

# ANNUAL REPORT 2017



# ANNUAL REPORT 2017



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# Letter from the Director



2017 was once again a year of intense activity for the Catalan Institute of Nanoscience and Nanotechnology (ICN2).

Our scientific activity has resulted in a total of 191 indexed publications and an average impact factor that has increased to a remarkable 6.88, with 79% of the publications in journals in the first quartile and 53% in the first decile. From the technology transfer side, the most important outcome for 2017 was the creation of new spin-off company Ahead Therapeutics, in which the ICN2 and ICREA participate as founding partners, together with the Institute for Health Science Research Germans Trias i Pujol (IGTP). The new company was created to advance the development of therapies for autoimmune diseases and pursue their application in a clinical setting. Just a few months in, the new company has already attracted 1.3 million euros in private investment.

Meanwhile, an important organisational change took place within the ICN2, in the form of the new structure and expanded role of the Strategy Development Office. First created in 2013, the aim of this office has always been to guide the institute's planning processes, promoting and managing key strategic actions, including institutional projects (Severo Ochoa, FEDER, etc.) and the coordination, preparation and execution of strategic plans. Building on the success of past actions, in 2017 we decided to enhance its scope with the goals of increasing its impact on competitive projects, providing greater support for the identification and submission of proposals to important funding calls (mainly from the European Union) and increasing the impact of our researchers' actions to transfer knowledge and know-how to industry and society. The office is led by Prof. Jose A. Garrido, who was also appointed as ICN2 vice-director.

Following a mandate from the Parliament of Catalonia, the CERCA Institution has been conducting its second round of evaluations of all affiliated centres, assessing their progress towards their founding missions. The ICN2 was evaluated in 2017, a process that concluded with an on-site visit by the external evaluation committee on 29 September 2017. The result of the assessment was very positive, culminating in a series of actionable recommendations and an overall rating of "outstanding" for the activities carried out at our institute.

The ICN2's most important institutional project, the Severo Ochoa Centre of Excellence research programme, is now in its final phase. After the very positive mid-term evaluation in 2016, we have worked very hard this year on our application to renew this award for a further four years. The Strategy Development Office led and coordinated all contributions to this proposal, and has been a key player in building what we feel is a very strong proposal, one which we hope will secure our Severo Ochoa status and funding for the 2018 to 2022 period.

Cooperation within the Barcelona Institute of Science and Technology (BIST) has also strengthened, thereby consolidating a research initiative that delivers high scores across all excellence indicators. During 2017, Dr Gabriel Silberman was appointed as the new BIST director, which has entailed a significant boost to all its activities. Overall, BIST continues to represent a strategic alliance for the future of all of its members, not least the ICN2.

On the negative side, 2017 has seen a clear deterioration in the regulatory landscape of research in our country, due to the increasing bureaucratic obstacles, limitations and controls imposed on the public sector. The situation has reached a critical level and poses a substantial threat to the future of many research institutions, which see the ability to carry out

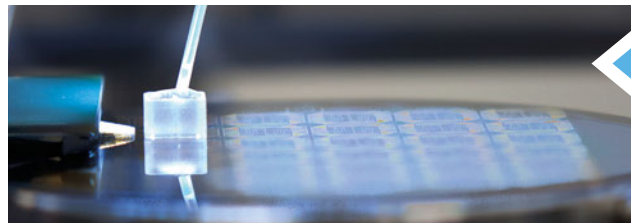
their daily work blocked by inflexible, unreasonable and sometimes contradictory rules. While some light can be glimpsed on the horizon (in form of parliamentary initiatives regarding personnel and taxes, for example) and makes us hopeful that the situation might improve in the future, the overall perspective is still quite dark and threatens to have a severe impact on institutes like the ICN2 and their efforts to remain globally competitive.

Overall 2017 has seen further consolidation of the ICN2 as one of Spain's top research centres. It is my pleasure to present this Annual Report, and I invite you to explore its pages and join us on our journey into the nanoworld.

