing e-waste and environmental damage. Metal halide perovskites (HaP) represent a breakthrough photovoltaic material class, achieving performance comparable to commercial solar cells, but their ionic and chemically dynamic nature leads to device instability and potentially harmful by-products.

We embrace these challenges by transforming the chemically dynamic properties of HaP into advantages. Leveraging their low formation energy and ionic mobility, PhoenixPV develops intrinsic self-healing strategies alongside extrinsic post-synthetic treatments that reverse degradation, restore performance, and safely capture toxic by-products. This dual approach not only extends device lifetime but also facilitates safer end-of-life recycling through targeted material separation methods. A key innovation is the integration of a high-throughput aging characterization system that enables parallel testing of numerous devices under controlled stress conditions, combined with in-operando diagnostic tools such as impedance spectroscopy to continuously monitor device health. Our goal is to position metal halide perovskites as foundational building blocks for repairable and recyclable photovoltaics, paving the way toward a more sustainable solar energy future.

Acknowledgments:

We acknowledge funding by Generalitat Valenciana for the funding via Pla Gent-T (grant ESGENT 010/2024).

Operando Spectroscopy Insights into Solar Fuel Photocatalysts

Soranyel Gonzalez Carrero [*a]

[a]*Instituto de Ciencia Molecular, Universidad de Valencia, 46980 Paterna, Spain*

Over the past decade, the efficiency of materials for solar fuel generation has improved notably. These advances have been driven not only by the development of new photocatalyst systems but also by the refinement of characterization techniques that provide a deeper understanding of fundamental material properties. In particular, advanced optical spectroscopy has been instrumental in linking material properties to performance, guiding the design of more efficient photocatalysts.[1] Despite these improvements, a persistent challenge remains: achieving effective separation and stabilization of photogenerated charges while minimizing recombination losses. This challenge is especially critical because catalytic transformations require charge carriers to remain active over relatively long lifetimes to drive reactions efficiently.

In this presentation, I will discuss our recent studies using operando optical spectroscopic analysis to address these challenges in photocatalyst materials for hydrogen production. [2] I will focus on charge separation and stabilization in emerging organic semiconductor systems, highlighting their remarkably long-lived photogenerated charges. These findings will be compared with results from more traditional inorganic photocatalysts, providing new insights into how material composition and structure influence solar-to-fuel conversion efficiency.

References:

[1] Choi, J.; Jung, W.; Gonzalez-Carrero, S.; Durrant, J. R.; Cha, H.; Park, T. Understanding charge carrier dynamics in organic photocatalysts for hydrogen evolution. Energy & Environmental Science 2024, 17 (21), 7999-8018

[2] Gonzalez-Carrero, S.; Kosco, J.; Fei, T.; McCulloch, I.; Durrant, J. R. Impact of water solvation on the charge carrier dynamics of organic heterojunction photocatalyst nanoparticle dispersions. Chemical Science 2024, 15 (45), 19044-19056

Acknowledgments:

We acknowledge financial support from Generalitat de Valenciana (CIDEIG/2023/17).

From Well-Defined Surfaces to Tunable Catalysts: Designing Electrochemical Pathways for Energy Conversion

Rosa M. Arán-Ais [*a]

[a]*Instituto de Electroquímica, Universidad de Alicante, Spain*

As the urgency of the climate crisis grows, the search for solutions that reduce fossil-fuel dependence and convert carbon-containing waste into valuable chemicals has become more pressing than ever. Electrochemistry plays a central role in this effort, enabling the interconversion of electrical and chemical energy and supporting the development of stable energy carriers. Strengthening electrochemical technologies and the materials behind them is therefore key to building a sustainable and resilient energy system.

In this context, Dr. Rosa M. Arán-Ais explores the fundamental interplay between surface structure—especially in well-defined single-crystal electrodes—and electrocatalytic reactions relevant to energy conversion and storage. Her work combines electrochemical measurements on single-crystal electrodes with nanocatalyst design, in-situ spectroscopy and microscopy, and mechanistic analysis to elucidate how atomic structure dictates activity and selectivity in reactions such as oxygen reduction, nitrate reduction, and the oxidation of organic molecules.

Her recent work highlights how controlled alloying of Pt and Pd on single-crystal surfaces influences the mechanisms and kinetics of the oxygen reduction reaction (ORR) and nitrate electroreduction (NO3RR). Additionally, her research explores the electrochemical oxidation of biomass-derived molecules (e.g., HMF) on single crystals to enable sustainable synthesis routes. Through the use of precisely defined materials and mechanistically guided analysis, this research advances the rational design of electrocatalysts capable of converting renewable electricity into value-added chemicals. The approach bridges fundamental electrochemistry with applied catalysis, offering broadly relevant insights across disciplines.

Two-dimensional Layered Hydroxides: From Molecular Control to Scalable Applications

Gonzalo Abellán [*a]

[a]*Instituto de Ciencia Molecular (ICMol), Universidad de Valencia, Valencia, Spain.*

Layered hydroxides (LHs) are exceptionally versatile materials with applications ranging from electrocatalysis and energy storage to magnetism. In this talk, I will present recent advances from the 2D-Chem Research Group (www.2dchem.es) in the synthesis and characterization of two-dimensional (2D) LHs.

We have developed a series of innovative synthetic strategies to fabricate functional LHs, including: (i) a microfluidic reaction–diffusion approach for producing self-supported layered double hydroxide (LDH) hollow architectures[1]; (ii) a co-precipitation strategy for obtaining graphene–LH nanocomposites[2]; and (iii) a room-temperature epoxide route that enables precise control over crystallographic phases—a key factor governing the electrochemical performance of LH materials[3]. Beyond structural control, covalent anion modification within the simonkolleite framework enhances both magnetic tunability[4,5] and electrochemical functionality[6].

To address industrial scalability, we introduce a room-temperature, atmospheric-pressure synthesis route for NiFe-LDHs via homogeneous alkalinization. Through chloride-mediated epoxide ring opening, we obtain low-dimensional, highly defective NiFe-LDHs exhibiting cation clustering. Advanced spectroscopic techniques (XANES, EXAFS, SAXS), combined with ab initio modeling, reveal the critical role of Fe clustering in optimizing catalytic behavior[7].

This energy-efficient and scalable methodology offers a cost-effective alternative to noble metal catalysts and paves the way for the large-scale implementation of LDH-based materials in water splitting, energy storage, sensing, and environmental remediation. Moreover, a spin-off company (Matteco) has been established to commercialize this technology, successfully distributing these materials worldwide.

