

ANNUAL REPORT 2023



Institut Català
de Nanociència
i Nanotecnologia

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**Institut Català
de Nanociència
i Nanotecnologia**



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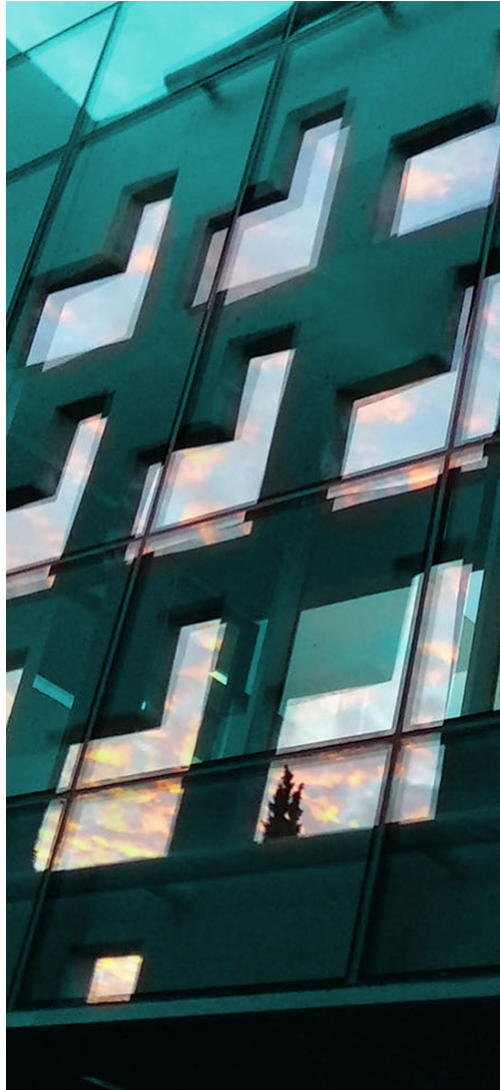
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LETTER FROM THE DIRECTOR



ICN2 is reaching maturity, after 10 years from its creation in 2013, when the former ICN incorporated the CSIC groups working at the extinct CIN2 Mixed Centre. It has been 10 years marked by the integration of groups, research priorities, common strategic goals, and a tremendous scientific success. During this period, ICN2 has been recognised with three consecutive Severo Ochoa Excellence Awards, the last of which just started in 2023 and will run until the end of 2026. The institute has also grown in size, quality and breadth of research topics, with a clear strategy to promote research lines ultimately leading to research outcomes of immediate relevance to society and industry.

The current Strategic Plan and our Severo Ochoa research program revolve around the concept of **Sustainability**. The research of ICN2 aims to provide unique solutions, offered by nanoscience and nanotechnology, for a sustainable future of our society. We focus on three global sustainability challenges: Medicine, Energy-efficient Information Processing, and Sustainable Energy Technologies. The path towards these nano-solutions starts at the fundamental research done at ICN2, which provides knowledge to develop technologies and eventually products. This focus on technology development founded on a solid basic research is a singular characteristic of ICN2 among other nanoscience centres in our environment. A proof of the success of this approach is the number of spin-off companies generated from the institute, some of them with a very bright future ahead. The case of InBrain Neuroelectronics is a clear example, with more than 30M€ of investment raised so far. Our policy for

protection of knowledge marks a highlight in 2023, when we have reached a record number of 42 active patents in our portfolio, with also a record ratio of 60% of our protected IP licenced to customers.

Two key projects for the future growth of ICN2 have received an important thrust in 2023. The first is the future BIST building at the Ciutadella del Coneixement, in Barcelona, which was announced in January, where ICN2 researchers will collaborate with groups from other BIST institutes on topics related to "Precision Medicine". The second is InnoFab, a proposal of the creation of an infrastructure for the fabrication of chips focused on next-generation semiconductors, with the capability of top-level research and development as well as pilot-line for industrial prototyping. With a budget well above 300 M€, InnoFab will be funded by the Spanish PERTE Chip and the Governement of Catalonia, and will position not only ICN2 but the whole innovation ecosystem of Catalonia in the frontline of European research and development in semiconductors.

2023 was plenty of other achievements and milestones for ICN2, which I invite you to explore in this Annual Report. All of this has been possible through the enthusiasm and talent of the whole ICN2 community, from the researchers, technicians, administration, students, visitors and collaborators. May this Annual Report serve to acknowledge their work and contribution to research and to society at large.

Sincerely,

Prof. **Pablo Ordejón**
Director, ICN2





We extend a warm welcome to the **ICN2 2023 Annual Scientific Report**. This document provides a summary of the activities undertaken by the Groups, Units and Facilities of the ICN2 during the year 2023. The **complete information** about their scientific production, projects, awards, and other impacts will be made **available on the ICN2 website**, where you can conveniently browse through all the science that we have produced.

For in-depth details about each Group, Unit and Facility presented in this document, a specific link and QR code are provided for your reference. We encourage you to explore this comprehensive report at your leisure and delve into all the data and scientific achievements of our community.

The **Institut Català de Nanociència i Nanotecnologia**, also known as the *Catalan Institute of Nanoscience and Nanotechnology (ICN2)*, is a non-profit international research institute located near Barcelona in Catalonia, Spain. It is committed to advancing knowledge, materials and devices in the fields of Information and Communication Technology (ICT), health, energy and the environment.

ICN2's expertise lies in the nanoscale, where it uncovers new properties, interactions and ways to exploit them in everyday life. The institute's objectives include bringing together scientists from diverse backgrounds to pursue better science, providing improved training for future generations of nanoscientists, and enhancing outreach to society, while also exploring new ways to engage with local and global industry.

ICN2 was accredited as a **Severo Ochoa Centre of Excellence** in 2014, a recognition that was renewed in 2018 for another 4-year period. The Severo Ochoa Programme, which is sponsored by the Spanish Ministry of Science, Innovation and Universities, aims to identify and support Spanish research centres that are among the world's best in their specialty. The ICN2's accreditation was renewed for the third time in a row, starting on 1 January 2023. This reflects the tremendous capability of the institute to continuously enhance its scientific and administrative processes to adapt to an increasingly diverse and complex society.

The trustees of ICN2 are the **Generalitat de Catalunya (Catalan Government)**, the **Spanish National Research Council (CSIC)** and the **Universitat Autònoma de Barcelona (UAB)**, where it is based. ICN2 is a **CERCA Centre** and also one of the founding members of the **Barcelona Institute of Science and Technology (BIST)** and the **Graphene Flagship**.

ICN2 is a global leader in nanoresearch, a place where both fundamental and applied research, as well as efforts to bring technology innovations to market, receive strong support. It is a proud creator of opportunities for dialogue and collaboration between researchers, industry, policymakers and society and a research institute committed to equal opportunities, fair selection processes and guaranteeing a healthy work/life balance.

WHAT DO WE DO?

At ICN2, we firmly believe that **nanoscience and nanotechnology will have an even more significant impact in the years to come**. We aspire to lead this impact by conducting excellent science, proposing innovative solutions to global challenges based on scientific knowledge, and engaging in dialogue with society about the benefits and potential risks of new technological advances. Our goal is to **collaborate with and provide expert advice to public and private institutions**, and to facilitate the adoption of newly generated knowledge **by industry, the health sector, and society at large**.

We are committed to achieving this with high standards of equality and diversity, attention to detail at every stage of the research career and providing the best possible work environment to ensure the safety and wellbeing of our community members. As you will discover in this report, our expertise in research and administration structures allows us to achieve these goals. Nanoscience and nanotechnology offer a close examination of the world around us. Understanding and controlling the sometimes-unexpected behaviour of matter at this scale has implications for all other sciences. ICN2 brings together chemists, physicists, biologists, materials scientists, and engineers to explore the uncharted corners of the nanoworld and determine how to turn acquired knowledge into applications that improve life and the world. Our researchers tackle this challenge from every angle, with teams working on the discovery, simulation, visualization, and experimental exploration of the

properties and behaviours of materials at the nanoscale, as well as the design and fabrication of devices that take advantage of their unique characteristics.

Research is at the heart of our mission, and therefore, we delve into it with detail in other sections of this document. In this introduction, we would like to focus on other aspects of our daily activities that enable us to achieve the desired levels of excellence.

CULTURE OF IMPACT

At ICN2, our research endeavours possess a dual focus: on one hand, we strive to push the boundaries of fundamental knowledge; on the other, we apply scientific insights to develop devices and solutions addressing major societal challenges.

The impact of ICN2 is exemplified through **various products that have already reached the market** in collaboration with multinational companies across diverse sectors. Our spin-off enterprises **create job opportunities and mobilise resources to make a difference** in medical, energy, and intelligent materials challenges. The ICN2 community is also deeply committed to **science outreach** and leads several **educational initiatives** that have a profound effect on society's understanding of the opportunities and challenges presented by nanotechnology.

ICN2 occupies a privileged position when measuring its influence in academic terms. However, **our research has a far-reaching impact beyond academia**, with the ultimate aim of constructing a more sustainable society

deeply engaged with scientific advancement. By bridging the gap between the scientific community and society, we are shaping a world where innovation, collaboration, and knowledge dissemination drive progress and address the pressing issues of our time.

EQUAL OPPORTUNITIES

ICN2 reaffirms its steadfast **commitment to fostering equal treatment and opportunities**, while managing diversity across all areas, preventing any direct or indirect discrimination based on factors such as gender, religion, culture, or other potentially discriminatory conditions. The institute diligently pursues measures to achieve genuine equality within our organisation by embedding equal opportunities as a strategic principle in our Corporate and Human Resources policies.

In 2023, a renewed Equal Opportunities and Diversity Committee has been working diligently to develop an ambitious **III Equal Opportunities and Diversity Plan**. This updated plan encompasses various aspects of the institute's institutional development, with a focus on promoting equality and diversity throughout the organisation.

Our **Human Resources policies** and practices uphold the principle of equal opportunities for individuals of all genders, cultures, nationalities, religions, or other distinguishing characteristics, covering areas such as selection, training, promotion, compensation, work-life balance, occupational risks, and occupational health. We maintain a strong commitment to preventing harassment and promoting conducive working conditions, implementing procedures for prevention and addressing complaints or claims promptly.

The **Women Talent Programme** specifically supports female researchers who aspire to achieve higher scientific goals. This programme complements other initiatives supported by the ICN2 Equal Opportunities Committee, including training activities, awards recognising female talent, and funding for seed projects led by female researchers.

By embracing these principles and initiatives, ICN2 **aims to create a more inclusive and diverse environment that nurtures talent and drives innovation**.

FOSTERING TALENT

The ICN2 prides itself on its ability to **attract skilled scientists, technicians, and support staff from all over the world**. Once these individuals join the institute, they can take advantage of various **training and professional development programs**. Furthermore, ICN2 scientists actively participate in regional, national, and international research communities. A significant number of those who complete their PhD or postdoctoral research at the ICN2 continue their careers at renowned institutions such as Harvard University, Yale University, the Max Planck Institutes, the French National Centre for Scientific Research (CNRS), and the French Alternative Energies and Atomic Energy Commission (CEA). This enables the ICN2 to continue offering positions to future nanoscientists. In 2023, the institute had an **average workforce of 327.31 members**.

	Total no. of full-time equivalents	31/12/2021 Total no. of persons	31/12/2021 Women	
			Number	%
Total	327.31	340	146	42.94%
1. Academic staff	202.85	214	82	38.32%
Group leader senior	18.36	19	3	15.79%
Group leader junior	1	1		0.00%
Staff Scientists	20.91	25	12	48%
Postdoctoral	54.58	55	14	25.45%
Predocctoral	66.49	72	33	45.83%
Academic Others	42.51	43	20	46.51%
2. Non-academic staff	124.46	126	64	50.79%
Administration	44.84	55	42	76.36%
Core scientific platforms	15.73	17	3	17.65%
Laboratory support	23.90	24	10	41.67%
IT staff	4.96	4	0	0.00%
Others	35.04	26	9	34.62%
TOTAL	327.31	340	146	42.94%

PHD PROGRAMME

The ICN2 is unwavering in its **commitment to fostering excellence** in its PhD Programme, designed to equip students with the unparalleled expertise and resources of the institute as a whole, while benefiting from the guidance and challenges presented by individual research groups.

Each year, our internal committee **offers invaluable advice to participants on essential formative experiences**, including

conference attendance, transferable skills, exposure, and publication records. Tailored to support students' development at every stage of their PhD journey, the comprehensive training calendar encompasses topics such as project planning, lab techniques, and scientific writing. In addition, our PhD students attend regular scientific seminars led by industry pioneers, participate in international

conferences and workshops, and seize opportunities for academic and industry placements with local and global partner institutions.

In 2023, the ICN2 PhD Programme continues to build upon the success of the **BIST Mentoring Programme** launched in 2021 in collaboration with BIST. This enhanced Mentoring Programme, an evolution of the previous internal initiative, empowers PhD students to overcome potential obstacles inherent in the PhD experience, focusing on career development and transition.

The ultimate goal of the ICN2 PhD Programme is to ensure that students maximise their experience at the institute and are thoroughly prepared to excel in their chosen professional paths.

POSTDOCTORAL TRAINING PROGRAMME

As part of the Severo Ochoa Programme and HRS4R budget, the ICN2 has meticulously crafted a Postdoctoral Training Plan dedicated to offering R2 and R3 Postdocs exceptional opportunities for professional and personal advancement. Conceived in 2020 and implemented in 2021, the plan encompasses a diverse array of activities included in the Annual Training Plan, all designed to empower Postdocs with cutting-edge tools and skills that elevate their proficiency, knowledge, and expertise in their respective fields.

The ICN2 remains steadfast in its commitment to ensuring that Postdocs are primed for **success in the next chapter of their careers, whether in academia or industry**. By focusing on nurturing their

talents and fostering their development, we are confident that our Postdocs will make substantial and lasting contributions to their chosen fields, driving innovation and shaping the future of research.

HUMAN RESOURCES STRATEGY FOR RESEARCHERS (HRS4R)

In May 2015, the ICN2 was bestowed with the prestigious Human Resources Strategy for Researchers (HRS4R) badge, a testament to excellence in Human Resources practices within research centres and closely associated with the European Charter for Researchers. This esteemed recognition serves as a strategic framework guiding the institution's efforts in recruitment, training, development, and equal opportunities initiatives.

In 2021, the ICN2 successfully secured the renewal of the HRS4R badge, extending its acknowledgement of distinction until at least 2024. The renewal process entailed updating the HR Action Plan and engaging with external experts. The meticulously devised actions for the current and previous periods can be accessed in the Careers section of the ICN2 website, showcasing our unwavering **commitment to fostering a supportive and dynamic environment for our researchers and staff**.



HR EXCELLENCE IN RESEARCH

In this part of the Annual Report, we are excited to share the significant impacts of our institutional, research, and innovation efforts during 2023. In the sections that follow, you will find a carefully selected collection of highlights and updates from the year, covering our achievements in important areas like sustainability, diversity, and scientific excellence.

We are proud to share these accomplishments with our stakeholders and look forward to continuing our mission to make a real difference.



In the year 2023, the ICN2 spearheaded a number of institutional events and initiatives aimed at generating fresh scientific prospects through the ICN2 community. The subsequent paragraphs present a summary of some of the key accomplishments that have been featured on the news section of the ICN2 website.

WellBIST: the psychological support programme for the BIST community

Human Resources, Health and Safety area and BIST, launched the **ICN2 Psychological support programme** to help those who need to improve their mental health. It also includes various training proposals on this topic.

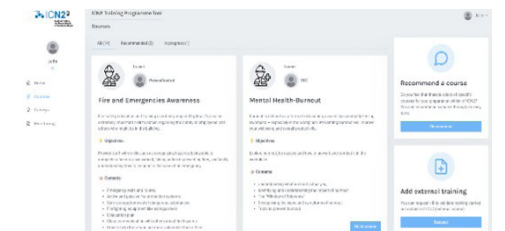


ICN2 values definition

During the 2023 and after a survey, discussion working group and personal interviews, ICN2 identified its Values. **Commitment, Collaboration and Transformation.** New material with messages related to this proposal is being prepared.

New ICN2 training platform

A new training page was launched to identify the training needs of our community, present the annual training plan, facilitate registration for our training activities, propose new courses, and manage surveys and certificates. Additionally, it includes a personal page to track individual training progress.



Construction for the 'Mercat del Peix' research complex kicks off with a big institutional event

The new research complex, which will host more than 1,200 researchers, will be fully operational in 2026. The **precision medicine-focused BIST building**, which will account for two-thirds of the total complex, will bring together researchers from CRG, IBEC, ICN2 and IRB Barcelona.



New electron microscope centre to advance in research in structural biology and new materials

The **Joint Electron Microscopy Center at ALBA (JEMCA)** was created thanks to the collaboration of different research entities to launch a new centre within the ALBA Synchrotron building offering electron microscope services to the scientific community. In specific, eight different partners will be using this centre: IBMB-CSIC, ICN2, IRB, CRG, ICMAB-CSIC, CSIC, UAB, and the ALBA Synchrotron.



ICN2 promotes the Coalition for Advancing Responsible Research Assessment (CoARA)

CoARA is a **global coalition devoted to implementing responsible and effective research assessment practices**, based on a set of 10 common principles and commitments. ICN2 is committed to devoting resources to reforming research assessment, reviewing and developing assessment criteria and tools, raising awareness of research assessment reform and providing transparent communication, guidance, and training on assessment criteria and processes.

ICN2 Unveils the III Equality of Opportunities & Diversity Management Plan 2023-2026

The plan sets key objectives such as guaranteeing **equality for all, promoting diversity and inclusion**, and eliminating barriers to workplace success. Strategic actions include improving communication, increasing transparency in staff selection and promotions, and conducting training on equal opportunities. The ICN2 community will collaborate to implement and evaluate the plan, working towards a more inclusive future.

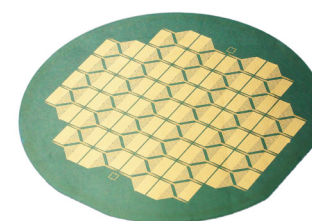


RESEARCH HIGHLIGHTS

In this section, we showcase some of the published results and projects that illustrate the high quality of broad diversity of interests, fundamental approaches, and potential applications of the ICN2 research lines. Here, we also show some of the most notable awards, recognitions and grants of 2023.

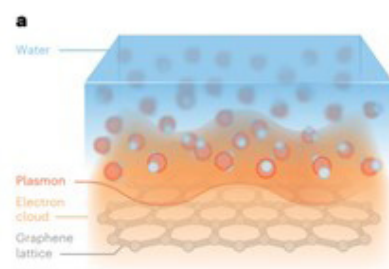
An EIC Transition Project will Help ICN2 and INBRAIN Neuroelectronics Develop Next-Generation Brain-Computer Interfaces Through Cutting-Edge Graphene Technology

With the ICN2 as a partner, the **'Graphene Transistors for High-Density Brain-Computer Interfaces' (GphT-BCI)** project, led by **INBRAIN Neuroelectronics**, kicked off on December 1, 2023. The GphT-BCI project, along with 19 other projects, was selected by the **European Innovation Council (EIC)** to receive a grant of €2.5M following the April 2023 EIC Transition programme cut-off. The goal of this funding is to turn cutting-edge science results into business opportunities for the innovation's future commercialization.



Electron cooling in graphene enhanced by plasmon-hydron resonance

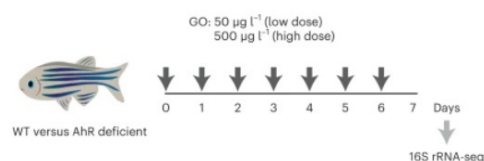
An international team of researchers, including Prof. **Klaas-Jan Tielrooij** from ICN2, reports that water can interact directly with the carbon's electrons: a quantum phenomenon that is very unusual in fluid dynamics. Experiments reveal that **water and carbon make a quantum couple**: the flow of water on a carbon surface is governed by an unusual phenomenon dubbed quantum friction. These results could lead to applications in water purification and desalination processes, and maybe even to liquid-based computers.



Xiaoqing Yu, Alessandro Principi, Klaas-Jan Tielrooij, Mischa Bonn and Nikita Kavokine. Electron cooling in graphene enhanced by plasmon-hydron resonance, *Nature Nanotechnology*, 2023. DOI: 10.1038/s41565-023-01421-3.