Sincerely,

Prof. **Pablo Ordejón**  
Director, ICN2

# What is the ICN2?



Global leader  
in nanoresearch

A place where both  
fundamental and applied  
research, and efforts to bring  
technology innovations to  
market receive strong support



Creator of opportunities for  
dialogue and collaboration  
between researchers, industry,  
policymakers and society

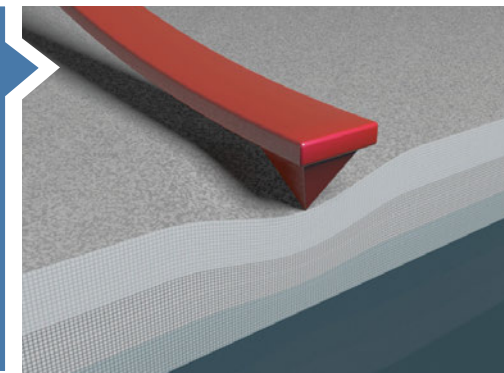
Commitment to equal  
opportunities, fair selection  
processes and the importance  
of the work/life balance



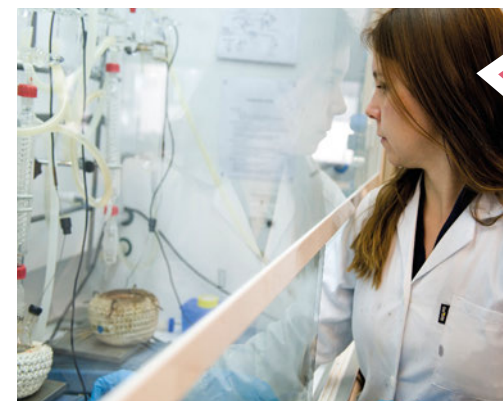
Trainer of the  
future generation of  
nanoscientists

# What do we do?

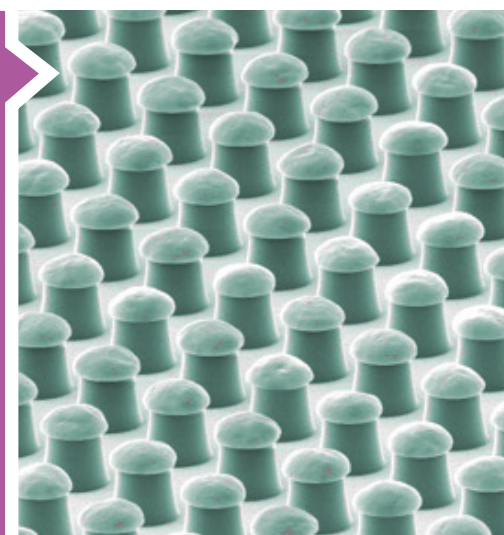
Nanoscience and nanotechnology  
take an extremely close look at the  
world around us. Understanding  
and learning to control the  
sometimes unexpected behaviour  
of matter at this tiny scale has  
implications for all other sciences.



The ICN2 brings together chemists,  
physicists, biologists, materials  
scientists and engineers to  
discover and explore uncharted  
corners of the nanoworld, and  
work out how to turn the insights  
gleaned into life- and world-  
improving applications.



Our researchers approach this  
challenge from all directions, with  
teams working on everything  
from the discovery, simulation,  
visualisation and experimental  
exploration of the properties and  
behaviours of materials at the  
nanoscale, to the design  
and fabrication of the  
devices they inspire.



# Organisation

At the ICN2 we firmly believe that people are our main asset. Scientists from diverse backgrounds are joined by technicians and administration professionals in the pursuit of the institute's many goals. We are also fortunate enough to have a knowledgeable Board of Trustees and Scientific Advisory Board made up of international peers.

## BOARD OF TRUSTEES

### President\*

**Emilio Lora-Tamayo**, President of the *Consejo Superior de Investigaciones Científicas* (CSIC)

### Vice-President\*

Minister for Business and Knowledge,  
*Generalitat de Catalunya*

### Secretary

**Francesc Ramon Subirada**, General Director for Research, *Generalitat de Catalunya*

### Members

**Margarita Arboix**, Rector of the *Universitat Autònoma de Barcelona*

**Lluís Calvo**, Institutional CSIC Coordinator in Catalonia

**Arcadi Navarro**, Secretary of Universities and Research, Ministry of Business and Knowledge, *Generalitat de Catalunya*

**José Ramón Urquijo**, Vice-President for Organisation and Institutional Relations, CSIC

\* The roles of president and vice-president alternate every two years.