References:

[1] M. Mattera, A. Sorrenti, L. De Gregorio Perpiñá, V. Oestreicher, S. Sevim, O. Arteaga, X. Chen, S. Pané, G. Abellán. Small, 20, 2307621 (2024).

[2] C. Jaramillo-Hernández, V. Oestreicher, M. Mizrahi, C. Huck-Iriart, C. Dolle, G. Abellán. Adv. Funct. Mater., https://doi.org/10.1002/adfm.202518088 (2025).

[3] C. Jaramillo-Hernández, A. Seijas-Da Silva, G. Abellán. Eur. J. Inorg. Chem., 28, e202400754 (2025).

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Atom-by-atom on-surface synthesis of nanomaterials: Fundamentals and applications

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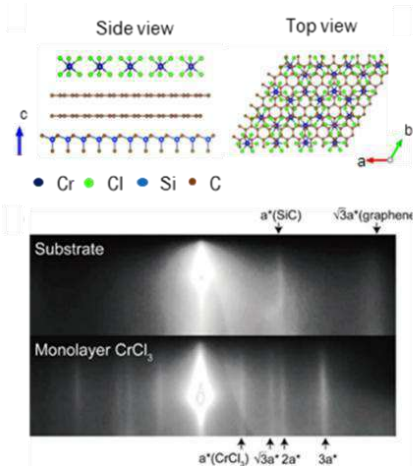
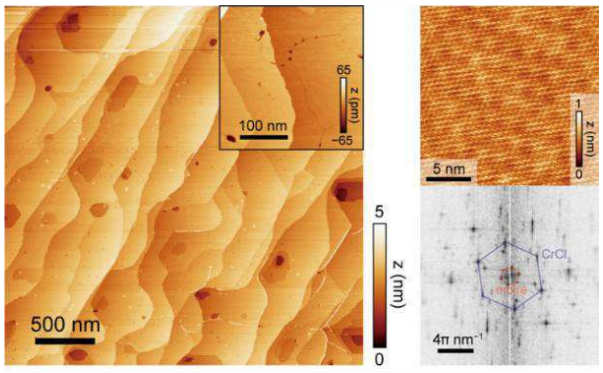
The properties of nanomaterials are governed not only by the nature of the elements that form them, but also by the way the atoms are positioned and arranged microscopically in the solid. Periodic arrangements of atoms, such as crystalline lattices, give rise to specific, well-defined electronic, optical and magnetic properties at the macroscopic scale. In this talk, I will show how to prepare crystalline nanomaterials by depositing atomic species on a surface with an ultra-high vacuum technique called molecular-beam epitaxy (MBE), and visualize how these atoms arrange periodically in real time with in-situ diffraction techniques. As a practical example, I will showcase the preparation of homogeneous two-dimensional, atomically-thin materials with unique magnetic properties [1], with potential applications in (spin) electronics.





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Engineering the properties of 2D van der Waals magnetic materials

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The advent of two-dimensional (2D) magnets has unlocked an exciting playground for solid-state physicists, offering a versatile platform to explore spintronic, magnonic and quantum phenomena at the atomic scale. In this talk, I will present our recent contributions to this fast-growing field. We will begin by exploring the tunability of spin waves in the air-stable 2D magnetic semiconductor CrSBr, taking advantage of its quasi-one-dimensional electronic structure and its exceptional response to external stimuli. By applying mechanical strain and controlling dielectric screening, we demonstrate how magnon dispersion and spin dynamics can be selectively modulated using first-principles calculations.[1] Next, we will move into the chemical domain, showing that the magnetic and magnonic properties of CrSBr can be finely tuned via molecular deposition. This chemical handle opens the door to molecularly controlled magnonics, enabling a new degree of freedom in spin-wave engineering. [2,3] We will also show that CrSBr holds promise as a sensitive platform for gas detection, with distinct changes in magnon spectra upon adsorption of environmental pollutants like NO, NO_2 and NH_3.[4] Shifting focus, we will discuss the origin of above-room-temperature ferromagnetism in Fe_3GaTe_2, highlighting the interplay between electronic structure, magnetic anisotropy and strain tunability.[5] Finally, we will explore hybrid quantum systems where molecular spin qubits are coupled to 2D magnets, unveiling coherent chemical control of magnon–qubit interactions[6] and will unveil the properties of graphendofullerene, a novel molecular 2D magnetic material based on endohedral metallofullerenes covalently linked forming a 2D network.[7]

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Enabling Human Digital Twins by intersecting Systems Biology and HPC

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This project, called SysBioHPC, aims to develop an innovative toolbox that integrates systems biology (SB) simulations optimized for high-performance computing (HPC) platforms and facilitates the use of artificial intelligence and machine learning (AI/ML) methods. The project addresses a critical gap in computational biology by scaling up the scope of systems biology modelling to handle complex, real-world biological scenarios.

Current SB modelling faces significant limitations when addressing large-scale simulations such as real-sized tumour simulations, temporal evolution of microbial communities, or clone-specific drug discovery. Despite the proven benefits of HPC in bioinformatics analyses, its application in SB modelling remains scarce, under-optimal, and not reproducible. Most SB modelling tools rarely use parallel processes, and existing efforts are typically one-shot adaptations without standardization.

The project is, first, developing HPC-optimized multiscale modelling software that allows integration of different types of modelling frameworks that span from the nanometre to the decimetre. Second, we are demonstrating the enhanced capabilities through two use case of digital twins: multiscale simulations of SARS-CoV-2 infection of human alveolar tissue, and real-sized bacterial communities' interactions and protection against drugs.

We are developing an advanced multiscale simulation environment. Building upon our PhysiBoSS, an agent-based multiscale modelling software, the team is developing HPC-optimized add-ons for ODE-based and metabolic modelling, integrate them with a distributed PhysiBoSS-MPI, and implement AI/ML tools for simulation orchestration and result analysis.

We are demonstrating the usefulness of our approach by modelling the SARS-CoV-2 infection. We are studying the SARS-CoV-2 infection of human alveolar tissue, incorporating detailed Boolean models of immune and alveolar cells enabling patient-specific drug treatment identification and simulation of high heterogeneity in patient responses. We

currently have a workflow in place that allows for the interactive simulation of a patient treatment, with different drug and clinical interventions.