Graphene oxide elicits microbiome-dependent type 2 immune responses via the aryl hydrocarbon receptor

An international group of researchers, including **Neus Lozano** from ICN2, showed that nanomaterials can **influence the crosstalk between the microbiome and immune system**. Oral exposure to graphene oxide (GO) modulates the composition of the gut microbiome in zebrafish. Also, GO was found to elicit AhR-dependent induction of *cyp1a* and homing of *Ick*⁺ cells to the gut in germ-free zebrafish larvae when combined with butyrate.



Guotao Peng, Hanna M Sinkko, Neus Lozano, Kostas Kostarelos, Lars Bräutigam and Bengt Fadeel. Graphene oxide elicits microbiome-dependent type 2 immune responses via the aryl hydrocarbon receptor, *Nat. Nanotechnol.*, 2023. DOI: 10.1038/s41565-022-01260-8.

New EU-funded 2D-BioPAD project kicks off in Thessaloniki

Members of the ICN2 Nanobioelectronics and Biosensors Group took part in the meeting that marked the start of the scientific activities of the recently funded 2D-BioPAD project. Thanks to €6M in funding, the project will develop a compact and easy-to-use device for the early diagnosis of Alzheimer's Disease.



MaX develops advanced simulation software for powerful supercomputers

In 2023 the **European High Performance Computing Joint Undertaking (EuroHPC JU)** launched 10 Centres of Excellence (CoEs) that will develop and scale up existing computing codes towards exascale performance in the next four years. The **MaX ("MAterials design at the eXascale")** European Centre of Excellence, dedicated to the development of advanced software for materials modelling and simulations, has renewed its funding from the European Union, entering a promising third phase of the project.



Funded by the European Union

EuroHPC Joint Undertaking



Javier Fonseca, Lingxin Meng, Inhar Imaz and Daniel Maspoch. Self-assembly of colloidal metal-organic framework (MOF) particles. *Chemical Society Reviews*, 2023. DOI: 10.1039/d2cs00858k.

Self-assembly of colloidal metal-organic framework (MOF) particles (Review)

This publication presented a comprehensive overview of strategies for the self-assembly of colloidal MOF particles into ordered superstructures of different dimensionalities, highlighting some of their properties and applications, and sharing thoughts on the self-assembly of MOF particles. This work was carried out by scientists from the **Supramolecular Nanochemistry and Materials Group** of ICN2, led by **Prof. Daniel Maspoch**.

MINIGRAPH kicks off scientific activities

The kick-off meeting of the project **MINIGRAPH**, coordinated by the ICN2 **Advanced Electronic Materials and Devices Group**, led by ICREA **Prof. Jose A. Garrido**, was held on 20-21 October at the Casa de Convalescència in Barcelona. The project has received €4M in funding from the European Commission through the 2021 European Innovation Council (EIC) Pathfinder Challenges call, plus another €1.2M from the Swiss Federal Government (State Secretariat for Education, Research and Innovation).



Funded by the European Union

MINIGRAPH

European Innovation Council



JORDI DÍAZ MARCOS
GERARD GUIMERÀ BALLESTA
JOAN MENDOZA GONZÁLEZ
PEDRO A. SERENA DOMINGO
MARÍA TENORIO TUÑAS
COORDINADORES

PRÓLOGO DE JAVIER GARCÍA MARTÍNEZ INCLUYE LIBRO ELECTRÓNICO THOMSON REUTERS PROVIEW™

A second volume of the White Paper of Nanotechnologies published

The “White Paper on Nanotechnologies II, state of the art of research, development and innovation” (Aranzadi, 2023) was published as a complement to the first White Paper, published in 2021, which aimed at providing an ethical and social vision of the advances in nanoscience and nanotechnology. Among the authors are several members of the ICN2, specifically (in alphabetical order): Dr Neus G. Bastús, Enric Calucho Palma, Dr María José Esplandiú Egido, Dr Jordi Fraxedas Calduch, Prof. Pedro Gómez Romero, Dr Inhar Imaz, ICREA Prof. Arben Merkoçi, and Dr Salvio Suárez-García.

Professor Arben Merkoçi Recognised as Top Scientist in Spain for Electronics and Electrical Engineering

Professor **Arben Merkoçi** was recognised by research.com as **the leading scientist in Electronics and Electrical Engineering** and ranked eighth in Materials Science in Spain. His research focuses on nanotechnology, biosensors, and nanoparticles, with significant implications for various industries. His interdisciplinary work and recognition highlight the importance of nanotechnology and biosensors in the advancement of technology.



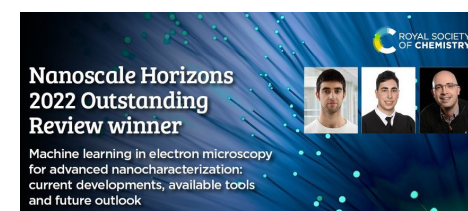
Prof. Laura Lechuga wins the Spanish National Nanotechnology Award

Prof. **Laura M. Lechuga Gómez**, leader of the ICN2 **NanoBiosensors and Bioanalytical Applications Group**, was the winner of the third edition of the **Spanish National Nanotechnology Award**, sponsored by the company NOB166. NOB166’s mission is to provide sustainable solutions and products for detergency, cosmetics, fibres, hard surfaces, and coatings, based on the use of nanotechnology.



Prof. Daniel Maspoch acknowledged with Rei Jaume I Award for exceptional contributions to New Technologies

Professor. **Daniel Maspoch Comamala**, Group Leader of the ICN2 **Supramolecular NanoChemistry and Materials Group**, was distinguished with **the New Technologies Rei Jaume I award** at the illustrious Rei Jaume I Awards ceremony. The Rei Jaume I Awards recipients were announced at a formal event at the Palau de la Generalitat Valenciana, presided over by the acting head of the Consell, Ximo Puig.



The Advanced Electron Nanoscopy Group receives “Nanoscale Horizons” Outstanding Review Award for a paper on machine learning

The award recognises the **exceptionally high-quality of the review**, which thoroughly discusses the application of machine learning and artificial intelligence to electron microscopy, authored by Marc Botifoll, Ivan Pinto-Huguet, and Group Leader ICREA Prof. **Jordi Arbiol** and published by the journal in 2022.

ERC Consolidator Grant awarded to Dr Elena Del Corro, senior researcher at the ICN2

Dr Elena Del Corro, senior researcher in the ICN2 **Advanced Electronic Materials and Devices Group**, is the recipient of one of the prestigious **Consolidator Grants 2023 of the the European Research Council**. She will develop the TriboMed project, aimed at integrating triboelectric energy generators into active implantable medical devices to improve life of patients suffering from diseases linked to the activity of the vagus nerve.



OUTREACH AND EDUCATIONAL HIGHLIGHTS

The participation of ICN2 in educational and outreach activities represents a long-term investment in raising the profile of nanoscience and the role of the ICN2 within society. Its efforts are having a growing impact with consolidated programmes and new initiatives opening new communication channels with a number of audiences. Actions in this area are a joint effort between the institute's Departments and scientists.



Crazy for Physics programme

The **Crazy for Physics** programme, promoted by **Fundació La Pedrera**, took place again in several sessions throughout 2023. It offers high school students exciting experiences that explore the biggest and smallest scales of the universe. It also provides a sense of what it's like to be a physics researcher.

NanoEduca 2023: final event and video contest award ceremony

The 2023 edition of the **NanoEduca Programme** ended with a special event for the teachers and students of the high schools that participated in the project. The winners of the NanoEduca 2023 Video Contest were awarded in a joyful ceremony.



LightNET project

ICN2's **LightNET** programme, supported by the **FCRI** and the **Catalan Department of Education**, introduces a citizen science project to test a novel carbon-capture technology to 164 schools across Catalonia. This project, occurring during **Science Week 2023**, not only educates students about innovative solutions to climate change but also actively involves them in data collection and analysis.

#100tífiques initiative brings female role models into schools

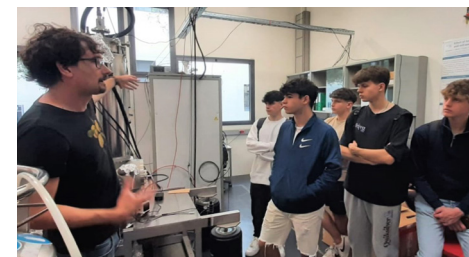
On the occasion of the International **Day of Women and Girls in Science**, the ICN2 took part in the fifth edition of #100tífiques, an initiative of the **Fundació Catalana per a la Recerca i la Innovació (FCRI)** and the **Barcelona Institute of Science and Technology (BIST)**, with the collaboration of the **Generalitat de Catalunya's Departments of Education, and of Research and Universities**. #100tífiques aims to highlight the **contribution of women in science and technology** and to provide young people with real role models.

#100tífiques



573 women researchers
505 schools
40,000 students

Thank you!

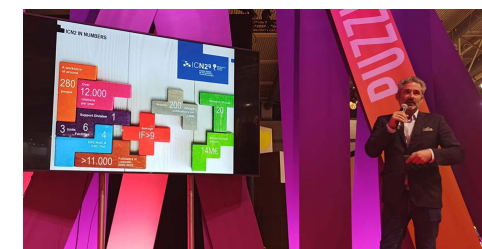


Great success of the 10alamos9 Nanoscience Festival 2023 at the UAB

On 25 April 2023, a **special day of activities for high school students** was organised at the Universitat Autònoma de Barcelona (UAB), in the framework of the **10alamos9 Nanoscience and Nanotechnology Festival**. The programme included visits to a few research centres in the campus (ICN2, ICMAB, IMB-CNM and the UAB itself) and a roundtable with young non-scientists.

ICN2 spearheads innovation dialogue at PuzzleX 2023

ICN2 Business and Innovation team, headed by **Pablo Pomposiello**, participated in **PuzzleX 2023** in Barcelona, engaging in vital **discussions about the future of technology**. With a focus on creating a sustainable and prosperous future, Pomposiello and his colleague Claudia Nieva sought new industry collaborations to further ICN2's innovative nanoscale research.



In line with the entrepreneurial spirit of the institute and its researchers, ICN2 continues to strive for excellence in Innovation and Impact. In this section, we highlight some of the major technology transfer and value creation actions that took place in 2023.

ICN2 captured the extraordinary opportunities in funding for Innovation

The year 2023 offered an extraordinary number of calls for applications in Innovation. ICN2 was able to secure an annualised grant income of more than €2.3M euro, almost a 300% increase over the total in 2022. These grants include collaborations with companies, providing not only robust funding to ICN2, but also a network of strategic partnerships.

INBRAIN Neuroelectronics was awarded a US-FDA designation of Breakthrough Technology for their graphene neural interphase

INBRAIN Neuroelectronics develops **graphene-based applications for neurological diseases** founded by researchers from IMB-CNM-CSIC, ICN2 and ICREA. The designation paves the way for a fast-track review through the approval process for clinical use.



ICN2 had a record year in Patent activity

The B&I Department handled the filing of 5 new Patents in 2023, a yearly number within our normal standards. The records came in Patents granted, with a record number of 4; and Patents Extended in National Markets, with a smashing record of 24 extensions. These robust numbers point at the strengthening of ICN2's IP base, the ultimate foundation for successful innovation and venturing.

Starting a Company from Within ICN2: the professional journey of a scientist turned into entrepreneur

Dr Juliana Jaramillo continued the **new series of seminars** launched by the ICN2 Department of Business and Innovation. The series of talks is titled The Innovators and highlights the experience of junior scientists turned technology entrepreneurs.



ICN2 developed a Pipeline of 3 New Spinoff Companies

ICN2 and CSIC partnered through 2023 to develop a pipeline of **3 new spinoff companies**, in the field of clinical diagnostics, tissue regeneration and carbon dioxide capture. The bases for investment, licensing and hosting of technology development services were established with a foundation target during 2024.

ADVANCING SCIENTIFIC FRONTIERS WITH THE THIRD SEVERO OCHOA CENTRE OF EXCELLENCE ACCREDITATION (2023-2026)

This year has seen the **kick-off of ICN2's third consecutive Severo Ochoa award**. In alignment with our current strategic plan, this Severo Ochoa project seeks to help ICN2 take major steps towards consolidating its international leadership and influence, as well as its impact. The scientific programme **"Nanosolutions for a Sustainable Society"** is being developed through three Application Domains (ADs) and four Enabling Research Areas (ERAs). ADs spearhead the delivery of transformative nanoscale solutions for concrete societal needs, being representative of ICN2 capabilities, resources, and strategic direction: Medicine, Energy-Efficient Information Processing and Sustainable Energy Technologies. Work in ADs is complemented and catalysed by ICN2's hubs of scientific expertise and knowhow pivotal to excellent science: Nanomaterials and Nanofabrication, Nanocharacterization, Modelling and Simulation and the Artificial Intelligence Computational Platform (AI@ICN2).

Main highlights for 2023 have been:

Governance

Setting up the project's governance, including the establishment of working groups (WGs) for each of the ADs and ERAs. These WGs are the heart of the Severo Ochoa (SO) project, proposing and deploying activities aligned with the project objectives. WGs are autonomous, chaired by members who are part of the SO Scientific Committee.

Human resources

During this first year, the ten SO predoctoral students assigned to the project were selected and incorporated to ICN2. So has the SO project manager. The selection processes for other profiles were launched, though incorporations have happened in 2024.

Infrastructure

275K€ were allocated for **equipment to the Investment Committee**, which launched two calls (one at the start of the year and another one at the end of 2023.) By the end of the year, over 100K€ had already been spent or committed. Furthermore, an investment of 100K€ was committed for a new computational cluster.

Internal calls

This year all first edition SO competitive calls were launched, and many resolved. The Internationalisation Committee allocated almost 15K€ for a total of 9 grants for the Outbound Mobility and the International Visitors Programmes. The Business and Innovation Office offered a total of 2 grants and 45K€ within the Technology Valorisation and the Venturing Programmes and the From Science to Business course. The 2023 Seed funding call was launched in October, to be resolved in 2024.

AI@ICN2 Platform

The **Artificial Intelligence Computational Platform** is one of the high impact activities of the SO programme. It is aimed at providing internal operational guidance and tools to the ICN2 community. This year we have set the bases for the platform by defining profiles and launching processes that have been concluded early 2024; exploring new strategic partnerships and designing specific trainings to be delivered inhouse. We have also mapped ICN2 research lines using or aiming to use AI/ML in the near future.

Other many actions, both cross-cutting and from the working groups were kicked-off this year and will see the light during 2024 and beyond. The journey towards developing nanosolutions for a sustainable society has started.



ORGANISATION

At ICN2, we take immense pride in recognising that our people are the driving force behind our success. Our dynamic team of scientists, hailing from a wide array of backgrounds, is bolstered by the invaluable expertise of our technicians and administration professionals, all working in unison towards the Institute's ambitious objectives. We are truly privileged to have the guidance and insights of our esteemed Board of Trustees and Scientific Advisory Board, composed of distinguished international peers, paving the way towards a bright future for the ICN2 community.

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DIRECTOR

The ICN2 is led by Director Prof. **Pablo Ordejón**, who also leads an ICN2 Group. He reports directly to the *Board of Trustees* and is advised by the *Scientific Advisory Board*. The Director works closely with the ICN2 Vice-Director, ICREA Prof. **Jose A. Garrido**, also Group Leader, the General Manager, Mr **Lluís Bellafont** and the Executive Assistant, **Cristina Granadero**.

Led by Dr **Margarita Navia**, this office works to provide a response to the different challenges faced by the institute on the short and long term, addressing issues at the national and international level, to improve the institute's responsiveness to an ever-changing global context. It oversees the development of the strategic plan, coordinates institutional projects like the Severo Ochoa Programme and provides advanced research development support to the ICN2 research community.

It works in close collaboration with both the research community and the administration departments, as well as the external collaboration network of the institute, and aims to bring insight and strategic manpower to research activities, hot topics like research data management, and ongoing initiatives to support the ICN2 in becoming a world-leading research institute.

MAIN ACTIVITIES

- » Design and management of the ICN2 Strategic Plan, supporting its translation into actionable goals and yearly plans, and monitoring overall progress towards bigger-picture objectives.
- » Delivering institutional strategic projects and initiatives.
- » Coordination of institutional projects and initiatives of strategic importance.
- » Supporting the direction in drawing new strategies and policies.
- » Co-identification of funding opportunities for research groups and researchers, plus dedicated pre-award information and support for calls considered strategic for the centre.
- » Cultivation of mutually beneficial relationships with key stakeholders.

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The Office of Business and Innovation is dedicated to **protect and commercialize ICN2's groundbreaking research results**, establishing R&D and licensing contracts with industry partners and fostering new collaborations within both private and public sectors. Our innovation instruments connect scientific discoveries to the market, expand our scientists' collaborative networks, and ensure that public science generates resources that fuel further scientific advancement. The Severo Ochoa Programme has facilitated a range of pioneering innovation activities, produced tangible outcomes and reinforced ICN2's status as a center of excellence. The Business and Innovation Office team aims to achieve excellence in innovation by providing robust support and empowerment to our researchers.

Initiated in 2019, **the Business and Innovation Office has been on a mission to become a true incubator for ICN2 technologies**, making significant strides towards integrating public science with the production of goods and services. Severo Ochoa funding has enabled internal support programs for Proof of Concept and Venturing. In the coming years, the Business and Innovation Office will deploy additional tools and mechanisms to ensure ICN2's continued leadership in innovation.

In 2023, the Business and Innovation Office focused on extending and strengthening our network through strategic communication efforts. In 2023, ICN2's Business and Innovation (B&I) team successfully accelerated the transition from scientific discoveries to market applications, emphasizing

its dedication to fostering knowledge transfer and innovation. The B&I team deposited 7 new patents, managed 42 active patent families, and negotiated 2 new Licenses, initiated 15 new R&D and Service projects. The B&I team reaffirms our unwavering commitment to bridging the gap between scientific research and real-world applications.

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Research activities at the ICN2 are directed by senior scientists of international repute who lead teams of PhD students, postdocs and other senior scientists in the development of their respective areas of expertise. In 2023 the ICN2 gathered 20 research groups that together cover much of the breadth of nanoresearch:

ADVANCED ELECTRON NANOSCOPY

ICREA Prof. **Jordi Arbiol**

ADVANCED ELECTRONIC MATERIALS AND DEVICES

ICREA Prof. **Jose A. Garrido**

ATOMIC MANIPULATION AND SPECTROSCOPY

ICREA Prof. **Aitor Mugarza**

INORGANIC NANOPARTICLES

ICREA Prof. **Víctor F. Puentes**

MAGNETIC NANOSTRUCTURES

ICREA Prof. **Josep Nogués**

NANOBIOELECTRONICS AND BIOSENSORS

ICREA Prof. **Arben Merkoçi**

NANOBIOSENSORS AND BIOANALYTICAL APPLICATIONS

Prof. **Laura M. Lechuga**

NANOELECTROCATALYSIS AND SUSTAINABLE CHEMISTRY

ICREA Prof. **María Escudero Escribano**

NANOMEDICINE

Prof. **Kostas Kostarelos**

NANOSTRUCTURED FUNCTIONAL MATERIALS

Dr **Daniel Ruiz-Molina**

NANOSTRUCTURED MATERIALS FOR PHOTOVOLTAIC ENERGY

Dr **Mónica Lira-Cantú**

NOVEL ENERGY-ORIENTED MATERIALS

Prof. **Pedro Gómez-Romero**

OXIDE NANOPHYSICS

ICREA Prof. **Gustau Catalán**

PHONONIC AND PHOTONIC NANOSTRUCTURES

ICREA Prof. Dr **Clivia M. Sotomayor-Torres**

PHYSICS AND ENGINEERING OF NANODEVICES

ICREA Prof. **Sergio O. Valenzuela**

SUPRAMOLECULAR NANOCHEMISTRY AND MATERIALS

ICREA Prof. **Daniel Maspoch**

THEORETICAL AND COMPUTATIONAL NANOSCIENCE

ICREA Prof. **Stephan Roche**

THEORY AND SIMULATION

Prof. **Pablo Ordejón**

THERMAL PROPERTIES OF NANOSCALE MATERIALS

Prof. **Javier Rodríguez-Viejo**

ULTRAFAST DYNAMICS IN NANOSCALE SYSTEMS

Dr **Klaas-Jan Tielrooij**

ADVANCED ELECTRON NANOSCOPY GROUP

JORDI ARBIOL

ICREA Research Professor and Group Leader



MAIN RESEARCH LINES

- Exploration by means of electron microscopy and related spectroscopies of the structure-properties relationships in nanomaterials for physical applications (photonics/plasmonics/ phononics/electronics/quantum technologies), adding AI-based methodologies for advanced automated data analysis and 3D atomic modelling (deep and machine learning).
- Understanding of the behaviour of nanomaterials for energy and environmental applications down to the atomic scale and creation of in-situ and correlative methodologies combining electron microscopy, synchrotron and AI.