## SCIENTIFIC ADVISORY BOARD

### President

Prof. **Miquel Salmerón**, Lawrence Berkeley National Laboratory and UC Berkeley, USA

### Members

Prof. **Jeff Bokor**, UC Berkeley and Lawrence Berkeley National Laboratory, USA

Prof. **Luisa de Cola**, Université de Strasbourg, France

Prof. **Sylvia Daunert**, University of Miami, USA

Prof. **Albert Fert**, CNRS/Thales, France

Prof. **Klaus Kern**, Max Planck Institut für Festkörperforschung, Germany

Prof. **Steven Louie**, UC Berkeley and Lawrence Berkeley National Laboratory, USA

Dr. **Tapani Ryhänen**, Nokia Technologies, Finland

Prof. **Clément Sánchez**, CNRS/Université Pierre et Marie Curie/Collège de France, France

Prof. **Nicholas D. Spencer**, ETH-Zürich, Switzerland

## DIRECTOR

The ICN2 is led by Director Prof. **Pablo Ordejón**. He reports directly to the *Board of Trustees* and is advised by the *Scientific Advisory Board*.

## STRATEGY DEVELOPMENT OFFICE

Led by Vice-Director Prof. **Jose A. Garrido**, this office pursues the double objective of improving the institute's resourcefulness when securing funds for future research and driving forward the business development and transfer of in-house technologies.

## RESEARCH GROUPS

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 total the institute currently has 17 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**
- Force Probe Microscopy and Surface Nanoengineering  
Dr **Jordi Fraxedas**
- Inorganic Nanoparticles  
ICREA Prof. **Víctor F. Puntès**
- Magnetic Nanostructures  
ICREA Prof. **Josep Nogués**
- Nanobioelectronics and Biosensors  
ICREA Prof. **Arben Merkoçi**
- Nanobiosensors and Bioanalytical Applications  
Prof. **Laura M. Lechuga**
- 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  
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**

## 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

- Nanofabrication
- Molecular Spectroscopy and Optical Microscopy
- X-Ray Diffraction
- Photoemission Spectroscopy
- Mechanical Workshop

## MANAGEMENT AND SERVICES

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 having its own head.

- Competitive Funding  
**Mireia Martí Barroso**
- Finance  
**Judit Vela**
- Human Resources  
**Rocío Pérez**
- Information Technologies  
**Jordi Prat Ribas**
- Legal Advisory  
**Joaquín Barberá Antolin**
- Maintenance and Safety  
**Xavier Ros**
- Marketing and Communication  
**Àlex Argemí**

## Equal opportunities

The ICN2 is an equal opportunities employer committed to diversity and the inclusion of people with disabilities. It strives to achieve a workforce that is diverse in age, nationality and gender.

## Fostering talent

The ICN2 prides itself on being able to attract talented scientists, technicians and support personnel from around the world. Once at the institute its researchers can opt into the many training and professional development programmes available.

Its scientists are active participants in the regional, national and international research scenes. Many of those who complete their PhD or postdoctoral research at the ICN2 move on to pursue their passion at the likes of Harvard, Yale, the Max Planck institutes, the French National Centre for Scientific Research (CNRS) and French Alternative Energies and Atomic Energy Commission (CEA). This in turn means that the ICN2 is able to keep on offering new positions to future nanoscientists.

Over the course of 2017 it had an average workforce of 266 employees.

## Culture of entrepreneurship

Meanwhile, the renewed prominence of strategy development this year reflects the institute's ongoing commitment to making real contributions to industry and society. The resulting culture of innovation and entrepreneurship will have the added benefit of preparing its researchers well for the more diverse, more imaginative manifestations of public-private research collaborations of the future.