We will next tackle bacterial communities and drug resistance. Combining PhysiBoSS with add-ons for Boolean modelling, metabolic modelling, and drug internalization to study community effects on antibacterial drug sensitivity, focusing on the relationship between metabolic interactions and drug protection.

The project represents a unique combination of skills bridging SB modelling, data analysis, AI/ML methods, and HPC computing. SysBioHPC is enabling the modelling of multi-body interactions, better reuse of published data, and implementation of computational standards for complex SB experiments. The toolbox is facilitating simulations closer to real scenarios, such as real-sized tumours with immune infiltrations and metastasis seeding.

The goal of the project is to deliver a comprehensive toolbox that scales up SB modelling capabilities, enabling researchers to tackle previously computationally intractable problems. The two use cases will demonstrate practical applications of digital twin modelling in COVID-19 research and antimicrobial resistance studies.

The interdisciplinary nature of this work, combining biology, applied mathematics, and high-performance computing, positions it to significantly advance these fields while opening new avenues for biotechnological and biomedical applications.

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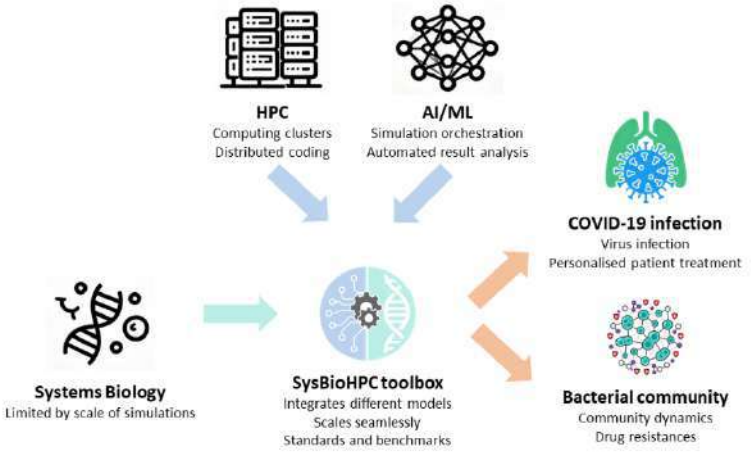
Arnau Montagud acknowledges funding from the Generalitat Valenciana's CIDE GenT programme under the project CIDEXG/2023/22.



Functional Characterization of Plant Aldo-Keto Reductases: Leveraging Knowledge from Mammalian Systems

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The Aldo-keto reductase (AKR) superfamily comprises a diverse group of monomeric NAD(P)(H)-dependent enzymes that catalyse the reduction of carbonyl compounds to their corresponding alcohols. AKRs play a key role in stress response mechanisms across all biological kingdoms. In mammals, however, they are also involved in a variety of metabolic pathways, including the biosynthesis of steroid hormones and prostaglandins. In contrast, the functional roles of AKRs in plants remain relatively understudied.

In the model plant *Arabidopsis thaliana*, four AKRs—AKR4C8 (*At2g37760*), AKR4C9 (*At2g37770*), AKR4C10 (*At2g37790*), and AKR4C11 (*At3g53880*)—have been identified based on sequence homology to the well-characterized human AKR1C family. Beyond these, an additional eighteen genes in *Arabidopsis* encode proteins with AKR-like features, yet their functions are still unknown.

To address this gap, we explored the hypothesis that *Arabidopsis* AKRs may share functional homology with their mammalian counterparts. These plant enzymes exhibit notable substrate promiscuity and potential functional redundancy, which pose challenges to their functional characterization. In this presentation, I will discuss how we integrate *in silico*, biochemical, and genetic approaches in our lab to uncover the physiological roles of AKRs in *Arabidopsis thaliana*.

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Intelligent Catalytic Reactors Enabled by Generative Design and Additive Manufacturing

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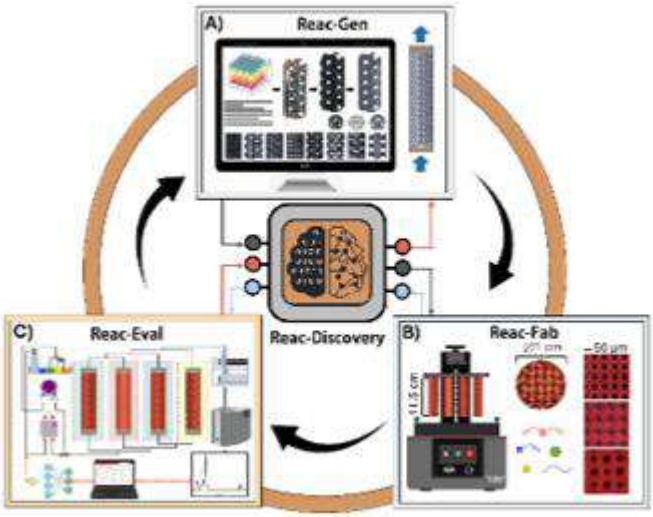
Reac-Discovery is presented as a digital platform that integrates parametric modelling, additive manufacturing, and machine learning for the design and optimization of catalytic reactors. The combination of periodic structures and autonomous optimization under continuous-flow conditions enables simultaneous adjustment of reactor geometry and reaction parameters, significantly improving the efficiency and sustainability of multiphasic catalytic processes.

Additive manufacturing (AM) has emerged as a key tool in reactor engineering, enabling the development of optimized structures that markedly enhance the efficiency of catalytic processes in continuous-flow systems. This study presents an innovative approach that integrates parametric modelling, high-resolution 3D printing, and artificial intelligence to design and fabricate reactors with advanced architectures that maximize mass and energy transfer. The implementation of open-cell periodic structures allows precise control of fluid dynamics and substantial improvements in mixing efficiency, overcoming the limitations of conventional systems. Furthermore, the integration of autonomous optimization platforms enables real-time adjustment of both reaction parameters and topological features through machine learning, establishing structure–activity correlations that accelerate the identification of optimal operating conditions. This approach has been successfully applied to the conversion and valorization of carbon dioxide (CO_2), demonstrating its potential to enhance catalytic efficiency and sustainability in chemical processes. The results highlight how digitally optimized reactors fabricated through additive techniques can provide tailored solutions for CO_2 utilization, outperforming traditional packed-bed systems. This work underscores the transformative role of intelligent manufacturing and automation in reactor engineering, paving the way toward the next generation of sustainable catalytic technologies.