NEW PROJECTS & MILESTONES

JEMCA has fulfilled the primary objective of the group, that of creating and leading a state-of-the-art research infrastructure in electron microscopy in Catalonia with strong international projection (thanks to e-DREAM). The new infrastructure and funded projects (**In-CAEM**, **SOLARUP**, **IMPRESS** and **ReMade@ARI**) will allow expanding the group's capabilities in the in-situ correlative electron / synchrotron microscopy / spectroscopy on energy,

environmental and quantum nanomaterials and will allow to open new research lines (see below). In parallel, we plan to continue working within e-DREAM as part of the Analytical Research Infrastructures in Europe (ARIE). One of our main objectives in ARIE and e-DREAM is the development of novel and disruptive correlative synergies and methodologies between different characterization technologies, as it can be between EM and Synchrotron light sources.

41 ARTICLES

11.855 MEAN IMPACT FACTOR

6 FUNDED PROJECTS

35 CONTRIBUTIONS

3 AWARDS

7 OUTREACH IMPACT

14 CONGRESSES ORGANISATION

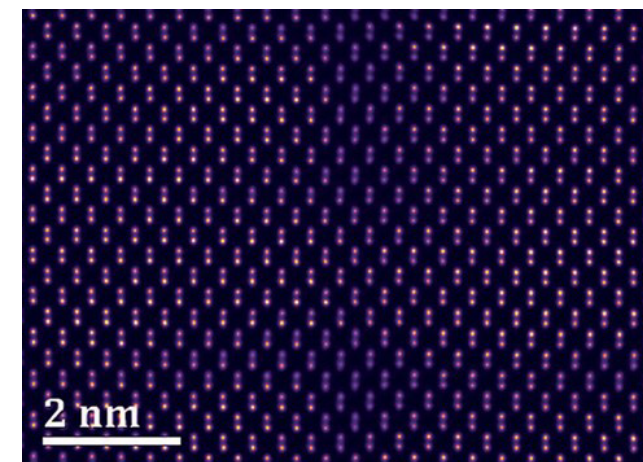
11 COURSES

New projects granted to the group in 2023 that will start in 2024 are **RIANA** (HORIZON EU), **EDISON** (AGAUR), **DeQD** (Danmarks Innovationsfond) and **NEXPECH2** (M-ERA. Net). In this way, two of the research topics we will explore, in addition to the research lines on which the group already works, are:

A) Development of AI-based methodologies for advanced automated data analysis

Our research line devoted to the direct correlation between atomic scale structure/ composition and sub-nanometer scale physical properties will benefit from the funds from the collaborative projects with Microsoft, the EU HORIZON EIC Pathfinder SOLARUP that Prof. Arbiol is coordinating and the IMPRESS project.

The new analysis capacities offered by JEMCA will allow for the study of newly designed hybrid semiconductor/ superconductor 1D and 2D nanomaterials for their application in quantum computing (Microsoft) as well as the photovoltaic (PV) cells developed within SOLARUP, and a better understanding of the physical phenomena involved in the



related devices. We will continue the search for Majorana- based or related quantum devices supported by our recent highlight in Nature 2022. In addition, as the new industry developments for quantum materials or novel nanostructured photovoltaic devices have as a priority objective the scalability of their systems (e.g.: scalable topological quantum networks or patterned PV nanostructures), it will be mandatory to combine detailed structural and compositional analyses at the atomic scale with a precise 3D modelling. Current such

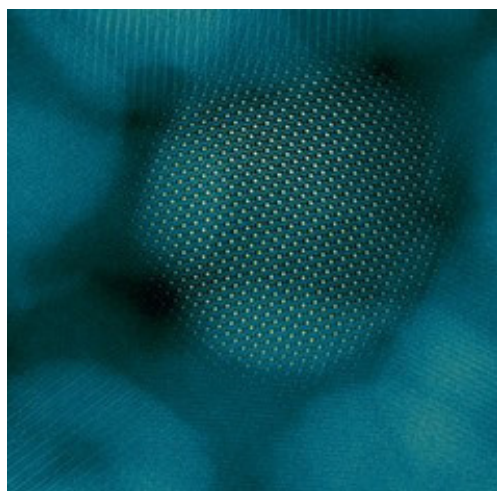
methodologies based on STEM imaging and related spectroscopies like EELS are limited by scale: conversion of the vast number of data points in a nanostructured system into the models needed for properties simulation is a mammoth task. In the next years, one of our main objectives will be to develop new methodologies for the automated processing of atomic-scale STEM-EELS data in order to obtain their direct conversion into the required nanoscale finite-element simulations input models. In order to do this, we will explore the application of AI methods based on machine/deep learning- enhanced pattern recognition (Nanoscale Horiz. 2022). The computing infrastructure necessary to develop such an ambitious AI-based project has been included in In-CAEM, which will provide the large data storage, data analysis and data treatment computing resources in collaboration with ALBA and PIC-IFAE.

B) In-situ and correlative study of energy nanomaterials

The next steps, moving forward in the energy nanomaterials research line, will be related to the development of in-situ / operando experiments in the electron microscopy to understand the physical and chemical phenomena promoting the different energy mechanisms (e.g.: (photo) electrochemical) with unprecedented resolution. Taking advantage of the synergy with ALBA, within In-CAEM and IMPRESS projects, we will work on developing correlative in-situ electron microscopy and Synchrotron experiments, in correlation to the developed theoretical models. In-CAEM provides not only the equipment but also the necessary synergies. Together with ALBA engineers and beam line scientists, we have already started to design the modifications

required to adapt some of the ALBA beam lines (e.g.: CIRCE, CLAESS, MSPD, MIRAS and NCD-SWEET) to allow the necessary in-situ correlative experiments with the new (S)TEMs. In-CAEM will also provide the computing resources for the in-situ data analysis and the availability of a large data storage capability.

In the following years, we will continue working hard to strengthen even more the JEMCA national and international alliances and synergies and apply for more funding to develop the future research ideas (several new proposals are right now being drafted and will be submitted in the coming 2023 HORIZON EU Calls).



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ADVANCED ELECTRONIC MATERIALS AND DEVICES GROUP

JOSE ANTONIO GARRIDO

ICREA Research Professor, Group Leader and Vice Director



MAIN RESEARCH LINES

- Technology and micro/nanofabrication for advanced electronic devices and systems based on 2D materials
- Chemical vapour deposition (CVD) of graphene and metal-organic CVD of transition metal dichalcogenide (e.g. MoS₂) films
- Fundamental electronic, electrochemical, and interfacial phenomena of 2D materials
- Bioelectronics and biomedical technologies: neural interfaces, neuroprosthetics, cell bioelectronics
- Electronic and electrochemical biosensors

NEW PROJECTS & MILESTONES

The AEMD group aims to explore fundamental electronic and electrochemical phenomena of novel materials, with a current particular emphasis on graphene and other 2D materials (e.g. MoS₂), and to develop the fabrication and processing technologies necessary to prepare advanced electronic devices and systems based

on them. A major focus of our work are applications related to neural interfaces and neuroelectronics.

2023 has been a year of great progress for the group. Our team has continued working together with the ICN2 Phononic and Photonic Nanostructures Group on the

5 ARTICLES

4.56 MEAN IMPACT FACTOR

14 FUNDED PROJECTS

19 CONTRIBUTIONS

1 THESIS

2 OUTREACH IMPACT

NANOSMART project for the development of wireless technology based on carbon and 2D materials finished on February 2023. As a highlight, the AEMD group developed 2D materials films at the cm scale, aiming at electronic applications. The group has also explored transfer and protection strategies to maintain the 2D materials crystallinity.

Within the EU Graphene Flagship, our group continued its participation in the Core 3 phase. During 2023, the group has kept collaboration with European partners for the advance of graphene biomedical technologies. In collaboration with Paris Vision Institute and University College London, we have developed a technique for simultaneous surface DC-coupled brain recordings and cerebral blood flow monitoring depth in the cortex using flexible graphene microtransistors and functional ultrasound imaging.

In **MINIGRAPH**, a EIC Pathfinder project coordinated by AEMD, we have advanced in the development of surface and depth bidirectional neural probes targeting neuromodulation in large animal models, a step closer to human translation. Moreover, we have progressed towards improved reliability and long-term operation of the neural interfaces.

We have been working in the **RESCUEGRAPH** project, focused on a functional stimulation system for rehabilitation after spinal cord injury using graphene-based nerve electrodes (under the FLAG ERA programme, led by Prof. Xavier Navarro from the UAB). We have demonstrated the capabilities of small graphene microelectrodes to stimulate selectively and with low current thresholds different fascicles within the sciatic nerve in acute and chronic animal experiments.

Our team is also working on the **i-VISION** project (funded by La Caixa Foundation), focused on the development of retinal implants for vision restoration, an endeavour carried out in collaboration with IFAE, ICFO, Barraquer Foundation and Paris Vision Institute. We conducted chronic in vivo experiments to assess the efficacy of retinal stimulation to evoked cortical activity, as evidenced by functional ultrasound monitoring. We have also worked in the integration of rGO electrodes with an application specific integrated circuit (ASIC) designed by IFAE for visual restoration.

We continue advancing our research as a Consolidated Research Group thanks to the support of the Catalan Government (2021 SGR 01534) and as part of a project

founded by the Spanish Ministry, focused on technologies based in 2D materials for biomedical applications, of which Dr Elena del Corro is co-PI. In the frame of this project we are developing a new graphene synthesis approach, we work on the automatization of the transfer process, on graphene protection strategies and on graphene selective functionalization towards the development of an universal sensor platform.

Additionally, the group has contributed to the project **"BrainGraph"**, led by Antón Guimerà from CNM-IMB and in collaboration with INBRAIN Neuroelectronics, focused on graphene based neurotechnology for advanced clinical brain monitoring. This project has been funded under the call *"Proyectos en líneas estratégicas"* funded by MCIN/AEI and by the European Union NextGenerationEU/ PRTR.

In 2023, we also started the **graphene transistor BCI (GphT-BCI)** project led by INBRAIN electronics and funded by the EU under the EIC Transition programme. This project will pave the way for the clinical translation of brain-mapping neural interfaces based on graphene-transistor arrays for brain-computer interfaces.

At individual level, Dr. Elena del Corro was awarded with an ERC Consolidator Grant to work on triboelectric energy generators for self-powered medical implants to improve the life of patients suffering from diseases linked to the activity of the vagus nerve. This project will start on September 2024.

Moreover, the project **TriBioNics** lead by Dr. Elena del Corro in collaboration with Samuel Sanchez Ordóñez from IBEC was selected in the BIST Ignite programme. This project combines for the first time three innovative technologies: 3D skeletal muscle printing, graphene bioelectronics and triboelectronics. The aim is to mould skeletal muscle and, among other things, develop new therapies for rehabilitation.

In addition, Dr. Amador Pérez started the project **LighNET** on October 2023 to develop solutions for climate neutral and even climate negative smart cities at a competitive cost. This project is a proprietary and innovative technology for developing urban spaces to capture CO₂.

Finally, Dr. Eduard Masvidal was awarded a Juan de la Cierva Postdoctoral Fellowship to develop advanced 2D materials-based neuroelectronic interfaces.

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ATOMIC MANIPULATION AND SPECTROSCOPY GROUP

AITOR MUGARZA EZPELETA

ICREA Research Professor and Group Leader



MAIN RESEARCH LINES

- Synthesis and advanced characterization of carbon-based 1D and 2D nanomaterials.
- Tailoring the quantum properties of 2D materials with atomically precise superlattices.

NEW PROJECTS & MILESTONES

The scientific research carried out by the Atomic Manipulation and Spectroscopy Group in 2023 was centred on two main topics: i) the synthesis of atomically precise graphene-based 2D nanostructures, the characterization of their chemical and physical properties, and exploring their potential application in different type of devices; ii) the engineering of the electronic properties of 2D quantum materials with tunable superlattices.

As an ongoing study of the on-surface synthesis of graphene nanostructures, we focused our efforts on exploring the flexibility of our method to produce atomically precise nanoporous graphene

(NPG) for varying pore geometry and shape, as well as chemical composition. We have demonstrated the integration of flexible phenylene bridges for tuning the quantum electronic coupling and anisotropy of NPG, with prospects on similar tunability of their nanosieving and thermoelectric properties. This research has been carried out within the **PORMOLSYS** project, funded by the State Research Agency. In parallel we are exploring different types of application of these graphene nanoarchitectures, such as the capability of imprinting superlattice potentials to trap excitons in 2D materials –in collaboration with ICFO partners within a BIST-IGNITE grant project– and their

3 ARTICLES

10.4 MEAN IMPACT FACTOR

8 FUNDED PROJECTS

14 CONTRIBUTIONS

1 CONGRESS ORGANISATION

3 COURSES

application as chemical sensors, which is done within **PORESENSE** and **SENSATION**, both funded by the State Research Agency. The former is devoted to the development of a proof-of-concept field-effect transistor chemical sensor based on nanoporous graphene, whereas the latter is more focused on developing the next generation of NPG materials with improved functional properties for sensing. In this context, and inspired by our recent achievement where the interdigitation of two type of graphene nanoribbons led to lateral heterostructure superlattices, we have explored the synthesis of hybrid heterostructures by including non-graphenoid components. We have also been carrying out an atomistic study of the interaction of NPG and derivatives with gaseous analytes by combining scanning probe microscopy with synchrotron-based spectroscopies.

As a parallel activity, we have continued previously established collaborations in the search for stabilizing and controlling magnetism in single molecular and atomic units. In particular, we have demonstrated that single rare earth atoms deposited on the surface of a topological insulator can induce a gap at the topological surface bands, a crucial prerequisite for the realization of the Quantum Anomalous hall Effect and other topological phenomena.

Finally, Prof. Aitor Mugarza is coordinating the development of a scanning probe microscopy (SPM) platform at ALBA synchrotron. The SPM platform, to be opened to users by the end of 2025, will consist of four different instruments that, together with several synchrotron beamlines, will be capable of carrying out correlative in-situ characterization of advanced materials.

This initiative is part of **InCAEM**, the Catalan project within the “Advanced Materials” programme of the Spanish Recovery, Transformation and Resilience Plan.

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INORGANIC NANOPARTICLES GROUP

VÍCTOR F. PUNTES

ICREA Research Professor and Group Leader



MAIN RESEARCH LINES

- Designing and development of synthetic strategies for the production of complex nanoparticles.
- Functionalizing nanoparticle surfaces with specific and relevant biomolecules.
- Studying of their physicochemical and fundamental properties and reactivity.
- Exploring the diverse applications of inorganic nanoparticles in biomedicine, spanning nanooncology, immunology, and antimicrobial fields, as well as their potential uses in energy harvesting and catalysis.
- Ensuring nanosafety through the development of toxicity and ecotoxicity testing models for nanoparticles, aimed at minimizing associated risks while maintaining desired properties.

NEW PROJECTS & MILESTONES

In 2022, the Inorganic Nanoparticles Group continued working on several ongoing projects devoted to designing and synthesising inorganic nanoparticles for interaction with biological systems and energy harvesting.

The **CONCORD** project, funded by the European Commission through the EuroNanoMed programme, aims to develop a new type of transfection nanovectors to improve current CAR-T cell therapy technology by using gold nanoparticles.

13 ARTICLES

7.831 MEAN IMPACT FACTOR

4 FUNDED PROJECTS

9 CONTRIBUTIONS

1 AWARD

1 THESIS

1 BOOK

2 OUTREACH IMPACT

1 BOOK CHAPTER

The project is coordinated by our team and can count on the expertise of the *Hospital Clínic de Barcelona*, the *Istituto di Ricerche Farmacologiche "Mario Negri"* in Milan (Italy) and the Tel Aviv University in Tel Aviv (Israel).

The project "*Nuevos sistemas de inmunoanálisis automatizados para la detección de alérgenos en alimentos*", supported by the *Consejo de Administración del Centro para el Desarrollo Tecnológico y la Innovación* (CDTI), is dedicated to the development and optimization of automated immunoanalysis systems. Specifically, it focuses on the preparation and functionalization of amorphous silica for subsequent utilization in turbidimetric detection, offering a competitive alternative to the current technology reliant on polystyrene nanoparticles.

The **SAPHNa** project is an innovative project supported by the Women Talent Postdoc Grant. Within this framework, the project is dedicated to pioneering the design and fabrication of a new breed of Pt-based hollow nanocrystals engineered to exhibit unparalleled catalytic efficacy.

Finally, the **ENDONANO** project, a Marie Skłodowska-Curie Initial Training Network (ITN) project funded by the European Commission, is devoted to quantitatively detecting bacterial endotoxins using novel nanotechnological approaches.

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MAGNETIC NANOSTRUCTURES GROUP

JOSEP NOGUÉS

ICREA Research Professor and Group Leader



MAIN RESEARCH LINES

- Exchange coupling in bi-magnetic core/shell nanoparticles and nanostructures.
- Magneto-optic nanostructures for biomedical applications.
- Nano/micro-structures for environmental remediation.
- (Photo)electrochemical nanostructures with self-motility and magnetic coupling.
- Novel magnetic and structural characterisation tools for nanoparticles.
- Innovative fabrication approaches.

NEW PROJECTS & MILESTONES

The group has concluded the work in the **PANTHER** project (led jointly by Prof. Josep Nogués and Dr Borja Sepúlveda) funded by the Spanish Ministry of Science and Innovation. It is devoted to the development of novel nanomaterials and actuation devices to enable highly efficient wireless nanotherapeutic actuation and detection of the actuation strength.

The group is also leading two Spanish Proof of Concept **STERILAIR** and **MAPSCALE** projects (led jointly by Prof. Josep Nogués and Dr Borja Sepúlveda). **STERILAIR** is devoted to the development of an efficient air disinfection system. **MAPSCALE** deals with the upscaling of the fabrication of magneto-plasmonic nanoparticles for bio-medical application.

7 ARTICLES

16.071 MEAN IMPACT FACTOR

6 FUNDED PROJECTS

2 CONTRIBUTIONS

2 THESES

2 CONGRESSES ORGANISATION

1 BOOK

5 OUTREACH IMPACT

6 COURSES

The **MOTYCAT** project (funded by the Ministry of Science and Innovation) has been running under the leadership of Dr Esplandiu. This project aims at the development of multicomponent and anisotropic micro/nanoreactors with motile capabilities for water remediation through photocatalytic degradation of pollutants under visible light or through pollutant capture via ion-exchange. The project also pursues the in-situ and direct synthesis of highly valuable compounds.

In 2023 the group has started to work in the **MOMTHER** project (led jointly by Dr Alejandro Gómez and Prof. Josep Nogués). The project is based on the fabrication of anisotropic magneto-opto-mechanical drug loaded nanocapsules for the wireless actuation and detection of amplified therapies for cancer and neurological diseases.

The group has continued to work in **BeMAGIC**, an EU Marie Curie-Skłodowska ITN project (led jointly by Prof. Josep Nogués and Dr Borja Sepúlveda), which deals with the fabrication and characterization of magneto-electric nanostructures for wireless neural and muscle stimulation.

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NANOBIOELECTRONICS AND BIOSENSORS GROUP

ARBEN MERKOÇI

ICREA Research Professor and Group Leader



MAIN RESEARCH LINES

- Innovative nanocomposites with improved electronic/catalytic properties, spatially-oriented anchoring substrates and highly sensitive electro/colorimetric readouts for sensing applications.
- Paper-based biosensors (e.g. lateral flow) modified with laser patterned rGO to enable electrochemical sensing on paper substrates without altering the paper microfluidic properties, thanks to the stamping method.
- Plug & play printing platforms for the ubiquitous fabrication of low-cost and environmental-friendly nanomaterial biosensors with nanofunctional inks, using commercially available office printers.
- Multilayered graphene and metal nanoparticle sensors printed on flexible polymers for the development of sensitive biosensors with impedimetric readout.