## Finances

### FINANCIAL ACCOUNTS 2017

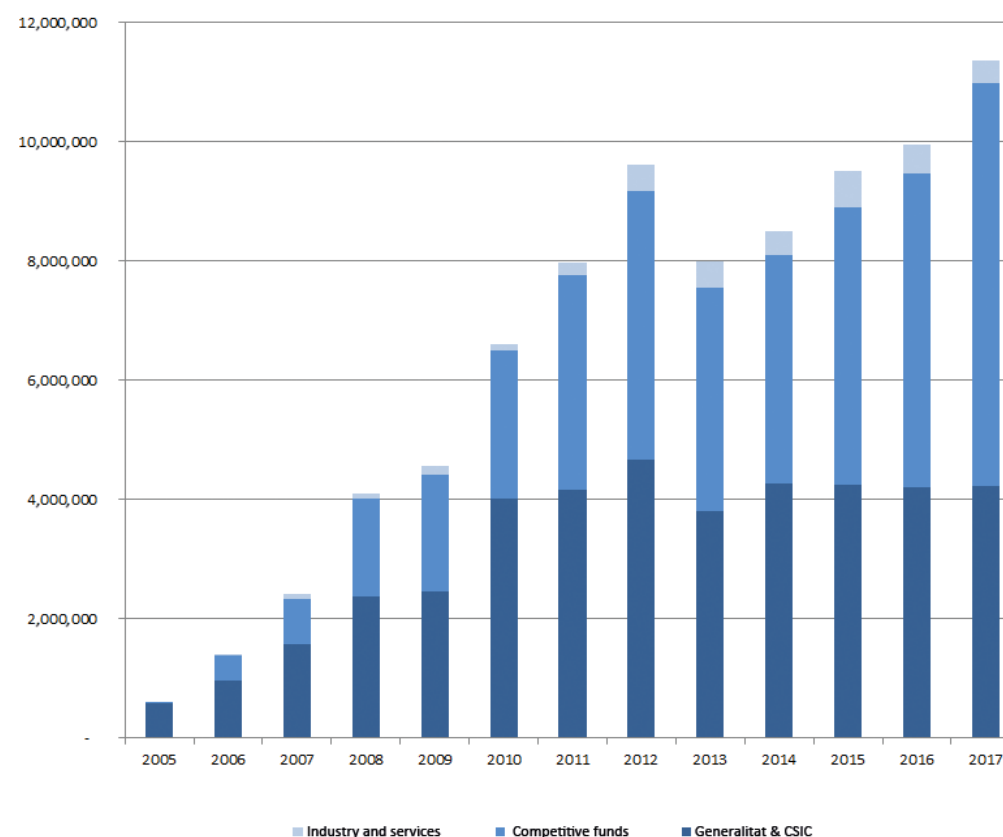
In 2017 the ICN2 Finance Department has continued to roll out the SAP Business One system, developing the web area where budget managers can monitor performance.

This year we have worked towards two goals: the first 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.

### INCOME

The ICN2's total operating funds in 2017 stood at €11,373,309, of which 37% were obtained from the Generalitat de Catalunya and the Spanish National Research Council (CSIC), 60% from competitive funding calls, and 3% from industry and services.

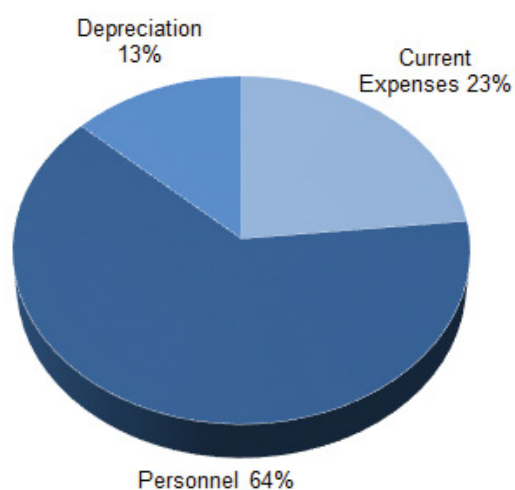
Evolution of ICN2 Operating Funds



## EXPENSES

Total expenditure in 2017 came to €11,060,742, including current expenses, personnel costs and depreciation.

### Expenditure in 2017



## Facilities and Equipment

Total accumulated investment by the ICN2 in scientific equipment, common services and general infrastructure as of year-end 2017 stood at €20,598,459.