A)
Reac-Gen
Reac-Discovery
C)
Reac-Eval
B)
Reac-Fab
11.5 cm
25 cm
50 µm

Nanoparticle based smart materials produced by additive manufacturing

Carlos Doñate Buendia [*a]

[a]*GROC-UJI, Institute of New Imaging Technologies, Universitat Jaume I, Castellón, Spain*

Photonics, Nanotechnology and Advanced Materials are considered by the European Commission as key enabling technology for the industrial development and improvement of human society lifestyle in the following decades. These technologies are key to improve imaging and treatment in medicine, material fabrication and processing or green energy harvesting systems, facilitating a sustainable human development. Pulsed laser ablation in liquid (PLAL), joins Photonics and Nanotechnology, representing a green synthesis technique of colloidal nanoparticles with a broad material and solvent library available that allow the straightforward synthesis of metallic, ceramic, organic, and alloy nanoparticles with compositional control. This versatility is a key feature for the development of advanced materials. The modification of currently existing materials to enhance or provide new functionalities represents the best approach to produce cost-effective smart materials for demanding applications. Smart materials provide extra functionalities, as sensing capabilities, or controlled motion (actuators)[1]. In this context, the production of smart materials with custom geometries and functionalities is a shared goal by researchers and industry. Additive manufacturing (AM) techniques offer the desired design freedom and represent a growing industrial market. In this contribution polymer materials (PLA, Nylon, TPU) are modified by the addition of laser generated nanoparticles to provide them on demand optical (by the addition of plasmonic nanoparticles)[2], magnetic (magnetite nanoparticles)[1], or enhanced mechanical, thermal and conductivity properties (carbon nanomaterials). The contribution covers all the process steps, starting with the upscaling and control (size, composition and phase) of the nanoparticle production by PLAL to meet industrial scale demands[3], going through ensuring homogeneous nanoparticle distribution in the materials employed for AM. Finally, optimizing the processing of the novel materials by AM techniques like laser powder bed fusion, stereolitography, and fused deposition modelling, and evaluating their recyclability by shredding and preparation of recycled based materials for AM to ensure the development of sustainable products. The aim is to develop novel materials with specific sensing, optoelectronic and/or magnetic performance easily and cost-effective printable into custom designs by AM.

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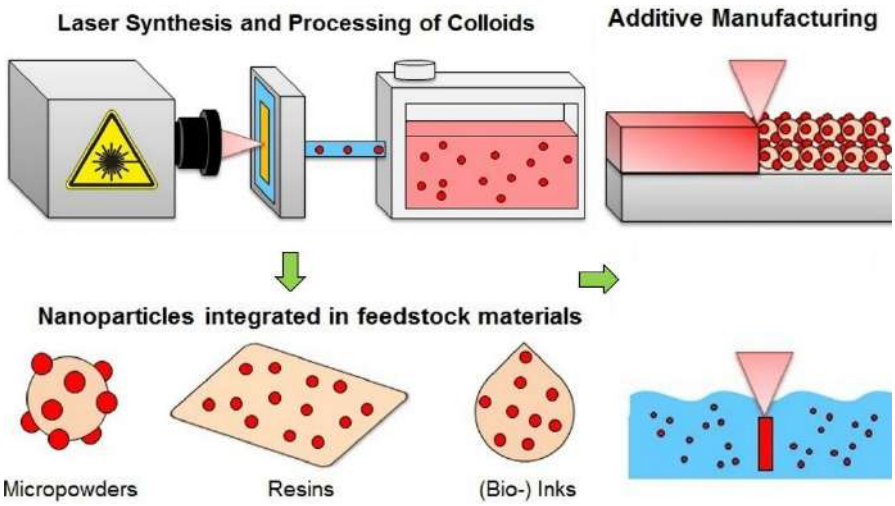

Innovative technologies for accelerator-based therapies and high-energy physics applications

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Particle accelerators are complex and powerful machines designed to generate, accelerate, and control charged particle beams. While they were originally developed to advance fundamental nuclear and particle physics, today they are also widely applied in other research fields as well as in industrial and medicine. At *Instituto de Física Corpuscular* (IFIC), research in advanced accelerator technologies has a long-standing tradition of complementing high-energy physics (HEP) experiments and, in recent years, has expanded toward innovative technologies for particle therapies. This contribution will review the accelerator technologies under development at IFIC, focusing on ongoing activities related to enhance both the efficacy and accessibility of advanced particle therapies.

Cancer treatment is one of the most impactful applications of accelerator technology. About half of cancer patients worldwide receive radiotherapy, typically with X-rays from linear accelerators. Hadron therapy (mainly protons and carbon ions) offers complementary advantages through precise energy deposition at the Bragg peak, sparing healthy tissue. Carbon ions are also 2–3 times more biologically effective. Proton therapy has grown rapidly thanks to technological and biomedical advances, while carbon-ion therapy remains less accessible due to the higher cost and complexity of accelerators and the limited availability of radiobiology facilities.

In the last decade, the concept of high frequency linacs for hadron therapy has gained greater interest thanks to its advantages, with respect to circular machines, of modularity and speed in the control of the beam energy. A linac is based on a chain of accelerating cavities that can be individually controlled allowing to change the energy of the final beam pulse by pulse in the order of a few microseconds. However, these machines require large facilities, making research on compact accelerating technologies essential. A key achievement presented in this contribution is the demonstrated accelerating gradient of 39 MV/m in a novel S-band accelerating cavity design [1], representing an important step toward compact hadron linear accelerators for medical applications.

Furthermore, at the end of 2023, IFIC was awarded by *Centro para el Desarrollo Tecnológico y la Innovación* with a grant in the program of an innovative public procurement for the construction of a 10 MeV/u carbon ion and protons accelerator by 2028 [2] for radiobiology and other research applications. This project leverages state-of-the-art technology to demonstrate what would represent the first stage of a treatment accelerator with carbon ions—technology that is not yet available at an industrial level, except in Japan. The construction of this infrastructure (ALMA, *Acelerador Lineal Multi-hAdrones*) is led by Spanish companies in collaboration with *Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas* (CIEMAT), the European Organization for Nuclear Research (CERN) and IFIC and will position IFIC at the forefront of accelerator facilities in Spain and internationally. Within this framework, we present the ALMA concept, covering the experimental beamline design and ongoing efforts to upgrade the linac energy from 10 MeV/u to 60 MeV/u, thereby extending penetration depth and broadening the range of supported studies. To exploit the ALMA facility, we are consolidating a multidisciplinary team to explore novel radiotherapy techniques. We also report exploratory research on combining particle beams with gold nanoparticles [3] to enhance proton therapy, with first proof-of-concept radiobiology experiments [4] at the *Centro Nacional de Aceleradores* in Seville showing promising results for improving irradiation efficiency.