NEW PROJECTS & MILESTONES

In 2023 the group has continued working on the following European projects, in addition to national projects. The first one, **MICROB-PREDICT** (Microbiome-based biomarkers to predict decompensation of liver cirrhosis and treatment response) aims to develop

personalised strategies to prevent and treat decompensated cirrhosis and acute-on-chronic liver failure by investigating the human gut microbiome. The second one, **CORE 3**, is part of the Graphene Flagship project and focuses on the development

7 ARTICLES

9.629 MEAN IMPACT FACTOR

11 FUNDED PROJECTS

37 CONTRIBUTIONS

2 THESES

3 CONGRESSES ORGANISATION

3 AWARDS

7 OUTREACH IMPACTS

4 COURSES

of graphene-based sensors. This project finished on September 2023. The third EU project is **EMERGE** (Emerging Printed Electronics Research Infrastructure). And finally, **SUSNANO** project, a Horizon Europe Twinning project together with UP /CATRIN (Czech Republic) as high-quality Twinning partner. The idea of this project is to boost the scientific excellence and innovation capacity in sustainable nanosensors for water pollution detection of Universiteti i Tiranës (UT). This is an important project which will contribute to strengthen the new NANOALB center in Albania.

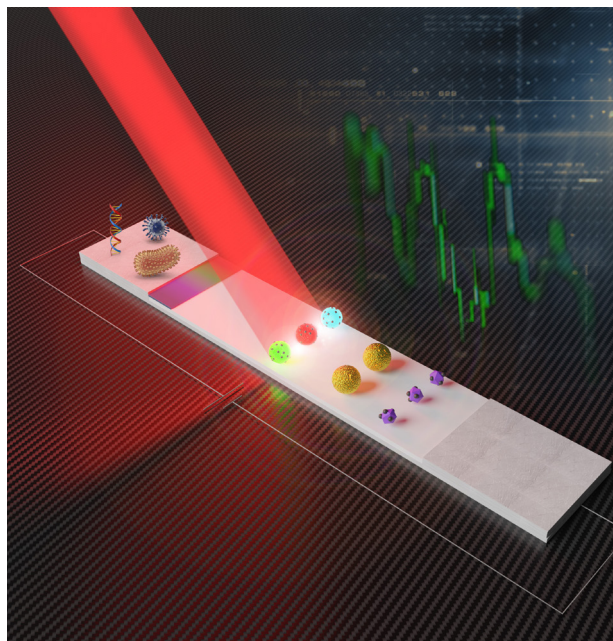
Another international project is **GLEBIOASSAY** in collaboration with the *Hospital Sant Joan de Déu* (Spain) and Palacký University Olomouc (UP) /CATRIN (Czech Republic). This project, funded through the EuroNanoMed-III call, aims to develop a multiplexed point-of-care nanobiosensing platform to monitor the efficacy of the naxitamab-based immunotherapy in neuroblastoma.

We also continued working on our three national projects: **NANOANAEMIA** (Multiplexed nanobiosensor for the instantaneous diagnosis and classification of anaemia at the point of care), **PAPYRUS** (Polymerase Amplification combined into a Paper-based electrochemical lateral flow array for antimicrobial Resistance quantification) and **FULLPOC** (Fully Integrated nanomaterial-based point-of-care devices for health-care applications).

Two new granted projects on which our group is involved started in 2023: A national project **ScreenEC** (Development of a non-invasive IVD for endometrial cancer screening on high-risk populations), and a Horizon Europe project **2D-BioPAD** (Supple Graphene Bio-Platform for point-of-care early detection and monitoring of Alzheimer's Disease).

During 2023 our group was the main contributor in the organisation of nano-Balkan International Conference (NB2023) with interest also for the NANOALB research center.

During 2023 two PhD students of the group defended their PhD thesis: Ana Rubio Monterde and Lei Zhao.



NANOBIOSENSORS AND BIOANALYTICAL APPLICATIONS GROUP

LAURA M. LECHUGA

CSIC Research Professor and Group Leader



MAIN RESEARCH LINES

- Plasmonics (SPR) and nanoplasmonics (LSPR) biosensors.
- Nanophotonic biosensors based on Silicon Photonics technology.
- Customised polymer microfluidic devices and flow delivery systems.
- Full integration in point-of-care biosensor analytical platforms.
- Universal biofunctionalisation techniques and biochip packaging.
- Bioanalytical applications in clinical, environmental and molecular biology, providing application-specific functionalities.

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NEW PROJECTS & MILESTONES

In 2023 the group has made significant progress in the development of integrated and multiplexed devices with interferometric nanophotonic and (nano) plasmonic biosensors, with the end goal of achieving sensitive, affordable, handheld and portable point-of-care devices. New multiplexed nanoplasmonic sensor devices have been implemented based on flexible substrates

for further integration in portable platforms. Novel designs of the multiplexed version of the nanointerferometric sensors together with multiplexed microfluidics have further expanded the capabilities of this ultrasensitive technology.

6 ARTICLES

10.017 MEAN IMPACT FACTOR

12 FUNDED PROJECTS

27 CONTRIBUTIONS

6 AWARDS

16 OUTREACH IMPACTS

1 BOOK

In parallel to the technological developments, we have demonstrated the feasibility of nanophotonic biosensor technology in several fields of application. We have maintained our focus on applications of clinical interest, including the detection of infectious diseases via a direct biosensor test in plasma. In our research line about dysregulation of cellular pathways evaluation, we have used our nanobiosensor technologies as alternative analytical techniques for the evaluation of different gene regulating pathways, with the aim of obtaining more informative and accurate cancer diagnoses and follow-up therapies.

These technologies also allow for a fast, direct and highly sensitive analysis of such regulating routes without the need for labelling or amplification. We have demonstrated a new and unique methodology for the direct detection of epigenetic marks (as methylation) in double strands of DNA and applied it to lung and ovarian cancer, two types of cancer which are difficult to detect in the early stages.

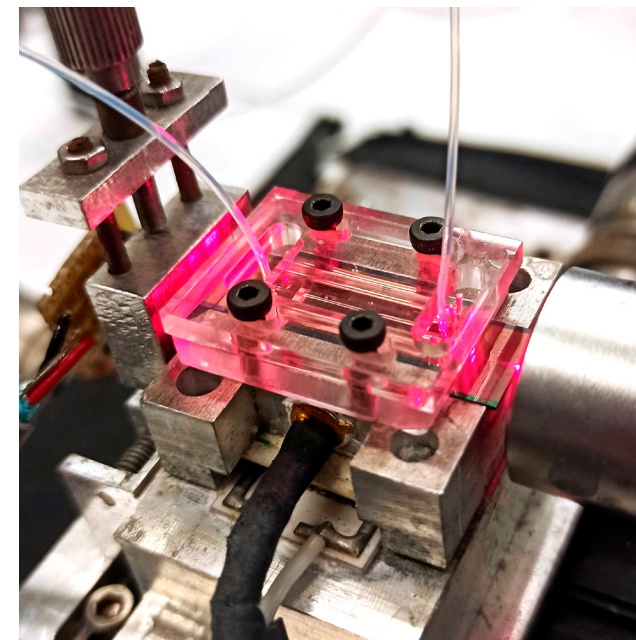
Within Next Generation funds project (**POINTED**), coordinated by the Group, we are developing a POC device intended to achieve a fully operative stand-alone Point-of-Care plasmonic biosensor with multiplexed capabilities for the simultaneous analysis of inflammatory biomarkers in complex human fluids (serum and plasma). The device is expected to provide label-free, highly sensitive detection of a panel of inflammatory biomarkers with relevance in acute inflammation processes diagnosis and prognosis derived from microbial infections.

During 2023 we have successfully finalised the project for an integrated and fully operational biosensor for Point-Of-Care (POC) diagnostics (**LEGOCHIP**). This was achieved by developing and applying pioneering multifunctional nanoporous graphene in nanophotonic BiMW biosensor devices, aimed at creating a universal and atomically precise functionalization interface. Additionally, we integrated highly specific sample filtration membranes for the direct analysis of clinical samples.

These new point-of-care biosensors are now be employed for a better surveillance and early warning to prevent and control future epidemics in the ICRA-EU granted project (**MUSECOV**), focused in providing a better understanding of the global circulation of animal coronavirus and their genetic evolution under different constraints and situations.

Within a granted Next Generation funds project (**PHITBAC**), coordinated by the Group, we are collaborating with academic institutes, hospitals and companies to provide a new, disruptive, and versatile point-of-care nanobiosensor technology for the diagnosis and clinical management of bacterial infectious diseases. The groundbreaking diagnostic device will provide rapid detection of most relevant pathogenic bacteria, including an on-site identification of antibiotic resistance, and a personalised monitoring of antimicrobial therapy effectivity.

Finally, in 2023, a new project funded by the European Union's Horizon Europe research and innovation programme (**NIAGARA**) was initiated. In this project, we are collaborating on the development, integration, and laboratory-scale validation of a multi-analyte biosensor based on nanophotonic interferometric chips. This biosensor is designed for the quantification of industrial, pharmaceutical, and microbiological residues in drinking water from drinking water treatment plants (DWTP).



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NANOELECTROCATALYSIS AND SUSTAINABLE CHEMISTRY GROUP

MARÍA ESCUDERO ESCRIBANO

ICREA Research Professor and Group Leader



4 ARTICLES

8.325 MEAN IMPACT FACTOR

2 FUNDED PROJECTS

8 CONTRIBUTIONS

2 AWARDS

2 CONGRESSES ORGANISATION

2 OUTREACH IMPACTS

MAIN RESEARCH LINES

- Electrocatalysis for renewable energy conversion (e.g. green hydrogen production and fuel cells).
- Electrochemical reduction of carbon dioxide into renewable fuels and chemicals.
- Electrochemical activation and partial oxidation of methane.
- Sustainable electrosynthesis of value-added chemicals.
- Surface nanostructuring and atomic ensemble control.
- Multimetallic and multifunctional nanomaterials.
- Mechanistic investigations of electrocatalytic reactions with spectroelectrochemistry.
- Electrochemical scanning probe microscopy for electrocatalysis.

NEW PROJECTS & MILESTONES

Our group combines electrochemistry, materials engineering and in-situ spectroscopic and microscopic characterisation to elucidate design principles for the discovery and development of novel electrocatalysts for renewable energy conversion, as well as the production of sustainable fuels and chemicals.

Electrocatalysis plays a key role in renewable energy conversion and storage technologies. Discovering and developing new materials that are active, stable, and selective catalysts remains a grand challenge for many important electrocatalytic reactions. Our research aims to address this challenge by investigating the structure of the catalytically active sites at the atomic level, developing advanced electrocatalyst nanomaterials, and gaining mechanistic understanding of relevant energy conversion reactions.

Some of our main research lines are focused on:

Electrocatalysis for renewable hydrogen production and fuel cell applications

Water electrolysis coupled with renewable energy sources allows direct conversion of clean electricity into chemical energy in the form of hydrogen molecules. Our group investigates novel electrocatalysts for the oxygen evolution reaction, a key reaction that determines the energy efficiency of water electrolyzers.

Fuel cells convert the chemical energy from hydrogen or liquid fuels directly into electricity. Our research in oxygen reduction has led to significant breakthroughs such as the discovery of novel electrocatalysts. We also investigate new catalyst materials for the oxidation of liquid fuels such as formic acid.

Electrochemical reduction of carbon dioxide into renewable fuels and chemicals

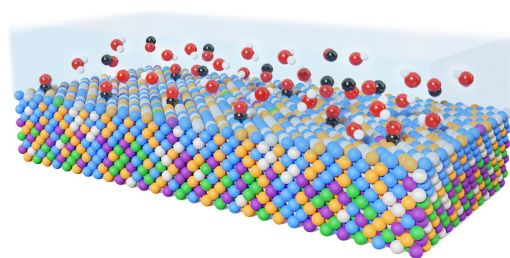
The use of renewable electricity to convert greenhouse gasses such as CO₂ into clean fuels and chemicals is very appealing. We are interested in engineering the structure of the electrode material at the atomic level as well as the electrolyte composition to understand and tune the structure-activity-selectivity relations for CO₂ electrocatalysis. Our goal is to rationally design highly efficient electrocatalysts for CO₂ reduction into renewable fuels and chemicals.

Electrochemical activation and partial oxidation of methane

Electrochemical methane activation and direct conversion to methanol is highly attractive – a dream reaction that would convert a greenhouse gas into a valuable liquid fuel in a dream device, on-site, and powered by renewable electricity. However, sustainable C-H activation and direct methane to methanol conversion at ambient conditions remain as great fundamental challenges. Within the ERC Consolidator Grant ATOMISTIC, we aim to elucidate the design principles and unveil the structure-reactivity-selectivity relations and the reaction mechanisms as well as the atomic-scale structure of the catalyst materials.

In situ and operando spectroscopic and microscopic characterisation of nanomaterials

Understanding, visualising, and engineering the active sites under reaction conditions is essential to design active, stable, and selective catalysts. We combine electrochemical methods with in-situ vibrational spectroscopy such as Raman and infrared spectroscopy, online mass spectrometry, gas chromatography, in situ scanning probe microscopy and in situ/operando synchrotron-based X-ray studies. In situ investigations are key to elucidate the design principles and unveil the structure-property relations and reaction mechanisms as well as the atomic-scale structure of the electrocatalyst materials.



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NANOMEDICINE LAB

KOSTAS KOSTARELOS

ICREA Research Professor, Severo Ochoa Distinguished Professor and Group Leader



MAIN RESEARCH LINES

- **Nanomaterials as vector systems for therapeutic and diagnostic applications.**
- **Development of graphene and 2D materials in medicine.**
- **Clinical translation of nanotechnology-based neurotechnology, bioelectronics and electroceutical devices.**
- **Discovery of novel biomarkers and therapeutic targets in oncology.**

The Nanomedicine Lab@ICN2, established at the end of 2019, is dedicated to the development of nanomaterials and devices for therapeutic and diagnostics applications. It has strong links with the *Nanomedicine Lab* at the **Faculty of Biology, Medicine and Health at the University of Manchester**, with Prof. Kostas Kostarelos leading both teams. Graphene and 2D materials have a central role in a number of research lines carried out by the group in the context of the Graphene Flagship and beyond, particularly in terms of the clinical translation of these advanced nanomaterials.

The group also develops liposomes and other nanoparticle systems for various biomedical applications, ranging from tools for biomarker discovery to cancer therapeutics and neurodegenerative disease interventions.

9 ARTICLES

13.356 MEAN IMPACT FACTOR

2 FUNDED PROJECTS

27 CONTRIBUTIONS

2 OUTREACH IMPACTS

3 CONGRESSES ORGANISATION

NANOSTRUCTURED FUNCTIONAL MATERIALS GROUP

DANIEL RUIZ-MOLINA

CSIC Professor and Group Leader



MAIN RESEARCH LINES

- Nanoscale functional polymers for brain diseases & regenerative medicine
 - Healthy aging
 - Inflammatory and infectious diseases
 - Regenerative medicine
- Chromogenic & emissive nanomaterials for energy efficient devices
 - Smart windows
 - Devices and security

NEW PROJECTS & MILESTONES

Molecular materials are uniquely placed to spur a revolution in the next decades, thanks to their ability to accommodate a wide span of functionalities, and the possibility to fine-tune them to suit a variety of technological purposes. However, while these materials already show optimal behaviour either in solution, as single crystals or as microcrystalline powders, their integration into functional devices still poses a scientific challenge, since, once incorporated into solid

matrices or hybrid devices, they often lose (at least partially) their inherent properties and/or their response efficiency.

The objective of the Nanostructured Functional Materials research group (NANOSFUN - nanosfun.com) is to develop **new strategies to obtain molecular (bio) nanostructures**, with adapted properties and smart responses to external stimuli, which can be incorporated into solid

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10 ARTICLES

9.29 MEAN IMPACT FACTOR

8 FUNDED PROJECTS

15 CONTRIBUTIONS

2 THESIS

1 COURSE

matrices, surfaces or as stable colloidal suspensions, while retaining their initial features and performance. For this, a wide range of molecular and biological building blocks are employed, using Nature as a strong source of inspiration. We work with the idea that ultimate control on every length scale and material interfaces is required to reach the intrinsic limits and functions of these (supra)molecular materials, and with the aim of finding applications for them oriented at improving our everyday life.

The group is upfront in terms of publications, research facilities and collaborations with other top score national and international research institutes and universities. Moreover, we push the research beyond the academic stage and always aiming to reach real applications. For this reason, NANOSFUN has various patents and has established long-term collaborations with small-medium-enterprises and multinational companies. More recently, researchers of the group also established two spin-off companies to speed-up the commercialization of two patented technologies. In addition to the laboratories dedicated to fundamental research, the group has a laboratory of more than 50 square meters exclusively devoted to works

and projects carried out in collaboration with companies, fully equipped and capable of scaled reactions up to volumes of 10 L.

Our main lines of research are the following:

Nanoscale functional polymers for Medicine

The NANOSFUN group will be deeply involved in the **development of polymeric nanoparticles and coatings for health and social welfare**. This embraces mostly, though not exclusively: I) Nanoparticles for diagnosis and therapy, II) Fine-tuning of the hydrophobic/hydrophilic balance, biocompatibility or other additional properties via surface (bio)functionalization and III) Thin films for the regeneration of human cells/tissues allowing for the proper functioning of organs or surgical adhesives and appliance bonding. We work both with commercial FDA-approved polymers, as well as with novel biopolymers, specifically designed for improved performance. A large part of our activities is devoted to the development of novel families of polymers based on coordination chemistry and catechol.

Chromogenic and emissive nanomaterials for energy efficient devices

We aim to develop advanced and smart nanostructured molecular materials that modify their optical properties (i.e. absorption and emission) in response to external stimuli, such as pH, temperature and light. These materials are key to the engineering of near-future commercial products that tackle social and environmental needs, such as sustainability, comfort and security. The main materials to be developed are: I) UV/vis/NIR-light induced color-changing films and coatings for rewritable devices, anticounterfeiting technologies and dynamic photoprotective coatings, II) Temperature-responsive fluorochromogenic micro / nanocomposites for thermal optical sensing and temperature-dependent optical filters, and III) Vis/NIR activated up-converting fluorescent materials for energy conversion, anticounterfeiting technologies and (bio)imaging.

For this, we follow novel and emerging concepts, principally based on the micro/nanoencapsulation of oil or phase-change materials mixtures of molecular dyes (such as spirooxazines, spiropyran, porphyrins and polycyclic aromatic hydrocarbons), which allow advanced, tuneable and customizable optical change effects of different degrees of sophistication: from highly fast to irreversible responses, multi-responsiveness, multiple outputs (colour, fluorescence), threshold-based changes, invisible (to the human eye) optical variations.

Collaborations with industry and technology transfer

We will continue our activity as a reference group in joint projects with the private sector, both with direct contracts and competitive grants, across three fundamental areas:

- » Micro/Nanoencapsulation of active ingredients
- » Photo/Thermochromism.
- » Smart and functional coatings

As seen before, NANOSFUN has strong activity in the validation of our technologies through collaborations with both companies and hospitals. An indicator of this strong tech transfer activity NANOSFUN has ongoing Spin-Off projects: *Futurechromes S.L.* and *DistInkt S.L.*

Additionally, another patented technology is being explored for its potential licensing to a new biotech-based Spin-Off devoted to the development of bioinspired membranes for tissue regeneration, which belongs to the European Patent "*Catecholamine-based membrane, process for its preparation and uses thereof*" (WO2022258780 A1).

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NANOSTRUCTURED MATERIALS FOR PHOTOVOLTAIC ENERGY GROUP

MÓNICA LIRA-CANTÚ

CSIC Research Professor and Group Leader



MAIN RESEARCH LINES

- Novel sustainable and green materials for Photovoltaics (Next-generation thin film, organic, hybrid, dye-sensitised, halide perovskite and all-oxide solar cells) and Photo(electro)catalysis.
- Green synthesis of nanomaterials by low-cost, low temperature and green solution processing methods.
- Solution processing methods for the fabrication of solar cells and printed electronics.
- Degradation studies of the stability of solar cells following ISOS protocols.
- Semiconductor oxides for energy, ICT applications, printed electronics.
- Self-powered, transparent, flexible electronic and optoelectronic devices.

NEW PROJECTS & MILESTONES

The NMPE group research objectives are focused on the **synthesis of novel nanomaterials and the control of their optoelectronic properties** through their manipulation at molecular level, with the aim of developing very stable and highly efficient perovskite solar cells. We search for novel Pb-free halide perovskites (both hybrid and inorganic).