During 2017 investment came to a total of €841,319, distributed as follows:

- Firewall security software
- Multi-mode microplate spectrophotometer
- Project management and reporting software
- Transistor characterisation setup
- Vector network analyzer
- Mass spectrometer for CVD graphene
- Compute nodes for HPC data centre
- Pulsed-laser deposition dual-laser setup
- Benchtop centrifuge (Allegra 64R)

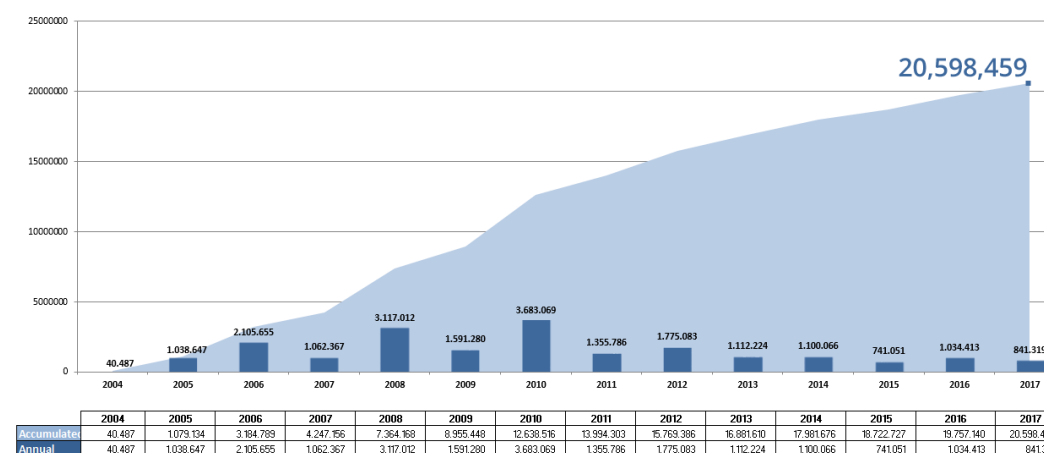
Equipment funded using Spanish ERDF ("FEDER") funds:

- Construction of a biosafety level 2 (BSL-2) laboratory
- Preparation of controlled-environment laboratories for nanofabrication
- Horizontal autoclave for sterilisation (Autester ST DRY PV" 18)
- ATEX certified spark-free fridge



**EUROPEAN UNION**  
European Regional Development Fund

### Evolution of Investments between 2004 and 2017

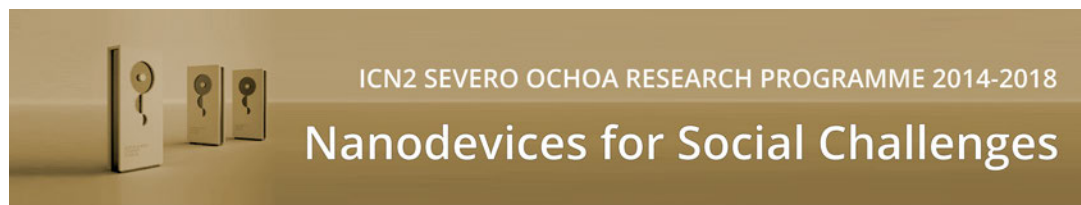


# Our Research





# Severo Ochoa Centre of Excellence



## 3 areas of application



## 4 interdisciplinary approaches



The ICN2 became a Severo Ochoa Centre of Excellence in 2014, earning itself a place alongside the top research centres in Spain. The associated research programme unites the institute's 17 research groups and support division in finding new ways to adapt and transform the wealth of knowledge generated in-house into real-world devices that offer innovative solutions to social challenges.

Based on four interdisciplinary approaches, the programme promotes the transformation of novel materials and know-how into patentable techniques and technologies in the areas of health, the environment, energy and ICT.

Other key areas of work lie in boosting the institute's international profile within academic circles, building on its first forays into technology transfer, and making the institute an attractive place to pursue a career within and beyond research. By doing so the ICN2 becomes more aligned with the needs and expectations of both the market and the research community, and forges ever closer ties with society.

## APPLICATION AREAS

To focus our efforts under the ICN2 Severo Ochoa research programme "Nanodevices for Social Challenges", we identified three core areas that broadly denote fields in which ICN2 research groups can make real contributions to the advancement of knowledge and technology innovation.