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Reactive Droplets as Self-assembly Directors

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I will show two types of "reactive coacervates"- that are able to carry our reactions within themselves and often the product is involved in hierarchical self-assemblies.

Reactive coacervates1 generate imine oligomers within and can transform into membranous constructs, or show life-like budding behavior. The imine product is also photo-switchable. This allows for interesting light responsive reversible transformations in these droplets. On the other hand, reactive coacervates 2 form as a result of a reaction within unstable surfactant coacervates (mother). The product is able to phase separate within the mother coacervates to give transient multi-phasic coacervates. The release of the gaseous byproduct in the reaction by these coacervates propels them in opposite direction to the gas exhaust. Under certain conditions, the gas if trapped in pockets around these coacervates compresses the spherical droplets into interesting non-spherical shapes.

I will therefore show how coupling reaction with liquid-liquid phase separation can lead to complex self-assemblies and materials with life-like properties.

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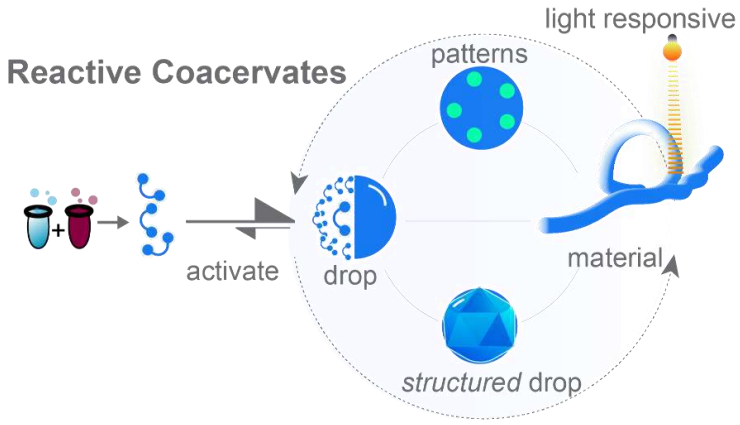

Engineering molecular cages for guest encapsulation, sensing, and biomedical applications

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Supramolecular chemists have developed a toolbox of methods that allow preparing molecular cages with cavities with customized sizes and properties, that allow the encapsulation of guest molecules with applications in catalysis, molecular recognition, sensing, gas separation, catalysis, materials chemistry, and emerging biomedical applications.[1-3] In general, cage synthesis involves the self-assembly of building blocks with precise shape and geometry under equilibrium control to yield the most stable cage structure.[4] The cage structure can be designed using molecular modelling to obtain any desired cavity size and shape with specific functional groups pointing towards the cavity.[5] This communication will show how to determine the cavity volume and hydrophobicity and ESP using CageCavityCalc,[5] and different synthetic strategies to obtain molecular cages from different building blocks to obtain porous organic cages and porous metal-organic cages.[6-8] The host-guest properties of the cages towards different guests, including anticancer drugs, will be presented.

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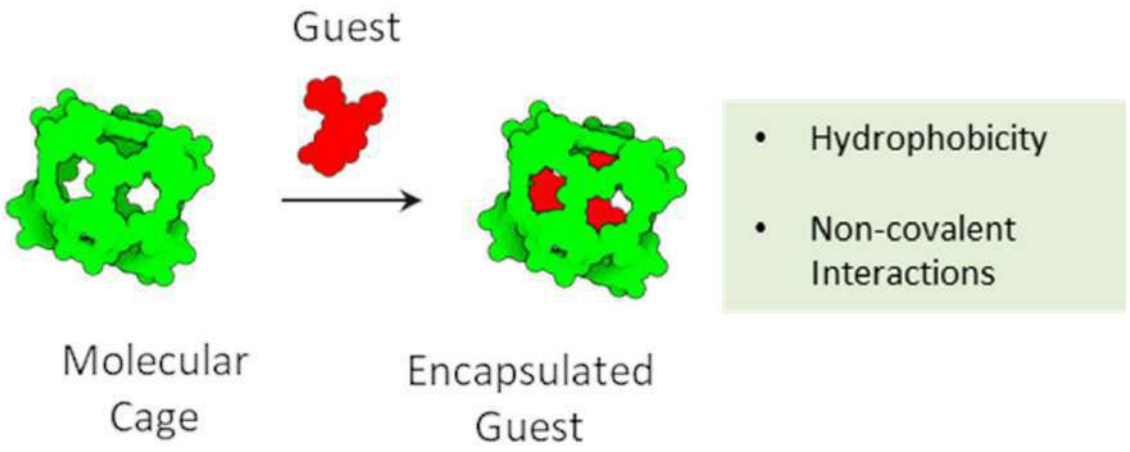

Solvent-free thermal defect engineering in metal-organic frameworks

Víctor Rubio-Giménez[*a], Sonia Martínez-Giménez [a], Alejandro Orellana-Silla [a], Marta Galbiati [a], Efrén Navarro-Moratalla [a], Braglia Luca [b], José Antonio Real [a], Sergio Tatay [*a], Carlos Martí-Gastaldo [*a]

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The controlled generation of defects in crystalline materials is widely used to tune properties for improved performance. This strategy is increasingly applied to metal-organic frameworks (MOFs), where coordination vacancies are commonly introduced in solution by exploiting the reversibility of metal–ligand bonds.[1] We present an innovative solvent-free approach for defect engineering in MOFs based on the selective thermal removal of neutral volatile linkers.[2] This method enables the generation of metal vacancies across a broad compositional space (0-100%) without requiring counterions, redox adjustments, or oxide formation to balance charge. Using a standard thermogravimetric analyser, we control the extent of linker sublimation with high precision and reproducibility. We identify key design criteria for applying this strategy and validate it with the Hofmann-type MOF $[Fe(pz)\{Pt(CN)_4\}]$ (pz = pyrazine).[3] Structural and spectroscopic analyses reveal a local transformation from FeN_6 to FeN_4 environments, leading to redox-stable unsaturated Fe^{II} sites that have unexpected effects on the spin crossover behaviour of the material. Furthermore, these open centres remain chemically accessible and can hence catalyse Lewis acid-type reactions. The ability to generate open metal sites without solvents or charge-balancing agents offers an alternative route for applications that require a precise control of defects, including the binding of molecules of biological ad catalytic interest.