Specifically, our contribution is in the area of solution processable metal oxides (classical and complex), halide perovskites (Pb-free, 2D and 3D) and, more recently, 2D materials and MXenes. We aim at the development of highly stable solar cells for industrial applications (e.g. building integration PV) and novel self-powered photovoltaic-based devices for Internet of things (IoT) applications (e.g. sensors, wearables, prin-

9 ARTICLES

15.338 MEAN IMPACT FACTOR

6 FUNDED PROJECTS

25 CONTRIBUTIONS

5 AWARDS

2 CONGRESSES ORGANISATION

1 COURSE

ted electronics). The group, with more than 15 years of experience in the field, is internationally recognised for its involvement in the enhancement of the operational stability of emerging photovoltaics and the development of ISOS protocols.

Fundamental Research Lines

Various of our lines of study are related to highly innovative and fundamental research within technology readiness levels (TRLs) below 3. We aim at the synthesis of materials as absorbers, transport layers and interfaces in solar cells. This line includes the synthesis of novel materials such as Pb-free halide perovskites, 2D materials and halide perovskites, novel anti-perovskites.

More recently, we have initiated the development of novel heterojunctions of MXenes (and 2D materials) with perovskites for their application in photovoltaics and photo(electro)catalysts. One of the objectives of this research is the manipulation of materials properties to enhance solar cells stability and the understanding of the mechanisms that permit their stability. We focus on the study and passivation of point defects of materials and interfaces.

We have also developed our own in-situ characterization methodology to study the materials and solar cell degradation under operando conditions. For this, we employ in-situ X-Ray diffraction analysis, Raman spectroscopy, Photoluminescence and Impedance Spectroscopy, among others. We employ indoor and outdoor stability procedures following ISOS protocols.

Another major goal of the group is the synthesis of nanostructured materials, especially those involving transition metal oxides (TMOs), via the application of low-cost and solution processing methods.

They have many possible applications as main active materials or barrier layers, but also as materials for external light management. The use of low-temperature synthesis methods (sol gel, hydrothermal, SILAR, among many others) permits tuning and controlling the properties of the final device. These oxides are being applied in our group as nanostructured

materials (nanorods, nanowires, nanotrees, core-shell, etc.) and dense thin films in the various next-generation solar cells, offering excellent performance in term of efficiency

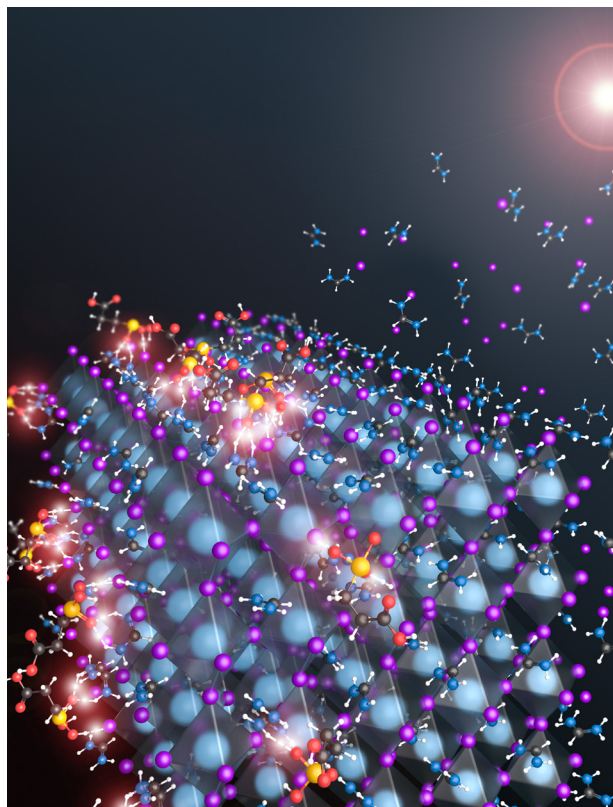
and lifetime. We are now functionalising these oxide surfaces by anchoring self-assembled monolayers with selected anchoring groups to interact simultaneously with the oxide and the active light harvesting material.

Applied Research Lines

Our applied research lines are dedicated to the development of novel and innovative devices whose technology readiness levels (TRLs) can be up to 7. We are working on **high-efficiency perovskite solar cells and novel printed electronic devices**, which can allow the group to collaborate with industry and to obtain intellectual property rights. We are also collaborating with top laboratories for the development of protocols and standards, with the aim to make the perovskite solar cell technology reach the market.

The group also works on the development of self-powered electronic and optoelectronic devices, as well as flexible and transparent devices for ICT and electronic applications.

We are employing machine learning for the elucidation of degradation mechanisms in Perovskite solar cells and the finding of a correlation between indoor and outdoor stability and accelerator factors for device degradation. Our aim is to employ machine learning also for the study of novel nanomaterials and data treatment.



NOVEL ENERGY-ORIENTED MATERIALS GROUP

PEDRO GÓMEZ-ROMERO

CSIC Research Professor and Group Leader



MAIN RESEARCH LINES

- Hybrid electrode materials for supercapacitors and hybrid energy storage devices.
- Nanocarbons (graphenes, nanotubes, porous nanocarbons) for batteries and supercapacitors.
- Nanomaterials for Zn-ion and Zn-Air batteries. Polyoxometalates.
- Nanopastes / Nanogels for energy applications.
- Harvestorage (triboelectric/supercapacitors) materials and devices.

NEW PROJECTS & MILESTONES

2023 has been a year of growth for the group. We have continued our work on materials and devices for ground-breaking energy storage. Dr. Rosa M. González Gil as a post-doc and project manager has consolidated as a structural part of the group.

The supply crisis got entangled with the inflation crisis. This, together with the growing climate emergency, adds urgency to reaching our goals. Our emphasis should change from the writing of highly-cited articles to the production of materials and energy storage technologies with direct impact on our society. In this respect, I totally despise and disregard the figures of "Mean Impact Factor" of the Journals in

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6 ARTICLES

7.65 MEAN IMPACT FACTOR

4 FUNDED PROJECTS

10 CONTRIBUTIONS

2 BOOKS

5 OUTREACH IMPACT

3 COURSES

2 TECHNOLOGY TRANSFER

which our publications appear, because they say nothing about the real impact of our work and go against the DORA declaration both ICN2 and CSIC have signed.

We don't forget about the fundamentals and the broad view of our field. In this respect, I have had the privilege to coordinate a multi-author contribution on the recent development in Energy applications as part of "*Libro Blanco de las Nanotecnologías II*" Cap. 6 (Editado por J. Diaz Marcos et al.) Aranzadi, 2023. ISBN: 978-84-1125-729-9

But in our group the fundamentals are put to work to contribute to solve grand challenges in the world of applications and in particular energy storage.

These applied targets have been fostered by the development of our projects, all focused on energy storage and at the same time quite complementary in their specific objectives:

Thus, **NANOPEISTORAGE** is a "*Proyecto de Generación de Conocimiento (Investigación Orientada)*" addressing fundamental aspects of the electrode- electrolyte interface

in energy storage devices based on nanopastes. The project **REVOLT**, on the other hand, deals with nanopastes as well but it is decidedly focused on the design of devices and their final application. REVOLT is funded within the programme of "Lineas Estratégicas" and is developed between ICN2 and the startup company "Napptilus Battery Labs" (NBL), originated as a spinoff rooted in the materials and technologies developed by our group. Our collaboration with NBL includes publicly funded projects like REVOLT but also privately funded contracts to optimize, advance the TRL and scale-up our technology. NBL results are very positive. The great dedication of Dr. Daniel Rueda and Veronica Fabian have a lot to do with this success. I strongly believe that the public-private collaboration of our group and center with Napptilus Battery Labs is exemplary.

Concerning other projects, we should highlight the very good results of our TED project to develop a new type of Zn-Air battery, based on polyoxometalates (POMs) as bifunctional electro-catalysts under near-neutral pH conditions. This is a project developed in collaboration with the group

of prof. Nieves Casañ-Pastor at ICMAB. In this topic of Zn-Air batteries, the work in the group of Dr Leandro N. Bengoa supported with a Marie S. Curie Fellowship has been crucial to success. This line has also been reinforced with the contract of Dr. Riccardo Argurio and with the incorporation of Andrea Inclán as a new PhD student.

In our group, presential congresses were reduced to a minimum, with online participation gaining weight during this 2023 year. Maybe we should keep using these more sustainable alternatives in the future. Shouldn't we?

Besides our enhanced technology transfer efforts, our group has continued working on the fundamentals of our NEO-Energy brand research, namely, hybrid electrode materials for hybrid energy storage. We focused not only on materials, but also on energy storage devices, which we strived to further develop, with emphasis on supercapacitors, batteries, and their hybrids.

We give more details about each research line in the following paragraphs.

From hybrid materials to hybrid devices for improved energy storage

The boundaries between batteries and capacitors are quickly blurring. Control over nanostructures is of great importance in the design of high-performance energy storage devices. We are developing materials with high specific surfaces, as well as ultra-dispersed molecular materials like polyoxometalates (POMs) for application

in electrochemical energy storage devices featuring the best properties of batteries (high energy density) and supercapacitors (high specific power, fast charging, long

cyclability). Two PhD thesis works are presently tackling this topic (Anukriti Pokhriyal and Lipeng Wang) from different points of view. We have recently published a review article on the employment of polyoxometalates in energy applications, a topic in which our group was a pioneer.

To flow or not to flow? Meet Nanopastes

We have worked on conventional batteries like LIBs but also on Flow Batteries. The knowledge of these two different technologies makes us converge in a middle point in the form of batteries formed by pastes, more specifically, nanopastes, in which solid electrode materials (preferably hybrid) are nanodispersed in liquid electrolytes (which could also be "hybrid". This leads to a complex but fascinating materials landscape from which final improved performance in energy storage could result.

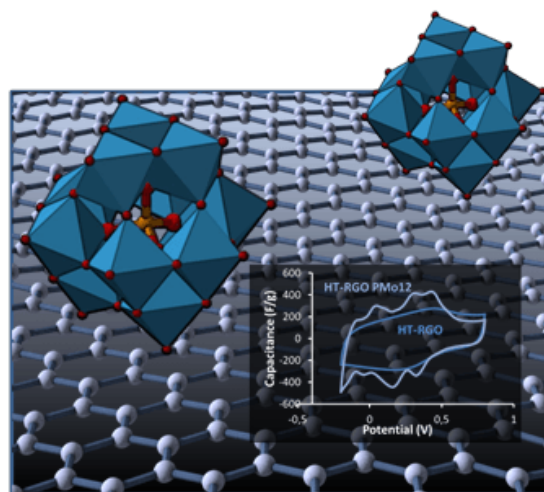
From Zn-Ion Capacitors to Zn-Ion batteries

Zinc is one of the most promising post-lithium technologies. We are presently working on an integrated scaled approach to advance in this technology: integrated because we pursue the simultaneous development of compatible and integrated components (anode, electrolyte cathode); scaled because we work stepwise on devices of increasing complexity, from Zn-Ion capacitors to Zn-Ion batteries to Zn-Air batteries. The ultimate goal is to develop Zn-Air batteries working at near neutral pH thanks to the bifunctional activity of Polyoxometalates.

Harvestorage materials

The coupling of our energy storage devices with harvesting devices was proposed in our strategic plan (as well as in the Severo Ochoa Programme 2018-2022). In 2022 Ms. Sharin M. Thomas keeps working on her PhD thesis on this topic.

Collaboration with a Portuguese group working on triboelectric nanogenerators is being initiated.



OXIDE NANOPHYSICS GROUP

GUSTAU CATALÁN

ICREA Research Professor and Group Leader



MAIN RESEARCH LINES

- Flexoelectricity and piezoelectricity: fundamentals and devices
- Ferroelectrics, antiferroelectrics, multiferroics, metal-insulator transitions
- Electronic and electromechanical properties of oxide thin films
- Domain wall nanoelectronics

NEW PROJECTS & MILESTONES

This year was an interesting one, with the official “group leader” away on sabbatical at NTNU in Norway. In his place, some management duties were taken up by Dr David Pesquera and Dr Kumara Cordero, who kept the boat afloat and managed to advance with their research too. In addition, David and Kumara co-wrote and got granted their own Plan Nacional project, **EPIQO**, to look for emergent phases in thin films of quantum (Mott) materials.

In terms of research outputs, we posted several manuscripts in arXiv, and these are now becoming fully-fledged peer-reviewed

publications in 2024. Two important papers that did get published in 2023 reflect two of our main research lines at the moment: antiferroelectricity and ferroelectric interfaces.

On antiferroelectricity, we reported the discovery that translational boundaries (aka antiphase boundaries) in antiferroelectric PbZrO_3 form ferrielectric (polar) domains. These ferrielectric domains are topologically protected by the incommensurability between their unit cell size (3 perovskite pseudocubes) and that of the antiferroelectric matrix

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3 ARTICLES

6.167 MEAN IMPACT FACTOR

9 FUNDED PROJECTS

9 CONTRIBUTIONS

3 AWARDS

(4 perovskite pseudocubes). This finding is our gateway into ferroelectricity, a property that can be used simultaneously for energy storage and memory storage. The work was first-authored by Dr Ying Liu, a Pro-BIST postdoc shared between the electron microscopy group of Jordi Arbiol and the oxide nanophysics group of Gustau Catalan, both of whom coauthored the work [Y. Liu et al, "Translational Boundaries as Incipient Ferroelectric Domains in Antiferroelectric PbZrO_3 " *Phys. Rev. Lett.* 130, 216801 (2023)].

Meanwhile, back on the more familiar ground of ferroelectrics, we are putting forward the concept of "molecular electrodes", or "chemical electrodes", which use charge transfer along chemically resonant structures (structures that share chemical formula but where a chemical bond can change location) to deliver compensating charge to ferroelectric surfaces. As our former PhD student (now Dr) Irena Spasojevic showed, such molecular electrodes have a much higher screening efficiency than conventional metal electrodes [I. Spasojevic et al., "Tunable Molecular Electrodes for Bistable Polarization Screening" *Small* 19 (30), 2207799 (2023)].

We have a FET-Open Project (**TSAR**, 'Topological Solitons in Antiferroics') to study topological structures in antiferroelectrics, a National Plan project to study functional oxide membranes (FO_xMe), and a "Strategic Project Oriented to the Ecological Transition and Digital Transition" to study pyroelectric and electrocaloric effects in low dimensional ferroelectrics (**PYROMETHER**), in collaboration with the ICN2 group of Thermal Properties of Nanoscale Materials. In addition, as mentioned, Dr Kumara Cordero and Dr David Pesquera have won and are leading a new Plan Nacional project of their own, called **EPIQO** ("Emergent Phases in Quantum Oxides").

Last but not least, we want to highlight the Juan de la Cierva award won by Dr Xin Wen, a postdoc in our group who is working on all things flexoelectric, including flexoelectric water ice. Stay tuned.

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PHONONIC AND PHOTONIC NANOSTRUCTURES GROUP

CLIVIA M. SOTOMAYOR TORRES

ICREA Research Professor and Group Leader



MAIN RESEARCH LINES

- Nanophononics and topological matter
- Nanophotonics
- Nanoscale thermal transport
- 2D materials
- Optomechanics
- Nanofabrication

NEW PROJECTS & MILESTONES

During 2023, the group worked on the following nine projects:

» **LEIT**, Lossless Information for Emerging Information Technologies, GA 101099125, ERC, AdG.

» **NANOPOLY**, Artificial permittivity and permeability engineering for future generation sub wavelength analogue integrated circuits and systems, GA 829061, H2020 FET Open project.

» **NANOSMART**, NANO components for electronic SMART wireless Systems, GA 825430, H2020 ICT project.

12 ARTICLES

7.1 MEAN IMPACT FACTOR

10 FUNDED PROJECTS

12 CONTRIBUTIONS

1 AWARD

4 CONGRESSES ORGANISATION

3 OUTREACH IMPACTS

2 COURSES

- » **MAGNIFIC**, Materials for a next-generation (nano-)opto-electro-mechanical systems, GA 101091968, HORIZON-CL4.
- » **MINERVA**, Making new electronic devices from amorphous materials, Ref. PCI2021- 122092 2A, NextGenerationEU/ PRTR.
- » **MUSICIAN**, Multifunctional silicon integrated NOEMS for broadband access networks, Ref. CI2022-135001-2, Plan Estatal de Investigación Científica y Técnica y de Innovación 2021-2023.
- » **D-SPA**, Diamond-based nanomaterials and nanostructures for advanced electronic and photonic applications, Ref. 734578, H2020-MSCA-RISE-2016
- » **LEONINE**, Monolayer and multilayer MoS₂-based sensors to evaluate noise and humidity levels on the sleep quality of the elderly, Ref. 22S09495-001, Subvencions per a projectes de recerca jove i emergent 2022, Ajuntament de Barcelona

- » **MOCCASIN-2D**, Monitoreo de gases del Cambio Climático con Sensores basados en Materiales 2D, Ref. TED2021-132040B-C22, Proyectos de Transición Ecológica y Transición Digital, AEI

In October 2023, Prof. Clivia Sotomayor Torres moved from her position at ICN2 to assume the role of Director General at the International Iberian Nanotechnology Laboratory (INL) in Braga, Portugal. Accompanying her, several members of her research team also transitioned to INL, while others remained at ICN2, integrating into different research groups.

PHYSICS AND ENGINEERING OF NANODEVICES GROUP

SERGIO VALENZUELA

ICREA Research Professor and Group Leader



MAIN RESEARCH LINES

- Development of novel nanodevice structures and nanofabrication methods to investigate the physical properties of materials at the nanoscale and their technological relevance
- Investigation of topological properties and low energy propagation of information in quantum anomalous edge states
- Spin and thermal transport in two-dimensional systems, including topological insulators, graphene and transition metal dichalcogenides
- Control of the magnetic state of ferromagnetic systems by means of the spin-orbit interaction and, particularly, the spin Hall and spin galvanic effects
- Coupling in hybrid magnon-phonon-photon systems
- Quantum circuitry and quantum transduction

NEW PROJECTS & MILESTONES

In 2023 the Physics and Engineering of Nanodevices Group (PEN) continued its work under the H2020 Graphene Flagship programme to develop spintronic

applications with graphene and related 2D materials. The group has explored the thermal properties of transition metal dichalcogenides and investigated the

2 ARTICLES

12.5 MEAN IMPACT FACTOR

9 FUNDED PROJECTS

15 CONTRIBUTIONS

2 OUTREACH IMPACTS

3 CONGRESSES ORGANISATION

1 COURSE

presence of proximity-induced spin orbit fields and magnetic exchange by means of spin transport methods. It has also continued making progress in exploring the spin properties of materials with large spin-orbit interaction—in particular, topological insulators grown in a dual-chamber molecular beam epitaxial (MBE) system—and has developed multilayer all-2D spin torque devices, demonstrating magnetization switching down to a few monolayers. Related work will continue with the support of a FLAG-ERA JTC 2021 Project: ‘2D MagNETic meMOries: Scalable growth and hYbrid electrical operation’ (**MNEMOSYN**).

Work has also been carried out within the context of the national project “Engineering the Spin and Thermoelectric Properties the Nanostructured Two-Dimensional Materials (**ENGINE2DM**)”, which was followed by **HEDOS**, “Van der Waals Heterostructures for Digital Technologies and Opto-Spintronics”, both supported by the Spanish Ministry of Economy, Industry and Competitiveness (MINECO). **ENGINE2M** was dedicated to the study of the spin Hall effect, of the

charge and spin transport properties of graphene, of the electrical injection and detection of hot carriers, and of the spin-to-charge conversion efficiency in graphene/metal hybrids. The aim of **HEDOS** is to deepen in those physical phenomena and expand the research activity of the group towards optoelectronic and opto-spintronic phenomena in van der Waals heterostructures.

The group coordinates two European projects launched in 2019 (**TOCHA** and **2DSPINMEM**, described below) and participates in the quantum initiative, coordinated by ICFO, to develop quantum transduction approaches. It is also a member of the SpinTronicFactory network, established to coordinate EU spintronics activities, and represents the Bellaterra node of the Spanish Spintronics Network.

The **TOCHA** project (“Dissipationless topological channels for information transfer and quantum metrology”, FET-PROACTIVE), funded under the Horizon 2020 EU Research and Development Programme, has the ambition of harnessing topological concepts for future generation of devices and architectures across which information can flow with low losses. This conceptually simple, yet technologically and fundamentally challenging requirements are crucial for the development of technologies in fields ranging from information processing to quantum communication and metrology. In each of these areas, the dissipation of information is a key hurdle that leads, for example, to unacceptable thermal loads or error rates.