### ICT

Information and communication technologies have a direct impact on virtually all aspects of modern society. The new working principles emerging from the study of materials at the nanoscale will enable faster, smaller and more energy-efficient devices. Our vision in this area goes beyond the conventional charge-manipulated-by-electrical-input paradigm to include the exploration of spin, phonons and photons as alternative state variables, and their manipulation using mechanical stress, light and heat.

### Energy

As part of its commitment to a low-carbon society, the EU has set ambitious objectives in energy. The development of novel nano materials, technologies and devices is key to solving the many technological challenges in this area. Graphene plays a leading role, being explored at the ICN2 as a means of boosting the lifetime of solar cells, and improving energy storage and charge transfer in flow batteries. But physical phenomena like ferro-, piezo- and flexoelectricities are also being studied in this context as a means of achieving superior performances and taking lead out of the equation.

### Life

Life is a broad term used to denote ICN2 research in health, food safety and the environment. Specifically, we harness the insights gleaned at the nanoscale to develop super sensitive devices capable of detecting analytes at very low concentrations, in increasingly small samples and with ever shorter turnaround times.

This enables the early detection of illnesses, health risks and pollution, which vastly improves the chances of a successful outcome. The same insights are also used to optimise actions in these areas, all with a view to making the devices environmentally-friendly, portable and low-cost. This in turn opens them up to users in remote locations and developing economies.

## INTERDISCIPLINARY PLATFORMS

We also established four interdisciplinary platforms within the ICN2 Severo Ochoa research programme. These aim to address challenges across the three application areas, while also producing highly relevant knowledge in their own right and developing new experimental and theoretical methodologies, materials and processes for the manufacture and understanding of novel nanostructures.

They have also proved to be great enablers of internal collaboration, bringing together ICN2 members from different areas of technical expertise and scientific disciplines.

### Theory & Simulation

The aim in this work package is to develop a portfolio of computerised modelling tools and algorithms to better understand and simulate the behaviour of matter at the nanoscale, and otherwise provide theoretical support to the ICN2 community across all three application areas.

## Nanomaterials Growth

The growth of new nanomaterials, their combination into multilayered nanocomposites and other hybrid materials, and the functionalisation of their surfaces for various applications lie at the heart of advances in device development. Discoveries in these areas have driven innovation in recent years, the most famous example being that of graphene, though other 2D materials, topological insulators and multifunctional oxides have also played their role. In this platform we devise and refine methodologies for said growth and preparation of materials with novel properties, for use in the three application areas and beyond.

## Nanofabrication

Even once we have the novel materials and a device concept, there is still work to be done. Advanced nanomanufacturing techniques are needed not only to build the devices, but to connect them up to the micro- and macro-scale world.

## Characterisation & Metrology

Last but not least, characterising new nano materials, structures and devices is critical to progress in the ICN2 Severo Ochoa research programme. Work has focused on addressing challenges in dimensional, shape and chemical metrology that affect the reproducibility (and consequent commercial viability) of a nanodevice. The ICN2 has solid in-house expertise in this area, plus an extensive network rooted in numerous EU projects.

[www.icn2.cat/en/severo-ochoa](http://www.icn2.cat/en/severo-ochoa)

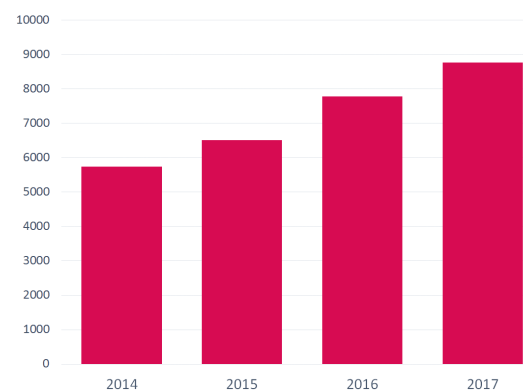
# Publications

Once again the ICN2 has performed well in terms of scientific publications. With 191 original papers published in the most influential journals, the average institutional impact factor (IF) has risen from 6.75 in 2016 to 6.88 in 2017.

We are particularly proud of the fact that 151 of these articles (79%) were accepted for publication in first-quartile journals, while 102 (53%) appeared in first-decile journals. Meanwhile, papers authored by ICN2 researchers were cited 8772 times in 2017.