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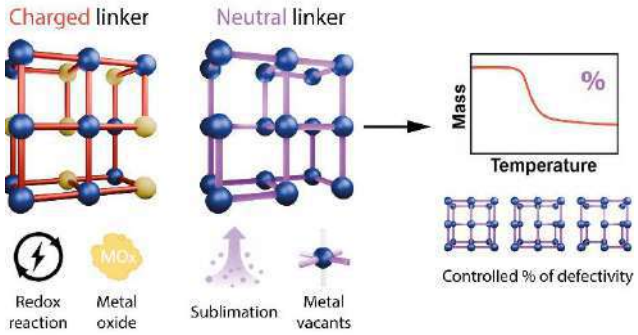

Quantum optics meets quantum technologies

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In this talk I will summarize my CIDEGENT proposal, in which we combine elements of quantum optics and many-body physics to search for new phenomena of use for quantum technologies. We put forward setups based on quantum simulators capable of stabilising exotic quantum phases of matter, such as supersolids or time crystals, which are extremely elusive in real materials. In addition, the project develops computational tools able to study the dissipative many-body problems required for this proposal, which pose one of the biggest computational challenges in physics. Finally, we consider more traditional quantum optical systems such as nonlinear optical cavities, but in regimes that are largely unexplored. For example, we consider the quantum properties of light emitted by cavities that undergo spontaneous time-translational symmetry breaking, that is, whose emitted light spontaneously oscillates in time, a regime that we can study thanks to the mathematical tools developed within our group.

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Catalyst Engineering as a Pathway to Sustainability

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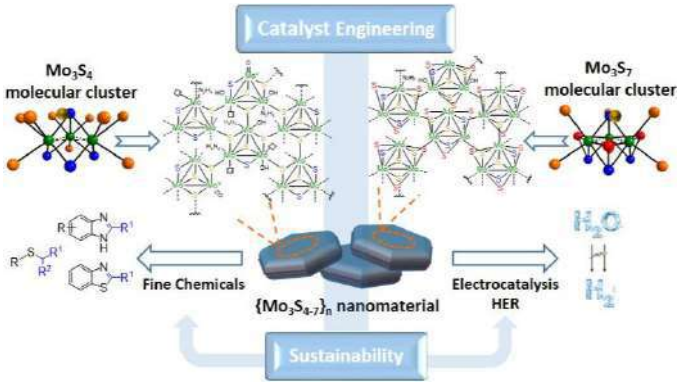
The depletion of fossil resources and growing environmental concerns associated with their use have underscored the need for abundant feedstocks, renewable energy sources, and atom-economical routes for the production of tailor-made chemicals and energy. Key to successfully reduce our fossil fuel overreliance relies on catalysis and, more specifically, on the development of highly active and inexpensive catalysts. In this communication, molybdenum sulfide-based nanomaterials, denoted as {Mo3S4−7}n, are presented as promising catalysts for advancing sustainability. It will be demonstrated how these nanomaterials can be precisely engineered at the nanoscale through an innovative bottom-up synthetic strategy that employs molecular clusters as precursors.[1]

The resulting nanomaterials comprise randomly agglomerated nanosheets that preserve the specific atomic arrangement of the original cluster motif, exhibiting unsaturated sulfur and metal atoms with Lewis basic and Lewis acid properties, respectively. Notably, these features inherently introduces defects at the naturally exposed edge sites and along the typically inert basal planes of the nanomaterials.[2],[3] Advantageously, these nanomaterials have been applied as multifunctional catalysts for one-pot hydrogenation and dehydrogenation reactions in fine chemical synthesis, and as electrocatalysts for the hydrogen evolution reaction (HER).[4]



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ABACuS: The Study of Copper Deficiency and ABA Regulation to Reduce Fruit Quality Loss in Tomato

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Copper (Cu) deficiency (CuD) represents a growing agronomic challenge in European arable soils, particularly pronounced in Spain, where the low bioavailability of this essential micronutrient compromises the development, yield, and quality of horticultural crops such as tomato (*Solanum lycopersicum*). Traditionally, this issue has been addressed through the application of inorganic fertilizers, but new European guidelines aimed at reducing the use of agrochemicals for environmental and public health reasons, together with the toxicity of Cu when in excess, have created the need to explore sustainable alternatives to maintain fruit safety, productivity and quality.

In response to this research need, the ABACuS project—led by the Postharvest Physiology and Biotechnology for Food Sustainability (PPB4FS Lab) at IATA-CSIC—focuses on unraveling the physiological, biochemical, and molecular mechanisms underlying Cu homeostasis in tomato, with particular emphasis on the regulatory role of the phytohormone abscisic acid (ABA). Our research line is supported by experimental designs using ABA-deficient mutant genotypes (*notabilis* and *flacca*), compared with the parental Ailsa Craig (AC), cultivated under Cu sufficiency (CuS) and CuD conditions in *in vitro*, hydroponic, and greenhouse systems, and studied across different fruit ripening stages.

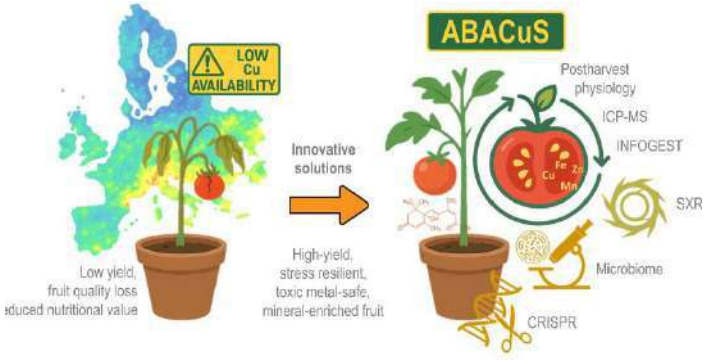
The results obtained reveal that CuD affects multiple aspects of fruit development and quality, including reduced maturity index, increased susceptibility to peel cracking, alterations in the accumulation of antioxidant compounds and micronutrients, and lower resistance to infection by the pathogen *Botrytis cinerea*. Furthermore, ABA has been shown to participate in the modulation of these responses, both in fruit physiology and gene expression during ripening. A particularly relevant finding is the role of ABA in the transgenerational transmission of CuD stress memory, which negatively affects seed germination and seedling growth in the next generation. This phenomenon is likely explained by the differential spatial distribution of Cu, Fe, Zn, and Mn in seeds derived from fruits grown under CuS and CuD conditions, as revealed by Synchrotron X-Ray Fluorescence imaging. This epigenetic dimension of nutritional stress opens new perspectives for designing biotechnological strategies to improve stress tolerance and fruit