The **2DSPINMEM** project (Functional 2D materials and heterostructures for hybrid spintronic-memristive devices, M-ERA) explores group-IV monochalcogenides (IV-MCs) materials and aims to perform the first ever evaluation of their potential as memristors, as well as to implement graphene-based heterostructures to control graphene spin properties by changing the memristive setting of the chalcogenides.

The group also participates in the EIC-Pathfinder Project “Phase-sensitive Alteration of Light colorAtioN in quadriparTite gaRnet cavity” (**PALANTIRI**), coordinated by Spintec (France), whose purpose is to develop quantum coherent frequency upscaling.

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SUPRAMOLECULAR NANOCHEMISTRY AND MATERIALS GROUP

DANIEL MASPOCH

ICREA Research Professor and Group Leader



MAIN RESEARCH LINES

- Metal-organic frameworks (MOFs), covalent-organic frameworks (COFs) and metal-organic polyhedra (MOPs).
- Functional delivery systems.

NEW PROJECTS & MILESTONES

In 2023, two projects carried out by the group came to an end, specifically: **SAFE-ON**, supported by the European Commission; and **HybMOFs**, supported by the Spanish Ministry of Science and Innovation – AEI under the *Acciones de dinamización “Europa Excelencia”* call.

In the framework of these projects, **SAFE-ON** aims to approach new antimicrobial coatings to the market and **HybMOFs** aims at using DNA nanotechnology and reticular chemistry to design hierarchical, multi-component, porous materials based on DNA-guided assembly of pre-synthesised nanoscale molecular cages.

The group has also continued working on **CLIPPOFF-CHEM**, which is supported by ERC under its Advanced Grant. This project aims to develop a highly innovative top-down synthetic method, based on controlling bond breaking in reticular materials to synthesize new molecules and materials. Also, the group has actively worked on **DISASSEMBLE** and **MOFTONIC**, both funded by the Spanish Ministry of Science and Innovation – AEI. These projects are focused on the full disassembly of reticular materials to obtain clusters and cages and on the self-assembly of colloidal MOF particles. The main objective of the fourth project, called **ReMOVEAs** and supported by the Spanish Ministry of Science and Innovation – AEI as well, is to develop

17 ARTICLES

9 FUNDED PROJECTS

9 AWARDS

1 OUTREACH IMPACT

3 THESES

13.482 MEAN IMPACT FACTOR

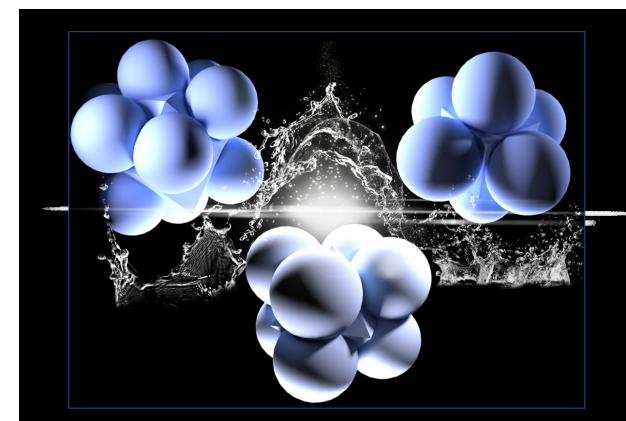
35 CONTRIBUTIONS

2 CONGRESSES ORGANISATION

4 COURSES

new porous composites for the removal of arsenic in water. And finally, the fifth project is **SGR 2021** (AGAUR), supported by the Catalan Government.

On the other hand, during 2023, the group has started two new projects: **CHITINMETICS** and **FUNCYCLING**, both funded by the Spanish Ministry of Science and Innovation – AEI. They are focused on the valorization of chitosan for the production of sustainable plastics for the cosmetics industry, and on the development and application of functional materials in sports clothing for cycling. The group has also continued to collaborate with companies to bring customised micro- and nano-encapsulation technologies to the market, working in parallel with different entities.



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THEORETICAL AND COMPUTATIONAL NANOSCIENCE GROUP

STEPHAN ROCHE

ICREA Research Professor and Group Leader



6 ARTICLES

8.46 MEAN IMPACT FACTOR

12 FUNDED PROJECTS

44 CONTRIBUTIONS

1 AWARD

4 CONGRESSES ORGANISATION

1 COURSE

MAIN RESEARCH LINES

- Theoretical research on quantum transport phenomena in topological quantum matter (topological insulators, Weyl semimetals) in equilibrium and non-equilibrium regimes.
- Spin dynamics and entanglement properties in Dirac matter (graphene, two-dimensional materials) and van der Waals heterostructures, with the search for new paradigm of quantum information manipulation.
- Artificial Intelligence and machine learning techniques to accelerate the building of realistic and adaptive structural and electronic models of highly disordered materials and heterostructures.
- Predictive modelling and multiscale numerical simulation of complex nanomaterials and quantum nanodevices.
- Molecular dynamics, thermal transport properties and thermoelectricity in nanomaterials of interest for microelectronics (amorphous graphene and boron nitride).

NEW PROJECTS & MILESTONES

In 2023 the group published the following relevant works:

Revealing the improved stability of amorphous boron-nitride upon carbon doping

We report on a large improvement of the thermal stability and mechanical properties of amorphous boron-nitride upon carbon doping. By generating versatile force fields using first-principles and machine learning simulations, we investigate the structural properties of amorphous boron-nitride with varying contents of carbon (from a few percent to 40%). We found that for 20% of carbon, the sp^3/sp^2 ratio reaches a maximum with a negligible graphitisation effect, resulting in an improvement of the thermal stability by up to 20% while the bulk Young's modulus increases by about 30%. These results provide a guide to experimentalists and engineers to further tailor the growth conditions of BN-based compounds as non-conductive diffusion barriers and ultralow dielectric coefficient materials for a number of applications including interconnect technology.

Observations of Aharonov-Bohm Conductance Oscillations in CVD-Grown Graphene Rings at 4K

In this work, we present the observations of Aharonov-Bohm (AB) oscillations in chemical vapor deposition (CVD)-grown graphene rings via magnetotransport measurements at 4K under out-of-plane external magnetic fields up to ± 2.1 T. Incorporating a baseline subtraction of the original conductance data allowed us to observe two-terminal conductance oscillations with a spacing of ΔB_{AB} of 3.66 to 32.9 mT from the ring with an inner radius of 200 nm and arm-width of 400 nm, and spacing of ΔB_{AB} from 2.1 mT to 8.2 mT from the ring with an inner radius of 400 nm and an arm-width of 400 nm. The fast-Fourier transform (FFT) data showed AB oscillation periods, with the interval of the h/e fundamental mode given by $30/T$ to $273/T$ for the ring with the inner radius of 200 nm and arm-width of 400 nm, and $122/T$ to $488/T$ for the ring with the inner radius of 400 nm. The broad spreading of FFT peaks is due to the aspect ratio of the

inner radius r_1 and the width w of the ring, $r/w \sim 1$. Systematic numerical simulations were performed to elucidate the relation between the AB oscillation frequency and the geometry of the ring. This work shows AB oscillations in CVD-grown graphene rings at an elevated temperature (4K).

Mechanistic Insights into Electronic Current Flow through Quinone Devices

Molecular switches based on **functionalised graphene nanoribbons (GNRs)** are of great interest in the development of nanoelectronics. In an experiment, it was found that a significant difference in the conductance of an anthraquinone derivative can be achieved by altering the environment's pH value. Building on this, in this work we investigate the underlying mechanism behind this effect and propose a general design principle for a pH based GNR-based switch. The electronic structure of the investigated systems is calculated using density functional theory and the transport properties at the quasi-stationary limit are described using nonequilibrium Green's function and the Landauer formalism. This approach enables the examination of the local and the global transport through the system. The electrons are shown to flow along the edges of the GNRs. The central carbonyl groups allow for tunable transport through control of the oxidation state via the pH environment. Finally, we also test different types of GNRs (zigzag vs. armchair) to determine which platform provides the best transport switchability.

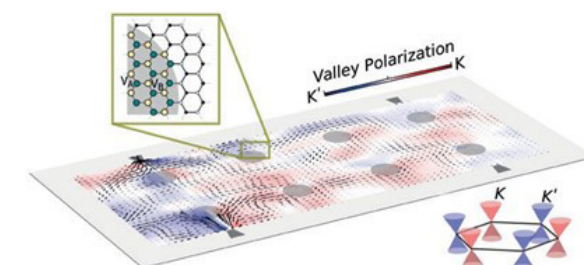
Connecting Higher-Order Topology with the Orbital Hall Effect in Monolayers of Transition Metal Dichalcogenides

Monolayers of **transition metal dichalcogenides (TMDs)** in the 2H structural phase have been recently classified as higher-order topological insulators (HOTIs), protected by C_3 rotation symmetry. In addition, theoretical calculations show an orbital Hall plateau in the insulating gap of TMDs, characterised by an orbital Chern number. We explore the correlation between these two phenomena in TMD monolayers in two structural phases: the noncentrosymmetric 2H and the centrosymmetric 1T. Using density functional theory, we confirm the characteristics of 2H TMDs and reveal that 1T TMDs are identified by a Z_4 topological invariant. As a result, when cut along appropriate directions, they host conducting edge states, which cross their bulk energy-band gaps and can transport orbital angular momentum. Our linear response calculations thus indicate that the HOTI phase is accompanied by an orbital Hall effect. Using general symmetry arguments, we establish a connection between the two phenomena with potential implications for orbitronics and spin orbitronics.

Emergent Spin Frustration in Neutral Mixed-Valence 2D Conjugated Polymers: A Potential Quantum Materials Platform

Two-dimensional conjugated polymers (2DCPs)—organic 2D materials composed of arrays of carbon sp^2 centers connected by π -conjugated linkers—are attracting increasing attention due to their potential applications in device technologies. This interest stems from the ability of 2DCPs to host a range of correlated electronic and magnetic states (e.g., Mott insulators). Substitution of all carbon sp^2 centers in 2DCPs by nitrogen or boron results in diamagnetic insulating states. Partial substitution of C sp^2 centers by B or N atoms has not yet been considered for extended 2DCPs but has been extensively studied in the analogous neutral mixed-valence molecular systems. Here, we employ accurate first-principles calculations to predict the electronic and magnetic properties of a new class of hexagonally connected neutral mixed-valence 2DCPs in which every other C sp^2 nodal center is substituted by either a N or B atom. We show that these neutral mixed-valence 2DCPs significantly energetically favor a state with emergent superexchange-mediated antiferromagnetic (AFM) interactions between C-based spin-1/2 centers on a triangular sublattice.

These AFM interactions are surprisingly strong and comparable to those in the parent compounds of cuprate superconductors. The rigid and covalently linked symmetric triangular AFM lattice in these materials thus provides a highly promising and robust basis for 2D spin frustration. As such, extended mixed-valence 2DCPs are a highly attractive platform for the future bottom-up realization of a new class of all-organic quantum materials, which could host exotic correlated electronic states (e.g., unusual magnetic ordering, quantum spin liquids).



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THEORY AND SIMULATION GROUP

PABLO ORDEJÓN

Distinguished Researcher, Group Leader and Director



MAIN RESEARCH LINES

- Development of theoretical methods, numerical algorithms and simulation tools for atomic-scale simulations towards massive HPC facilities.
- First-principles simulations at the nanoscale.
- Physical properties and chemical processes in materials.

NEW PROJECTS & MILESTONES

In 2023, the Theory and Simulation group (T&S) started new relevant projects for the group:

MaX - Materials design at the eXascale, one of the fifteen European Centres of Excellence in high-performance computing (HPC) Applications supported by The European High-Performance Computing Joint Undertaking (EuroHPC JU) and The Spanish State Research Agency (AEI).

MaX supports developers and end users of advanced applications for materials simulations, design and discovery, and works at the frontiers of current and

future HPC technologies. It brings together leading developers and users of materials applications, together with top experts in HPC. After two periods of three years (2015-2018 and 2018-2021), the grant was renewed for the 2023-2026 term, with an increased budget and the inclusion of new groups and codes to the team.

Work during this year has been centred on adapting **SIESTA** for its execution in GPU-accelerated architectures. These will be the building blocks of the coming European pre-Exascale supercomputers financed by the European High-Performance Computing Joint Undertaking (EuroHPC JU), which are

5 ARTICLES

3.74 MEAN IMPACT FACTOR

9 FUNDED PROJECTS

16 CONTRIBUTIONS

1 THESIS

2 CONGRESSES ORGANISATION

4 OUTREACH IMPACTS

currently being commissioned in three HPC centres (BSC in Spain, CINECA in Italy, CSC in Finland and IZUM in Slovenia).

ALCOAT - Recycled aluminium alloy coatings with chemically tailored electrochemical potential for safe protection of steel structures is a European project funded under the "Research Fund for Coal and Steel" call. Its period is between 2023 and 2027 and a highly industry-oriented project, with the participation of several industries in the steel area, and with target TLRs as high as 5, its goal is to develop new, efficient, sustainable and "green" coatings for the inhibition of the corrosion of steel, based on Aluminium scrap (aluminium from waste and parts rejected or discarded). T&S is focusing on Work Package 4, which is related to advanced material modelling.

SIESTA ecosystem of materials simulation techniques, after two periods SIESTA development projects (2016-2018 and 2019-2022), the grant was renewed for the 2023-2026 (PID2022-139776NB-C62) term funded by The Spanish State Research Agency (AEI). These are the continuation of a series of collaborative, coordinated projects starting

in 1996, by the core group of developers of SIESTA, which provide the main base funding for the development of the code and its associated methodologies.

The project aims to develop an ecosystem of revolutionary methods, algorithms, and computer codes for simulating atomic-level condensed matter systems.

NFFAEurope, a project funded under the H2020-INFRAIA-2018-2020 call "Integrating and opening existing national and regional research infrastructures of European interest". The Nanoscience Foundries and Fine Analysis (NFFA) is a platform for interdisciplinary research at the nanoscale, in which our group participates as an "installation" offering computational support for experimental users' projects. T&S is part of the **Nanoscience Foundries and Fine Analysis Project - Europa|PILOT** (NNFA-NEP), during 2023, the proposal of services "Molecular Modeling of electron transfer reaction in self-assembled monolayers" was accepted. The group will continue providing services to transnational users during the next years.

In addition, in 2013, the T&S achieved to execute the first year of the **MAGNIFIC - Materials for a next-generation (nano-) opto-electro-mechanical systems** project, a Horizon Europe-funded project which will continue until the end of 2026. T&S group is responsible for the theoretical model of the dynamics of nc-Si, as well as ALN and the interface formed by ALN/nc-Si. This year, work was focused on developments on phonon dynamics and interactions in silicon grain boundaries.

Besides, we continue with our work within the project supported by the AEI (PDC2022-133467-I00), entitled **THERMOS - Industry-grade software for the simulation of thermal properties of materials**. A "Proof of Concepts" project, to explore the commercialization of the software developed by the group for the calculation of the thermal properties of materials. Work during this year has been centred on mapping the functionalities and interfaces of the different layers of the workflow structure to the technologies and modes of operation required.

Next year is expected to start with **HANAMI- Hpc AlliaNce for Applications and supercoMputing Innovation: the Europe-Japan collaboration** funded by European High-Performance Computing Joint Undertaking.

Significant results were obtained by T&S group, an example of this was DFT and QM/MM simulations of electrified interfaces using Non-Equilibrium Green's Functions, which offers a viable solution to the computational challenges of investigating the dynamics of liquid water interacting with electrified surfaces, providing a good balance between accuracy and

computational cost. The T&S group was invited to present results at the 2023 March Meeting of the American Physical Society. Where it also presented the works about the understanding thermal transport properties of 2D 2D-bonded Transition Metal Dichalcogenides (TMDs).

Outstanding international collaborations aligned with the objectives of the group continue, such as the collaboration with Prof. Ivan Cole's group, RMIT (Australia), on the development of first-principles methods to deal with problems related to electrochemistry, such as the corrosion of metals. The collaboration was formalised through a Framework Collaboration Agreement signed between ICN2 and RMIT, currently share three PhD students (2 of them hired by RMIT and 1 by ICN2), and 2 postdocs (1 hired by ICN2 and 1 by RMIT).

Also, another outstanding international collaboration merging of the codes developed by T&S (SIESTA) with those developed by Prof. O. Hellman (Weizmann Institute), and using them to compute the thermal properties of several materials, including 2D transition metal dichalcogenides. The collaboration has given rise to a software which we are now exploring the possibility to commercialise, through our spin-off company SIMUNE.

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THERMAL PROPERTIES OF NANOSCALE MATERIALS GROUP

JAVIER RODRÍGUEZ-VIEJO

UAB Professor and Senior Group Leader



MAIN RESEARCH LINES

- Heat capacity of low-dimensional materials.
- Phase transitions with emphasis on size effects; influence of external fields on heat capacity and phase transitions.
- Cross-plane and in-plane thermal transport in thin films and low-dimensional materials, including membranes, 2D materials and single nanowires, characterised by DC and AC-methods.
- Design, development and characterization of microthermoelectric devices for energy harvesting and sensing applications.
- Growth and characterization of ultrastable organic thin film glasses with applications in OLEDs and solar cells.

NEW PROJECTS & MILESTONES

Prof. Rodríguez-Viejo joined the ICN2 in 2021, where he started the new **Thermal Properties of Nanoscale Materials** group (while keeping his research group at the UAB). During 2022 the two laboratories, AFM and nanocalorimetry lab, have become fully operational. They include a high-vacuum nanocalorimetric setup, to measure phase

transitions in ultrathin layers, and a high-vacuum evaporation chamber, to allow for co-evaporation of small organic molecules and simultaneous characterization by *in-situ* nanocalorimetry, as well as several topographic AFM with temperature stages to follow *in-situ* the kinetics of phase transitions.

4 ARTICLES

11.7 MEAN IMPACT FACTOR

6 FUNDED PROJECTS

20 CONTRIBUTIONS

4 OUTREACH IMPACTS

16 COURSES

ULTRAFAST DYNAMICS IN NANOSCALE SYSTEMS GROUP

KLAAS-JAN TIELROOIJ

Senior Group Leader



In collaboration with the Oxyde Nanophysics group we have started a new project: **PYROelectric free-standing Membranes for THERmal Energy Recovery (PYROMETHER)**, TED2021-131363B-I00.

The goal is to investigate pyroelectric and electrocaloric effects of single-crystal free-standing (anti)ferroelectric oxide membranes using the nanocalorimetric chips as suitable platforms for direct measurements. We also aim to analyse the suitability of oxide AFE/FE membranes as potential materials towards an efficient pyroelectric energy conversion of heat into electricity. As a first step during 2022 we are measuring the heat capacity of thin film oxide membranes.

The group has also demonstrated a novel methodology to measure the heterogeneous transformation of ultrathin ultrastable glasses. It benefits from the mechanical instabilities created in tri-layer stacks during the melting of an intermediate layer to image by AFM the changes in topography. This work is based on the upgrade of a commercial Atomic Force Microscope for real-time imaging of temperature dependent phase transitions.

Within the EU project **EMPIR Nanowires**, and in collaboration with IMB-CNM-CSIC, we have developed suspended platforms to measure thermal transport in single nanowires.

Within the EU **NFFA-PILOT** project, thin silicon nitride membranes have been fabricated, in collaboration with IMB-CNM-CSIC, and assembled in UHV-compatible liquid cells for HAXPES (Hard X-rays Photoelectron Spectroscopy) experiments using synchrotron radiation at the GALAXIES beamline in SOLEIL (France). 20 nm thick membranes have been successfully tested in electrochemistry experiments.

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MAIN RESEARCH LINES

- Quantum materials.
- Ultrafast transport and dynamics of heat and charge.
- Terahertz technologies.
- Photodetection.

NEW PROJECTS & MILESTONES

In 2023, the UDNS group reached important milestones. The most impactful one is that part of the group members and group's ERC-funded equipment moved to Eindhoven University of Technology in the Netherlands. At the same time, the group is continuing several activities at the ICN2, with a number of group members and experimental setups.

Another important milestone was the starting of the **ICN2 Quantum Synergy Lab**. This is a joint lab facility for ICN2 groups working on quantum-related projects. Besides the UDNS group, this particularly

involves the PEN group of Prof. Sergio Valenzuela and the TCN group of Prof. Stephan Roche.