## CITATIONS

### Evolution of Citations



Source: Scopus

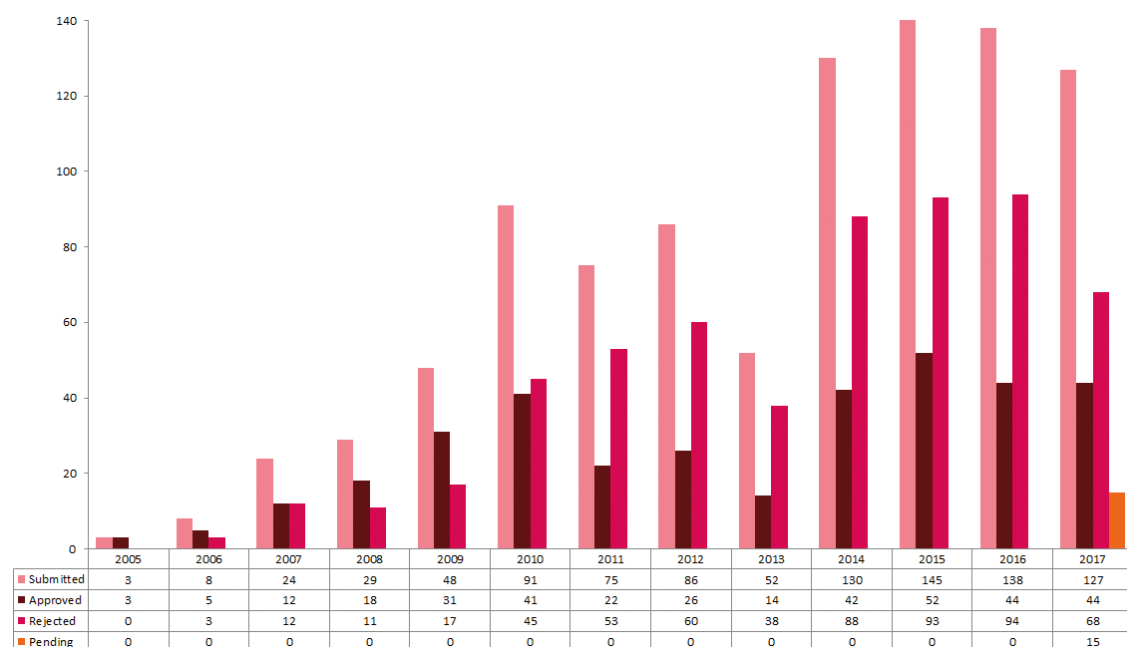
## TOP 10 JOURNALS

Journal	IF	No. articles
<i>Chemical Society Reviews</i>	38.618	1
<i>Progress in Materials Science</i>	31.14	1
<i>Energy and Environmental Science</i>	29.518	2
<i>Advanced Materials</i>	19.791	3
<i>Advanced Energy Materials</i>	16.721	2
<i>ACS Nano</i>	13.942	2
<i>Journal of the American Chemical Society</i>	13.858	2
<i>Nano Letters</i>	12.712	7
<i>Nano Energy</i>	12.343	1
<i>Advanced Functional Materials</i>	12.124	3