quality without resorting to intensive agricultural practices. In turn, transcriptomic studies have identified ABA-dependent expression patterns involving genes related to detoxification of reactive oxygen species (ROS), metal transport, cell wall metabolism, and developmental processes such as endosperm maturation. Building on these findings, a set of candidate genes has been selected for CRISPR edition in both AC and *notabilis* backgrounds, aiming to develop high-yield CuD resilient tomato plants, safe from toxic metal accumulation and enriched in essential minerals in the fruit. Our current efforts also aim to determine how CuD affects the fruit's surface microbiome, potentially influencing postharvest pathogen resistance and, consequently, food safety and marketability.

Overall, this research lies at the intersection of plant physiology, fruit nutritional and mineral quality, postharvest biotechnology, and agricultural sustainability. Its goal is to generate applicable knowledge for the development of crops that are more resilient to micronutrient deficiencies and the impact of climate change, thereby contributing to food safety and security and improving the nutritional quality of horticultural products.

Acknowledgments:

We gratefully acknowledge the collaboration of Prof. Olena Vatamaniuk and her team at the School of Integrative Plant Science, Cornell University, for the SXRF imaging analyses. We also acknowledge the contribution of Prof. Bárbara Blanco-Ulate from the Postharvest Section at UC Davis in the generation of the CRISPR-edited tomato lines. The help and technical assistance of J. Coll from the Microscopy Facility at IATA-CSIC and of V. Sentandreu from the Genome Facility at SCSIE-UV are also gratefully acknowledged.



FunGIALab: Connecting Fungal Diversity, Evolution, and Biotechnological Applications

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Microorganisms are the invisible architects of life on Earth. Among them, fungi—and especially yeasts—play essential roles in ecosystems and human industries. Despite their importance, most fungal species remain undescribed, and their potential largely untapped. Understanding this hidden biodiversity is not only a scientific challenge but also a gateway to developing sustainable solutions in food production, health, and environmental resilience.

In a first part of my talk, I am excited to introduce our research lines at FunGIALab (Fungal Genomics and Industrial Applications Lab). Our team focuses on:

i) Uncovering fungal diversity and understanding their ecological roles;

ii) Studying mechanisms driving fungal evolution, with an emphasis on speciation and domestication;

iii) Developing molecular tools to engineer fungi that address specific biotechnological challenges; and

iv) Creating robust bioinformatics pipelines to analyze the large datasets generated by our work.

In the second part, I will spotlight Sacchar2Omics, a project funded by the GenT CIDEGENT and CIESGT programs of the Generalitat Valenciana. This project focus in *Saccharomyces*, a genus particularly valuable, not only for their historical role in food (bread, wine, and beer) and beverage production, but also as model organisms for studying evolution, genetics, and biotechnology. Sacchar2Omics aim is to uncover the hidden diversity within *Saccharomyces*, understand how these yeasts adapt to natural and industrial environments, identify the genetic and phenotypic features that define populations and

their ecological roles, and discover traits that can be harnessed for sustainable innovation. The project not only generates fundamental insights into microbial evolution but also provides practical tools and resources for applied research and industrial development.

As a member of AccenT, I am excited to share the vision and progress of FunGIALab at this first international conference. Beyond its scientific contributions, our lab actively fosters collaboration with biotech companies and promotes public engagement through outreach and education. By bridging basic research and applied innovation, we contribute to global efforts in biodiversity conservation, sustainable production, and the development of a circular bioeconomy.

I believe that by connecting evolutionary biology, genomics, and biotechnology, we can create meaningful synergies across disciplines and explore new frontiers in science and innovation.

Acknowledgments:

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We are especially grateful to our collaborators for their contributions to joint projects and PhD supervision: Estéfani García Ríos, Inger Skrede, Sergi Puig, Paula Alepuz, Pedro María Martín Sánchez, Víctor García Bustos, and Nerve Zhou.

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Development of fungal biorefineries for the sustainable production of proteins and metabolites of industrial interest

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Europe is in transition towards an economy based on the technological application of biological knowledge (bioeconomy) to significantly reduce harmful and greenhouse gas emissions, promoting sustainable industrial practices. The European Green Deal and the Farm to Fork Strategy represent commitments by the European Union to create a sustainable, resilient and fair food system[1]. Central to these initiatives is the role of food biotechnology, which offers innovative solutions to some of the most pressing challenges in food production. Among these, play a key role by converting agri-food by-products and waste into high-value products, fostering a circular and sustainable economy[2]. Fungi are particularly promising in this context, as they can transform agri-food residues into molecules of interest for applications in agriculture, food, and health. The use of fungi as cell factories for the sustainable bioproduction of high-value molecules is well aligned at the international level, with the Sustainable Development Goals (SDGs) formulated by the United Nations[3], and regionally, with the S3-CV 2021-2027 strategic framework of the Valencian Community[4].

Considering the above mentioned framework, my research focuses in the development of sustainable, safe and cost-effective approaches to exploit fungi as cell factories for the synthesis of metabolites and enzymes with applications in food biotechnology. Within my research group (FungalFact, IATA-CSIC), we are developing processes for the production of high-value carotenoids from naturally accumulating yeast species, supported by projects NANOXFUN (CIDEXG/2023/20), VALOCIX (CNS2024-154560) and YEAST4VALUE (INNEST/2025/122). Additionally, through the FUNGIPRO project (PID2024-162829OB-I00), we are engineering filamentous fungi strains to enhance the production of proteins and enzymes relevant to the agri-food value chain, including plastic-degrading enzymes and antifreeze proteins.