Our scientific highlights of 2023 include the development of a novel technique to extract the thermal diffusivity of thin films, which does not require any material input parameters: *Rev. Sci. Instr.* 94, 034903 (2023); and the measurement of the thermal conductivity of carbon nanotube networks that can be used as pellicles in extreme ultraviolet lithography applications: *ACS. Appl. Mater. Int.* 15, 51876 (2023).

6 ARTICLES

13 MEAN IMPACT FACTOR

5 FUNDED PROJECTS

15 CONTRIBUTIONS

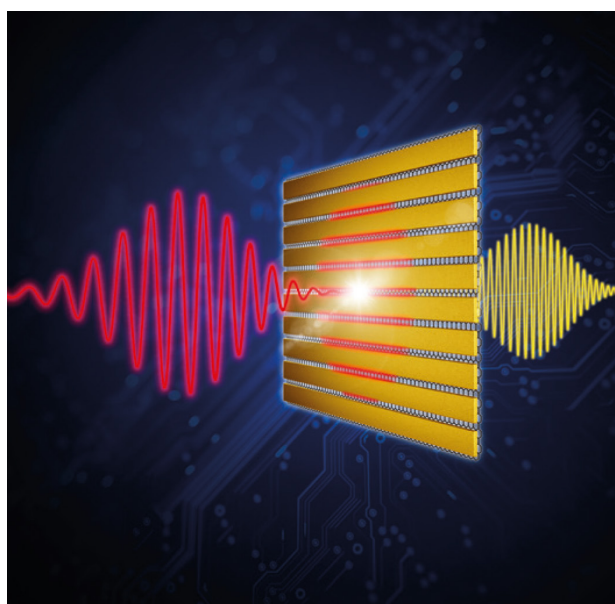
1 OUTREACH IMPACT

The group also published several works with long-term collaborators, in particular the Max Planck Institute for Polymer Research in Mainz (Germany): *Nat. Nanotechnol.* 18 898 (2023) and *Nano Lett.* 23, 1850 (2023); the Institute of Photonic Sciences in Castelldefels (Spain): *ACS Photonics* 10, 1850 (2023); and Helmholtz-Zentrum Dresden-Rossendorf (Germany): *Nano Lett.* 23, 3872 (2023); on a range of topics related to the ultrafast dynamics of quantum materials.

In 2023, the group continued its work on ERC Starting Grant **CUHL**, ERC Proof of Concept grant **COOLGRAELE**, and Flag-ERA project **ENPHOCAL** with partners IMEC (Belgium), UGent (Belgium) and MPIP (Germany), coordinated by K.J. Tielrooij.

Furthermore, the group was awarded a new Plan Nacional project, called **HYDROPTO**.

Francesc Alzina Sureda joined the group as Senior Researcher, Patricia Alquilar Merino started as a doctoral student, shared with the PEN group, and Ronny De La Bastida Chiza continued in the group after successfully finishing his MSc degree in Physics at the UAB.



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RESEARCH SUPPORT DIVISION

Research at the ICN2 is supported by a centralised support infrastructure that provides shared access to specialised equipment, services and expertise. It is made up of three research support units, and a set of technical facilities run by specialised technicians.

RESEARCH SUPPORT UNITS

INSTRUMENTATION UNIT

Dr **Gustavo Ceballos**

ELECTRON MICROSCOPY UNIT

Dr **Belén Ballesteros**

NANOMATERIALS GROWTH UNIT

Dr **José Santiso**

CORE RESEARCH FACILITIES

- » Biolab Facility
- » Mechanical Workshop
- » Molecular Spectroscopy Facility
- » Nanofabrication Facility
- » Photoemission Spectroscopy (XPS&UPS) Facility
- » X-Ray Diffraction Facility

ELECTRON MICROSCOPY UNIT

BELÉN BALLESTEROS

Unit Leader



MAIN RESEARCH LINES

- Use of advanced electron microscopy techniques for nanoscience and nanotechnology research and applications.
- Scientific-technical support for both internal ICN2 research groups and external scientists and companies.
- Study of the structure and chemistry of functional carbon nanotubes and graphene.
- Exploration of 2D layered inorganic nanotube systems.
- Electron microscopy studies of the interaction of nanomaterials and biological entities.

NEW PROJECTS & MILESTONES

The electron microscopy unit focuses on the use of electron microscopy techniques for nanoscience and nanotechnology research and applications. The Unit's main objective is to **provide scientific-technical support to the ICN2 research groups** and to other research centres and companies, as well as to develop and implement novel techniques.

During 2023, the new Double Aberration-Corrected Transmission Electron Microscope with monochromator and a Focused Ion Beam installed in the JEMCA and ICN2 respectively were commissioned, and initial experiments were carried out by groups of their founding institutions. These state-of-the-art equipment, partially funded with ERDF funds and with contributions of ICN2,

1 ARTICLES

10.9 MEAN IMPACT FACTOR

6 FUNDED PROJECTS

3 CONTRIBUTIONS

4 OUTREACH IMPACTS

1 COURSE

CSIC, ICMAB, UAB and ALBA, represent a leap in quality in the tools that the Unit provides to the local scientific community.

In 2023 the Unit incorporated a new member, Dr Kapil Gupta. The Unit also hosted Marta Villaret as visiting undergraduate students from the UAB.

Aside from their daily fundamental activities, during 2023 the members of the Unit were involved in the organization of the third edition of the *ICN2 ArtMeetsNano Image Contest*. Also, Dr Ballesteros took part in the organization of the *LeaderSHE* seminars, a series of lectures given by outstanding women who succeeded in reaching leadership positions in different professional fields. This initiative, promoted by the Equal Opportunities Committee, aims at inspiring young female researchers and professionals to pursue leading roles in academia, industry or any other work environment.

As in previous years, the team actively participated in the *BIST Winter School on Microscopy and Imaging Sciences*, which is part of the BIST-UPF Master of Multidisciplinary Research in Experimental Sciences. Moreover, the Unit participated in the outreach activities organised at the ICN2, such as the *Bojos per la Física* (Crazy for Physics) programme.

The Unit devoted efforts to the **NFFA- Europe** and the **ReMADE@ARI** infrastructure projects, providing access to the ICN2 electron microscopy facilities to a number of researchers from other institutions.

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INSTRUMENTATION UNIT

GUSTAVO CEBALLOS

Head of Research Support Division - Instrumentation Unit



1 FUNDED PROJECT

1 THESIS

1 COURSE

MAIN ACTIVITIES

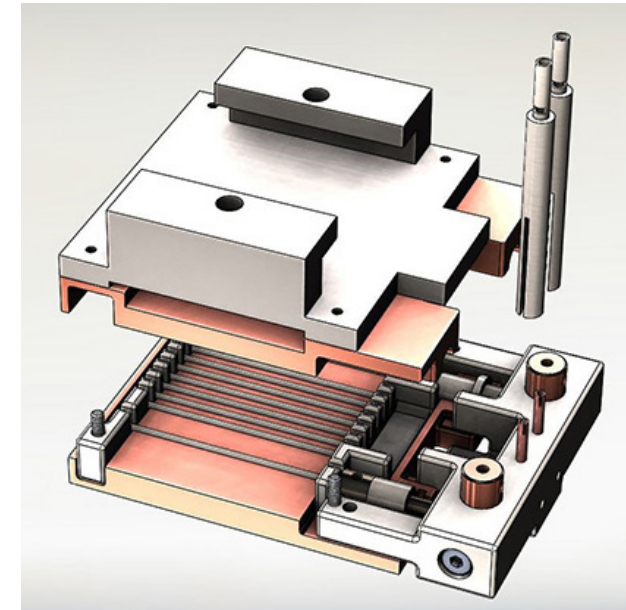
The Instrumentation Unit at ICN2 is involved in various activities aimed at providing scientific and technical support in applied physics, precision instrumentation, microengineering, nanotechnology, scientific computing, and 3D design of precision devices. The main activities of the unit include:

- Designing, developing, and improving advanced precision instrumentation.
- Modifying commercial instrumentation to meet specific experimental requirements.
- Scientific computing for data analysis and modeling.
- Data acquisition for experimental measurements.
- 3D computer-aided design (CAD) of precision devices.
- Expertise in vacuum technology, including high vacuum (HV) and ultra-high vacuum (UHV) systems.
- Cryogenics for experiments requiring low-temperature environments.

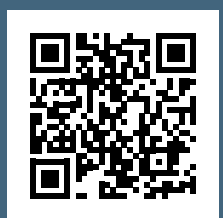
Additionally, the Instrumentation Unit collaborates with several institute Spin-offs, participating in the prototyping and final development of devices.

NEW PROJECTS & MILESTONES

In 2023, the Instrumentation Unit achieved several milestones and contributed to new projects. The unit developed **innovative setups to facilitate experiments in various fields** such as magnetometry, spectroscopy, nanomaterial synthesis, photovoltaics, and bio-sensing. Furthermore, the unit actively participated in dissemination activities, utilizing their expertise to design and construct prototypes and technology demonstrations.



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NANOMATERIALS GROWTH UNIT

JOSÉ SANTISO

CSIC Tenured Scientist and Unit Leader



MAIN ACTIVITIES

- Pulsed laser deposition of epitaxial thin films and free-standing membranes of different materials (mainly oxides), looking at strain and relaxation mechanisms, and the microstructural and functional properties (metal-insulating transitions, ferroelectric, ferromagnetic, oxide ionic conducting, thermoelectric, transparent conducting, resistive switching, etc.)
- MOCVD growth of 2D layers of transition metal dichalcogenides.
- Structural characterisation by RHEED and advanced XRD and electronic transport properties.
- Fundamental aspects of interfacial phenomena in layered oxide materials and multilayers for their use as components in ionic and protonic solid oxide fuel cells (SOFCs), as well as in resistive switching devices.
- Accurate structural characterization of epitaxial thin films making use of advanced X-ray diffraction techniques (reciprocal space mapping under non-ambient conditions and external stimuli: gas change, voltage, illumination).

6 ARTICLES

7.25 MEAN IMPACT FACTOR

3 FUNDED PROJECTS

1 COURSE

NEW PROJECTS & MILESTONES

Our unit produces films by means of **pulsed laser deposition and metal organic chemical vapour deposition (MOCVD) techniques** and works in close collaboration with many ICN2 research groups, as well as with external teams. A recently developed two-laser PLD setup allows co-ablation of two targets for deposition of films with composition gradient new mixed composition materials. Our unit carries out advanced structural characterisation of thin films, primarily by X-ray diffraction (XRD), and work on developing advanced methods for the characterisation by XRD of epitaxial thin films. These include in-plane diffraction, Grazing Incidence XRD (GIXRD) analysis, as well as 3D reciprocal space mapping. This microstructure research is complemented with High-Resolution Transmission Electron Microscopy (HRTEM) characterisation.

We are particularly interested in surface and interfacial phenomena, such as oxygen exchange kinetics. For this purpose we have developed a time-resolved XRD technique that monitors the subtle chemical expansion produced in transition metal oxide thin films when changing their oxygen stoichiometry.

We aim to perform in-situ and operando characterisation by XRD in different solid state electrochemical devices. These

studies have also been extended to in-situ structural analysis of ferroelectric materials, and materials showing resistive switching.

We have also continued working on the development of a thin film MOCVD process for the growth of high-quality ultrathin transition metal dichalcogenides, starting with MoS₂, in collaboration with the ICN2 group led by Prof. José A. Garrido.

In 2020, we started working in collaboration of Prof. Gustau Catalan's group on the fabrication of single-crystal free-standing membranes of perovskite oxides by using water-soluble sacrificial epitaxial layers in an attempt to implement functional oxides in a new generation of electronic devices. Currently, we are engaged in the fabrication of free-standing membranes of different ferroic oxide materials to analyse the intrinsic characteristics of strain-free ultrathin films.

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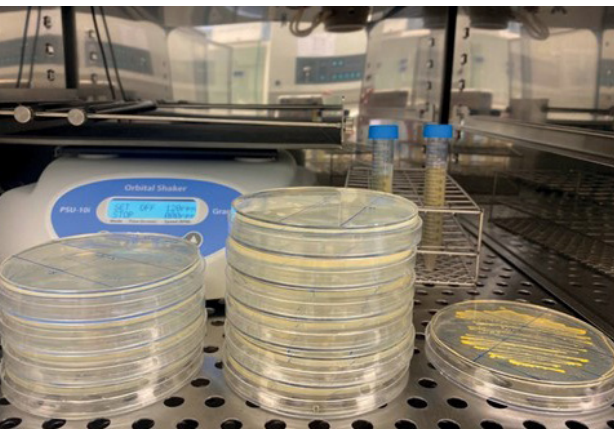
BIOLAB FACILITY

AVAILABLE TECHNIQUES

- » Biological Safety Cabinets (class II)
- » CO₂ Incubators
- » Cryopreservation of cells in cryogenic tank
- » Microbiological incubator
- » Bench-top microcentrifuges
- » Refrigerated centrifuge
- » Autoclaves
- » Inverted optical microscopy
- » Orbital shakers
- » Cell density meter
- » Portable vacuum aspiration system
- » Water bath, vortex, pipettes
- » Refrigerators, freezer and ultra-freezers

NEW PROJECTS & MILESTONES

In 2023, the Biolab Facility has continued to offer its service to scientists of ICN2 and other research centres and companies on the UAB campus. In particular, scientists from the neighbouring *Institute of Materials Science of Barcelona (ICMAB)* made use of the service provided by the Biolab Facility. The central cell strain collection of animal and bacterial cells that the Biolab had started to establish in 2021 was expanded with further cell lines. This institutional strain collection offers the users of the Biolab Facility the possibility to acquire rapidly and cost-efficiently a variety of cells for their studies. New equipment has been acquired and installed, amongst them a PC and a compact inverted microscope with camera for easier cell observation. 2023 was also the year of a thorough revision of the Institutional Biosafety Programme and the Biolab Facility and its safety procedures by the Biosafety Committee of the UAB. The Biosafety Committee of the UAB accredited the Biolab a very high standard for a BSL-2 facility in all aspects.



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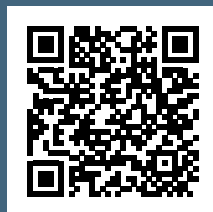
MECHANICAL WORKSHOP

AVAILABLE TECHNIQUES

- » Precision milling, turning and grinding
- » Close tolerance machining
- » Mechanical assembly
- » Computer-aided design (CAD)
- » Computer-aided machining (CAM)
- » Computer numerical control (CNC)
- » Tungsten inert gas (TIG) welding
- » Bending and cutting machine
- » 3D Printing of thermoplastics
- » Sand Blast Cabinet



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MOLECULAR SPECTROSCOPY FACILITY

AVAILABLE TECHNIQUES

FT-IR spectroscopy

- » Detectors available for MIR, NIR and FIR measurements
- » Powders, films and surfaces
- » Variable temperature (73 K - 500 K)
- » Polarization modulation-infrared reflection-absorption spectroscopy (PM-IRRAS)
- » Vibrational circular dichroism (VCD)

UV-Vis spectroscopy

- » Two ranges available: 175 - 900 nm/ 190 - 1100 nm (only for liquid samples)
- » Liquids, films, surfaces and powders
- » Integrating sphere
- » Variable temperature (r.t. - 372 K)

Microspectroscopy

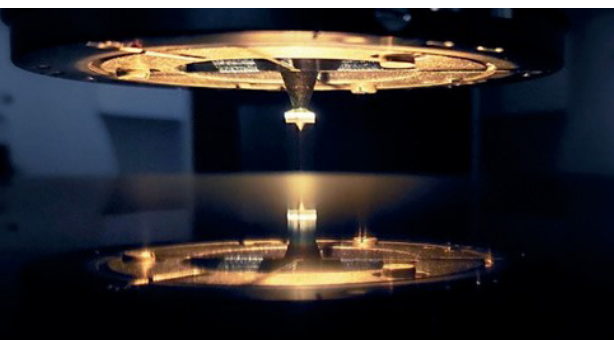
- » FTIR and Vis-NIR measurements
- » Solids, films and surfaces
- » Objectives:
 - 15x reflection/transmission
 - 36x (only reflection)
 - Grazing angle
 - ATR
- » Vis and IR polarizers available

Dynamic light scattering and zeta potential

- » Dip cell for measurements of zeta potential in organic solvents available

Static contact angle

- » Static and dynamic
- » Surface free energy of solids
- » Surface and interfacial tension of liquids
- » Work of adhesion
- » Advancing and receding contact angles and evaluation of a roll off angle by tilting table method



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NANOFABRICATION FACILITY

AVAILABLE TECHNIQUES

- » Electron-beam lithography (EBL)
- » Direct write laser UV lithography (DWL)
- » UV mask aligner
- » E-beam evaporation
- » ICP-RIE plasma dry etching
- » Plasma cleaning
- » Wedge wire bonding
- » Spin coating
- » Optical microscopy
- » 3D optical profiler
- » Stylus profilometer

NEW PROJECTS & MILESTONES

In 2023, the Nanofabrication Facility activities focused on the **improvement of standard protocols and procedures for micro- and nano-fabrication techniques** linked to key equipment and to the most common processes involved in the facility users' work. A new ultra-high resolution ebeam lithography system was installed to allow sub-10nm resolution patterning on substrates up to 6" in size. The facility has kept growing in the number of active users and processes developed, some of them from ICN2 spin-off companies that are making intensive use of the facility. New processes have been developed that enhance the existing nanofabrication services and improve users experience regarding these techniques. With a focus on dry etching and photolithography processes (combined with the existing thin film evaporation systems), the new processing protocols will allow the development and fabrication of fully functional micro- and nano-devices.

In addition to providing essential micro- and nano-fabrication capabilities for research in electronics, optoelectronics, and 2D materials and devices, this facility is intended to contribute to the pursuit of research in other emerging, interdisciplinary, and rapidly growing areas of study, such as biomedical and biochemical lab-on-a-chip devices, heterogeneous integrated circuits, and photonic and phononic devices.

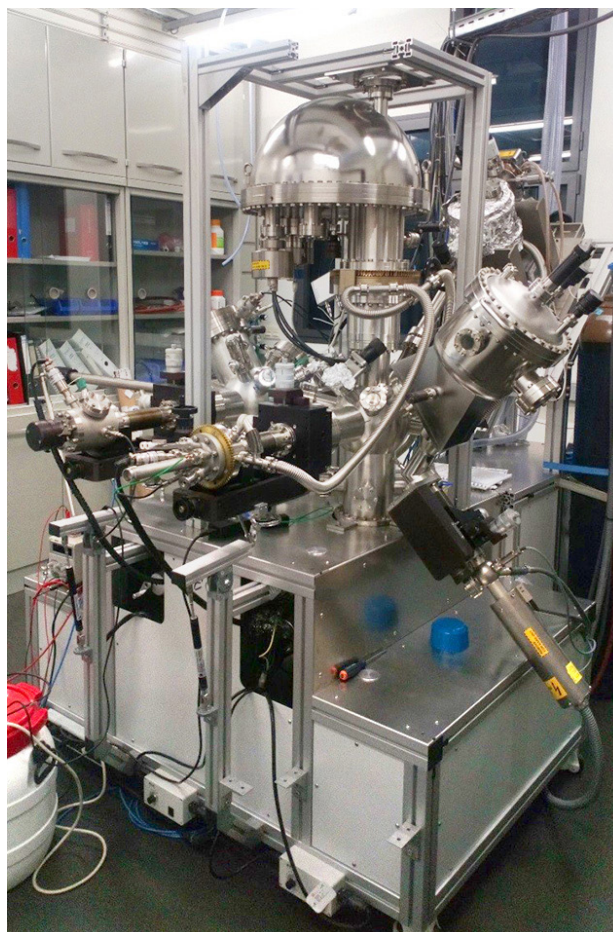
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PHOTOEMISSION SPECTROSCOPY (XPS&UPS) FACILITY

AVAILABLE TECHNIQUES

- » Elemental composition
- » Detection of contaminants
- » Quantitative analysis
- » Determination of chemical or electronic state of each element on the surface
- » Layer ordering in the first 8-10 nm (relative depth plot)
- » Work function, ionization energy and valence band measurement using UPS
- » Direct band mapping using ARUPS
- » Temperature-dependent XPS measurements
- » In-situ preparation of materials by thermal evaporation for later analysis



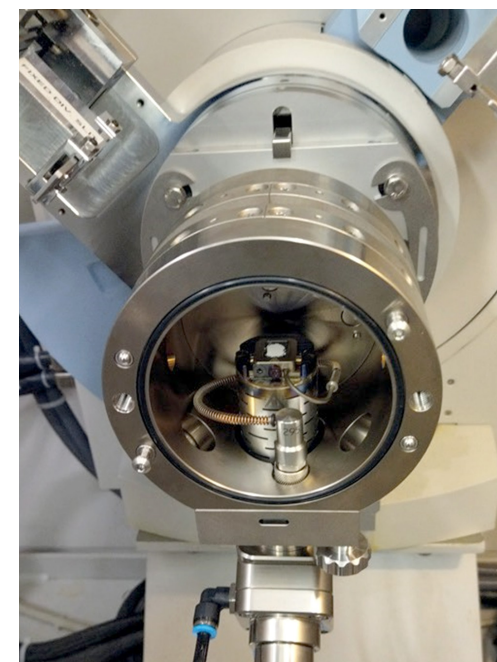
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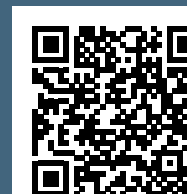
X-RAY DIFFRACTION FACILITY

AVAILABLE TECHNIQUES

- » XRD of powder materials for the structural analysis of phases in both reflection and transmission geometries
- » Capillary measurements in transmission mode for liquid specimens or air sensitive powder materials
- » Small-angle X-ray scattering (SAXS) for flat nanopowder samples in transmission geometry
- » In-situ powder characterization of the crystal structure in organic and inorganic materials, and pharmaceutical materials. Studies of structural phase transitions as a function of temperature, oxidation states and cell parameters evolution.
- » XRD of thin films to identify phases and determine cell parameters, domain orientation and stress on epitaxy and polycrystalline films (at normal and high resolution)
- » In-situ thin films characterization applying:
 - Gas exchanges at elevated temperatures (redox kinetics, oxide ionic materials)
 - Applied voltage bias (piezoelectric, ferroelectric, electrostriction, resistive switching)
 - Exchange between wet and dry atmosphere (water uptake, protonic conducting materials)
 - Simultaneous atmosphere exchange and electrical conductivity
 - LED illumination at RT and applying low temperature (up to 100 °C) with controlled atmosphere (photoactivated phase transitions, photostriction, etc.)