Early-Life Exposure to Arsenic and Toxic Metals: Epidemiological Perspectives

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The ARSENCIA project (Exposure to arsenic in the presence of other metals, metabolism, and health effects in childhood and adolescence, CIDEGENT/2020/050 - ESGENT/003/2024), funded by the Generalitat Valenciana, has fostered progress in understanding the implications of chronic exposure to inorganic arsenic and mixtures of other toxic metals through diet in vulnerable populations such as children. These effects are evident even at low levels, relevant to the general population, and the available evidence suggests that early exposure may increase the risk of neurological, cardiovascular, and metabolic diseases throughout life. Led at Miguel Hernández University, ARSENCIA is supported by internationally recognized cohorts such as INMA, NELA, NHBCS, and PREDIMED-Plus. The project focuses on updating databases on metals in biomarkers and foods, evaluating the role of dietary patterns such as the Mediterranean diet in exposure to and detoxification of arsenic and metal mixtures, analyzing the relationship between exposure and growth, respiratory health, neurodevelopment, and hormonal function using advanced statistical models, proposing innovative strategies to reduce the presence of metals in the food chain, and promoting the transfer of knowledge to society and regulation. The project has also enabled the establishment at UMH of a reference mass spectrometry laboratory for trace elements, with the capacity to analyze arsenic speciation through chromatography in various matrices. Overall, ARSENCIA has consolidated at UMH a strategic line in trace element epidemiology, advancing the understanding of the effects of exposure to toxic metals in vulnerable populations and in the development of strategies for their reduction. The results contribute scientific evidence to guide interventions and improve public health policies.

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Cell Division and Cohesinopathies

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How eukaryotes, including humans, inherit their nuclear genome is a fundamental question in biology that has direct clinical implications, as chromosome missegregation is a leading cause of miscarriages and birth defects, and is tightly linked to the progression of malignant tumours.

Our research interest is focused on studying cell division and Rare Diseases. We investigate the fundamental mechanisms that control chromosome segregation and mitotic progression during the cell cycle. Recently, numerous observations suggested that cohesin has an important role in the organisation of the chromosome architecture. In this project, our main objective is to study how the cohesin and Nipbl mutations found in CdLS patients cause the disease phenotypes.

Separase is a master mitotic regulator that, upon activation, will lead to chromosome segregation, Cdc14 activation, spindle elongation and condensation and resolution of the rDNA. The direct separase targets in most of the mitotic events triggered by separase remain unknown. Our major aim is the identification of separase interacting proteins and/or substrates using state-of-the-art genomic and proteomic screenings.

On the other hand, we also study the functions of a chromosome segregation-associated complex, the cohesin complex, in a human rare disease such as the Cornelia de Lange Syndrome. Recently, numerous observations suggested that cohesin has an important role in the organisation of the chromosome architecture. In this project, our main objective is to study how the cohesin and Nipbl mutations found in CdLS patients cause the disease phenotypes.

Targeting Telomeric G-quadruplex using Supramolecular Strategies

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Non-canonical nucleic acid structures have attracted considerable attention of researchers from many science fields, including chemistry, biology, physics, materials and nanotechnology. They include triplexes, *i*-motifs, three/four-way junctions or G-quadruplexes (G4). The later one is a supramolecular assembly of two or more tetrads, which arise from the hydrogen bonding network of four coplanar guanines. The stability and topology of G4 structures are mainly controlled by the alkali metal cation employed, the base sequence and the nature of the nucleic acid (DNA or RNA). Strikingly, a large number of putative G-quadruplex forming sequences have been identified in the genomes of human, microorganisms and viruses, and evidences suggest their pivotal role in key biological processes.[1] In particular, telomeres are regions enriched with putative G4-forming DNA sequences and have been associated to ageing and cancer. Therefore, G4 structures are currently tested as a therapeutic target to block telomere elongation in cancer cells.[2-3] Telomere sequences comprise hundreds of the hexanucleotide TTAGGG repeats which forms superstructures containing multiple consecutive G4 structures.

Herein, we present our rational desing to develop supramolecular systems able to bind selectively telomeric G-quadruplexes. Initially, we developed several series of triphenylamine-based ligands and metal complexes capable to interact strongly by G4s.[4] A range of biophysical assays (FRET melting, fluorescence spectroscopy and gel electrophoresis) has been used to characterise the interaction towards telomeric and other G4s in addition to duplexes. Our results point out the importance of the organic core scaffold, the number and class of the substituents, the molecule net charge and the reinforced structure of the ligands to bind strongly telomeric G4s.

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Acknowledgments:

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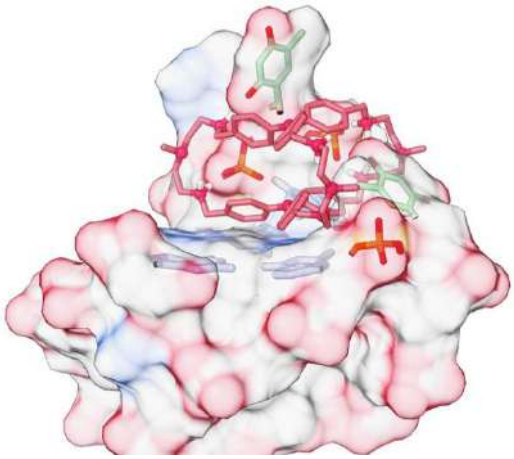

Role of APC-driven actin nucleation in collective cell migration and its impact on gut diseases

Mari Angeles Juanes[*] [a]

[a]*CIPF (ES)*

Colorectal cancer (CRC) is the second-leading cause of cancer death worldwide, and its incidence continues to rise. Early detection is essential to reverse this trend, improving treatment success and reducing the societal and economic burden associated with CRC. In 85% of CRC cases, cancer-initiating mutations occur in the tumour suppressor Adenomatous Polyposis Coli (APC) gene. APC was first identified as a potent actin nucleator in vitro using single-molecule assays, and we later confirmed to nucleate actin within cells. Through the Plan GenT CIDEGENT project, we employed a separation-of-function APC mutant (APC-m4, defective in actin nucleation) alongside biochemical, cell biology, and AI-driven approaches to investigate the relevance of APC-dependent actin nucleation in 2D and 3D models. Our findings revealed that APC-mediated actin nucleation is critical for focal adhesion turnover, cell-cell adhesion dynamics, and collective cell migration. Moreover, APC-driven actin filaments facilitate the formation and elongation of invasive structures emanating from cancer spheroids. We also observed that this pool of actin cooperates with other actin nucleators, collectively enabling protrusion formation but not elongation. Currently, we are validating these findings in in vivo models. Ultimately, this research aims to stratify patients and develop personalized anti-invasive therapies. Our work underscores the importance of investing in molecular mechanism studies to address unmet clinical needs, with significant benefits for patient well-being, healthcare systems, and the economy of the country.

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