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Research is also underpinned, protected and promoted by a comprehensive set of management and support services. Overall responsibility for ICN2 administration lies with the ICN2 General Manager Mr **Lluís Bellafont**, with each department and area having its own head.

COMPETITIVE FUNDING

Mireia Martí Barroso

FINANCE

Judit Vela

HEALTH AND SAFETY AREA

Jose Antonio Pérez

HUMAN RESOURCES

Julio Pérez

INFORMATION TECHNOLOGIES

Javier González

MAINTENANCE AND SERVICES

Xavier Ros

MARKETING, COMMUNICATION AND FUNDRAISING

Àlex Argemí / Anna Rovira

TECHNICAL MANAGEMENT SUPPORT AREA

Estefanía Latorre



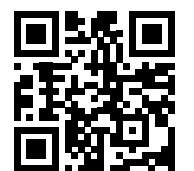
Throughout 2023, the ICN2 Management and Services Department experienced significant developments, enhancing its operational efficiency, and expanding its team to better support the institution's scientific endeavours. One of the key changes of the year was the **appointment of Anna Rovira as the new Director of Marketing, Communication, and Fundraising** towards the end of the year. Her role focuses on driving strategic initiatives, improving planning processes, and enhancing fundraising efforts to support ICN2's mission. Her leadership is expected to align the department's activities with the broader goals of ICN2, ensuring effective communication and engagement with a wide range of stakeholders.

Another major development in 2023 was the incorporation of ten new members from the *"Programa de Primera Experiència Professional en les Administracions Públiques"* (First Professional Experience in the Public Administration Programme), financed by the Catalan Employment Service. These individuals have been integrated into various departments, providing essential support, and bringing fresh perspectives to the organization. The objective of this initiative is to **enhance ICN2's operational capability** and guarantee the smooth and efficient functioning of all departments.

The restructuring and strategic additions made in 2023 reflect ICN2's commitment to maintaining a high standard of service and support for its scientific community. These changes are designed to create a more dynamic and responsive environment, capable of meeting the evolving needs of both researchers and administrative staff. The enhancements in the department are part of the overall strategy of ICN2 to foster a cooperative and innovative research environment.

For further details on our activities and services, please visit the ICN2 website.

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ICN2 IN NUMBERS

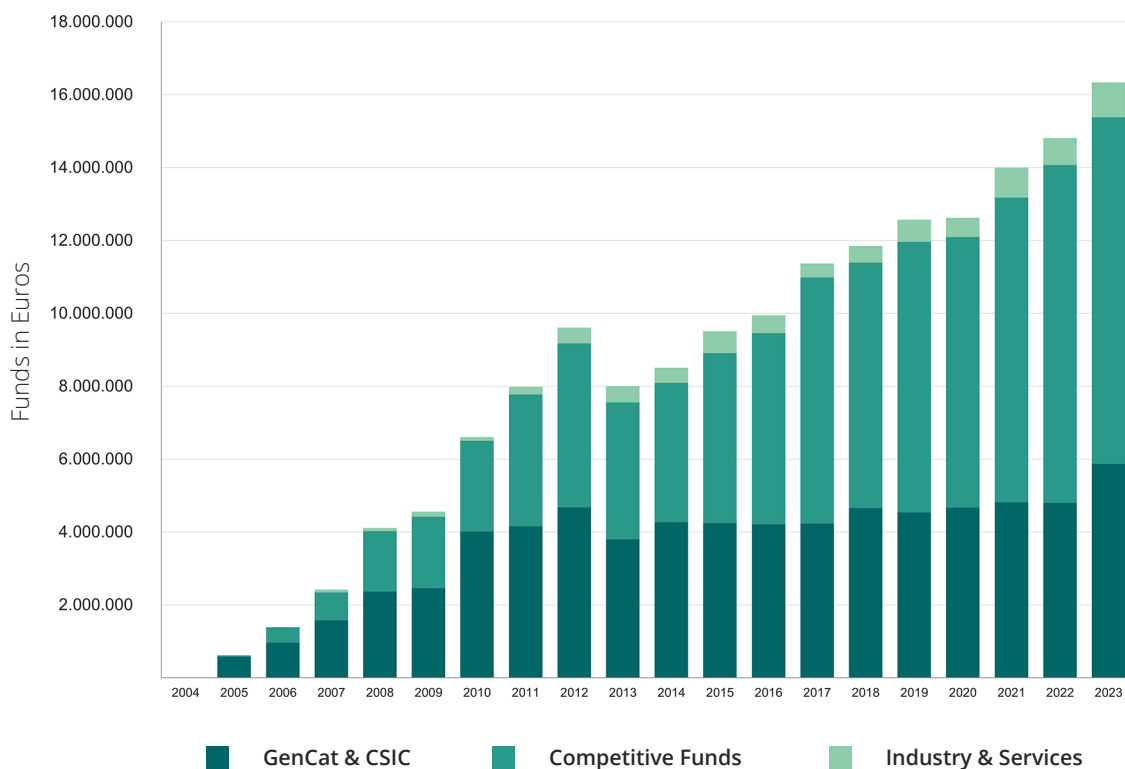
FINANCE

FINANCIAL ACCOUNTS 2023

In 2023 the ICN2 Finance Department has continued with the digitalization of its processes to increase the efficiency of the department, developing a web solution for purchasing and travel management.

This year we have worked towards consolidating two goals: the first is to **improve communication and tailor the service to the needs of the different groups and departments**, and the second to begin to offer financial information to all users.

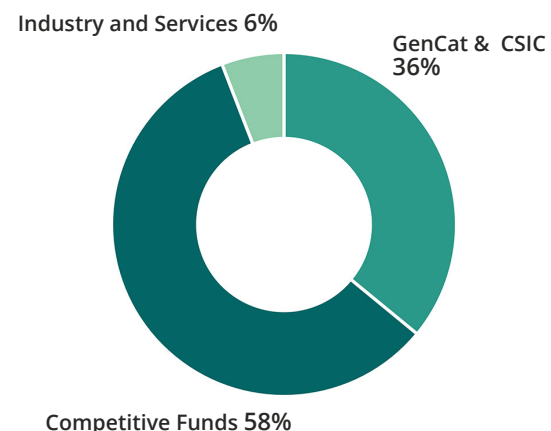
Evolution of ICN2 Operational Funds



INCOME

The ICN2's total operating funds in 2023 stood at €16,339,192, of which 36% were obtained from the Generalitat de Catalunya and the Spanish National Research Council (CSIC), 58% from competitive funding calls, and 6% from industry and services.

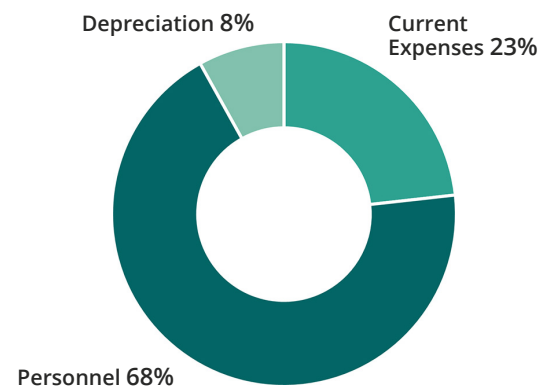
Funds Distribution 2023



EXPENSES

Total expenditure in 2023 reached €13,426,152 including current expenses, personnel costs and depreciation.

Expenditure in 2023



FACILITIES AND EQUIPMENT

Total accumulated investment by the ICN2 in scientific equipment, common services and general infrastructure as of year-end 2023 stood at €32,565,646.

During 2023 investment reached a total of €5,268,476, being the most important investments:

- » Ebeam Lithography System
- » Encapsulator
- » Micro-Manipulador xyz con Controladores
- » Planta Piloto Tratamiento Aguas
- » 3d Rotator for Dilution Fridge
- » Gas Chromatography
- » Estimulador X--XDAQ-One-R1024-S128
- » Vitrina de Gases Lab. -1019 de 1500mm
- » Picosecond Supercontium Laser

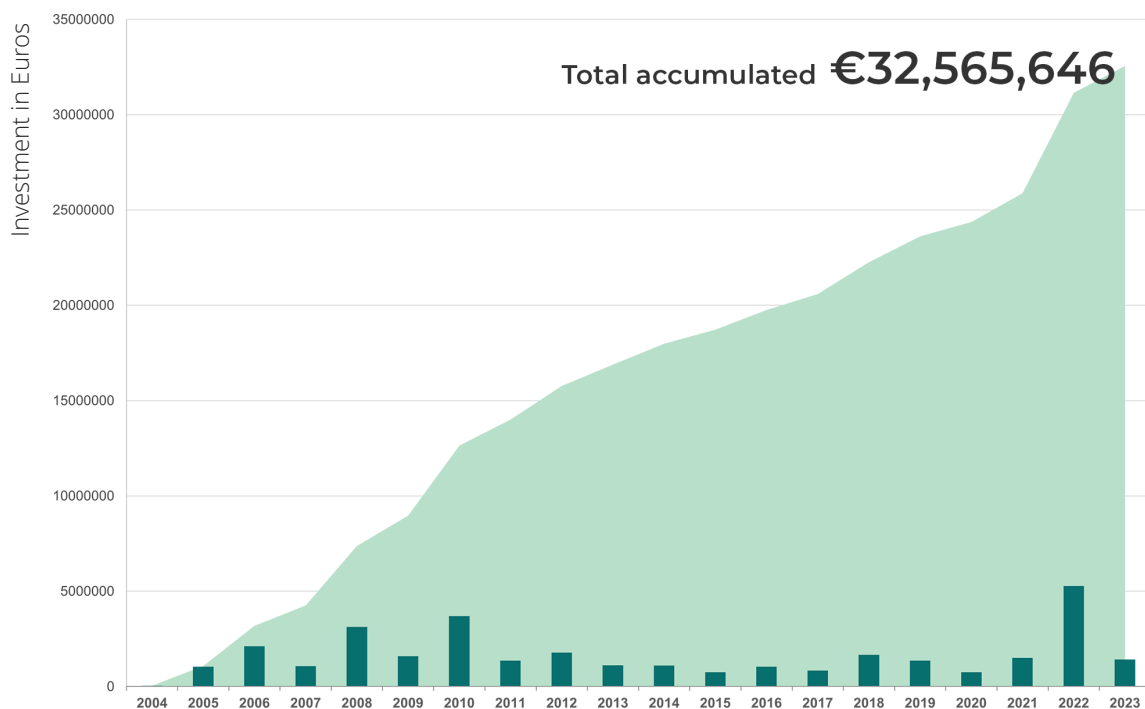
Equipment funded using Spanish ERDF ("FEDER") funds:

- » Placa Agitadora
- » HP Slim Desktop S01-pF2028ns Intel Core i5-12400/16GB/512GB SSD
- » Monitor BENQ DESIGNVUE PD3205U
- » 2 Pistola Spray Drier
- » HP OMEN 40L GT21-0022ns AMD Ryzen 5 5600X/16GB/512GB SSD/RTX 3060
- » PC HP Pro SFF 400 G9 i7 16/512 GB
- » Electrode
- » Bloque Térmico IKA
- » Balanza Analítica ENTRIS II. SARTORIUS. Modelo BCE224i-1S
- » Microscopio Óptico

- » Horno - Estufa Universal Aire Forzado 53L MEMMERT
- » Magneto-Optic Microscope 2
- » Multiagitador con Calefacción
- » Circulation Pump And Flow Meter Regulator
- » Laser Diode Controller
- » Ultraturrax T25 Disperser and Accesories
- » Impresora VOLTERA V-ONE
- » Optical Table
- » Mass Flow Controller
- » Bomba Turbomolecular
- » XYZ Motorised Translation Stage
- » Probes and Positioner Manipulators
- » nXDS6i Dry Pump
- » Capacitive Guage
- » Chemistry Diaphragm Pump
- » Activeline Control Software
- » Bomba De Vacio RV3
- » Laser 808 nm
- » Micro-Heater MPN:CMH-7019
- » Valve Gate CF 35 Manual Operated
- » CNI-MGL-III-532-300-2%-LED
- » Bomba Pfeiffer DUO 6 Ref: PK 195 488-T
- » Dewar Refrigeracion
- » THR64000 Spectrometer
- » Baño Para Rotavapor
- » Bomba Vacio Aceite con Sensor



Evolution of Investments between 2004 and 2023



RESEARCH OUTPUTS

PUBLICATIONS

175

JOURNAL ARTICLES 2023 (Indexed)

78% Q1 → **39%** D1 (JCR - WoS)

98% Q1 → **70%** D1 (SJR - SCOPUS)

76,6% OPEN ACCESS (138 art.)

70% INCLUDED IN DDD (123 art.)

10.565

AVERAGE IMPACT FACTOR (JCR - WoS)

149

ICN2 DOCUMENTS H-INDEX (JCR - WoS)

13

VERY HIGH IMPACT ARTICLES (IF > 20)

67

HIGH IMPACT ARTICLES (IF > 10)

3

JOURNAL COVERS

5

NON-INDEXED JOURNAL ARTICLES

INSTITUTIONAL ICN2 EVENTS

48

TOTAL

13 THESES **8** NANOSEMINARS
23 SEMINARS **1** INNOVATORS TALK
3 MANUEL CARDONA LECTURES

PARTICIPATED EVENTS

318

ORAL CONTRIBUTIONS

173

INVITED

42

ORGANISING
COMMITTEES

80

POSTERS

MEDIA IMPACT

656

ONLINE

-2,96% vs 2022 *

79

OFFLINE (PRINT, RADIO, TV)

+0% vs 2022

* This year's media impact data revealed the need to boost brand visibility and increase scientific publications online.

SOCIAL NETWORKS



8,114

FOLLOWERS

+13,49% vs 2022



1,452

SUBSCRIBERS

+24,10% vs 2022

9,856

TWEETS

+14,26% vs 2022

41

VIDEOS

-55,92% vs 2022 *

* During 2023 we reduced YouTube video production to focus on other social media platforms and align with our strategic plan.



14,453

FOLLOWERS

+14,26% vs 2022

BUSINESS AND INNOVATION

34
NDAS SIGNED

116
COMPANIES ENGAGED

42
ACTIVE PATENTS

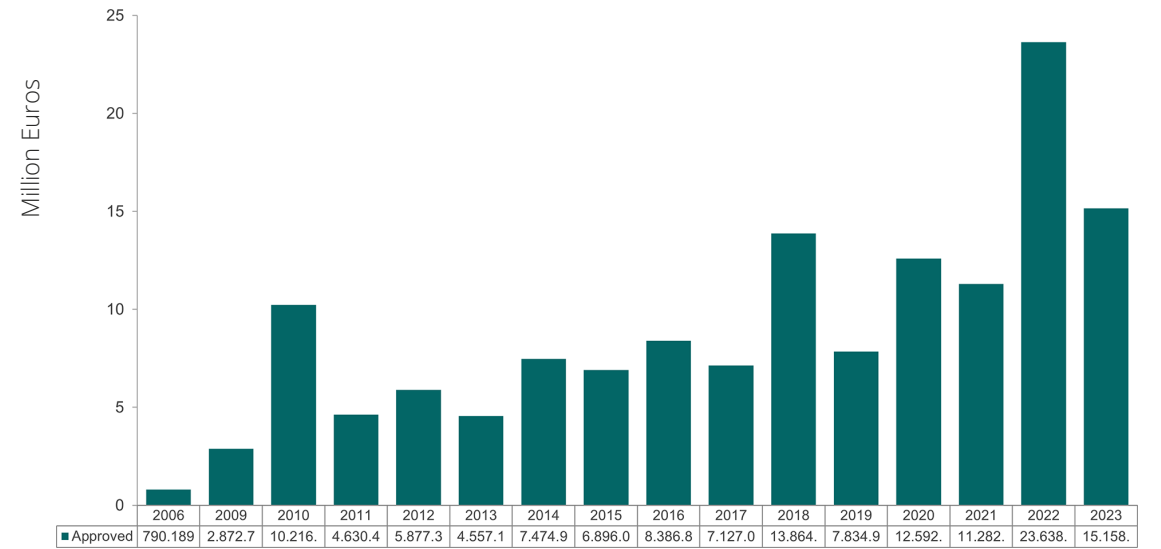
5
NEW PATENTS

2
NEW LICENSES

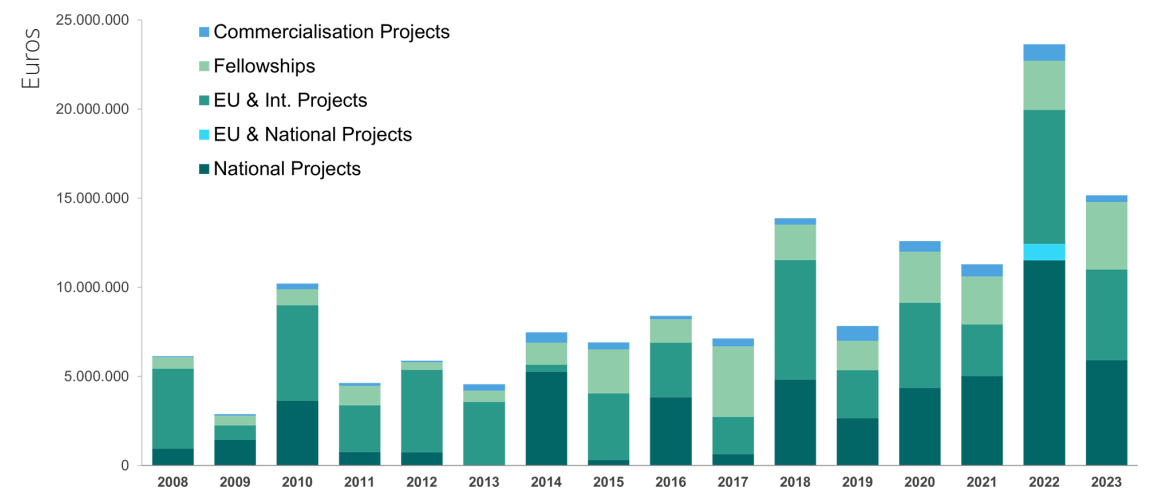
9
R&D CONTRACTS

PROJECTS

Evolution of Competitive Funding Approvals 2008-2023



Evolution of income from approved competitive proposals by source



Annual Report 2023

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Marketing, Communication and Fundraising Department

May 2024