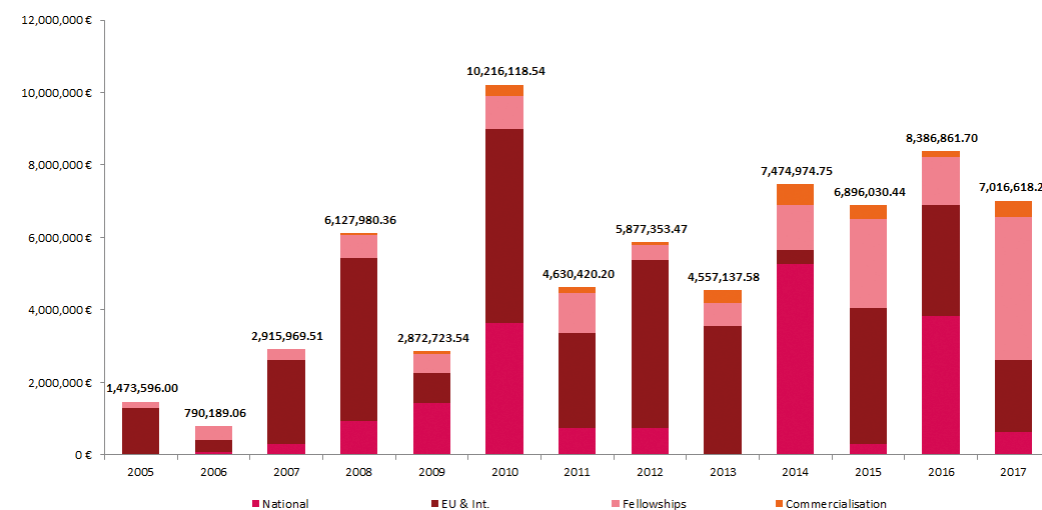
# Projects

In 2017 the ICN2 researcher community submitted slightly fewer proposals than in previous years. However, we can expect our success rate to be in line with previous years once all pending calls are resolved. Meanwhile, income from competitive projects has decreased relative to 2016, which can be explained by the fact that two large national funding calls were launched and resolved in that reporting period.

Outcome of Proposals Submitted by Year  
(as of 15/04/2018)



Evolution of Income from Approved Proposals by Source



Year	National	EU & Int.	Fellowships	Commercialisation	Total	Accumulated
2005	-	1,298,196.00	175,400.00	-	1,473,596.00	1,473,596.00
2006	81,174.06	341,415.00	367,600.00	-	790,189.06	2,263,785.06
2007	297,485.00	2,333,548.90	284,935.61	-	2,915,969.51	5,179,754.57
2008	945,388.69	4,486,646.00	642,236.80	53,708.87	6,127,980.36	11,307,734.93
2009	1,436,035.15	817,276.80	544,832.00	74,579.59	2,872,723.54	14,180,458.47
2010	3,628,829.15	5,368,981.70	892,343.20	325,964.49	10,216,118.54	24,396,577.01
2011	752,896.69	2,615,392.74	1,100,560.77	161,570.00	4,630,420.20	29,026,997.21
2012	741,886.22	4,627,620.00	416,372.05	91,475.20	5,877,353.47	34,904,350.68
2013	-	3,564,229.18	627,672.40	365,236.00	4,557,137.58	39,461,488.26
2014	5,260,418.26	400,143.00	1,228,292.64	586,120.85	7,474,974.75	46,936,463.01
2015	314,048.27	3,729,431.00	2,466,735.17	385,816.00	6,896,030.44	53,832,493.45
2016	3,821,062.00	3,065,066.50	1,320,638.72	180,094.48	8,386,861.70	62,219,355.15
2017	636,509.32	1,974,111.25	3,951,704.72	454,293.00	7,016,618.29	69,235,973.44
	<b>17,915,732.81</b>	<b>34,622,058.07</b>	<b>14,019,324.08</b>	<b>2,678,858.48</b>	<b>69,235,973.44</b>	

# Technology Transfer

In 2017 the Knowledge and Technology Transfer Department furthered its efforts to protect and commercialise ICN2 research results, establishing new R&D and licensing contracts with industry, new collaborations with the private and public sectors, new spin-offs and new networking channels.

## INTELLECTUAL PROPERTY AND SPIN-OFFS

### Four new European patent (EP) applications:

- *Sensors for translocating analytes comprising nanometer or sub-nanometer thick heterostructured functional layers and a method for sensing translocating analytes*  
Nanobiosensors and Bioanalytical Applications Group  
Antoni Homs
- *A system for detecting an analyte from a sample in an analytical test substrate and a portable device for carrying out said detection*  
Nanobioelectronics and Biosensors Group  
Arben Merkoçi Hyka, Ruslan Alvarez, Jahir Orozco
- *A method for tuning the magnetic coercivity of a nanoporous film*  
Magnetic Nanostructures Group  
Josep Nogués
- *Chatecol derivatives and use thereof*  
Nanostructured Functional Materials Group  
Daniel Ruiz-Molina, Josep Sedó, Juan Mancebo

### One Spanish patent (ES) application:

- *A method for tuning the magnetic coercivity of a nanoporous film*  
Magnetic Nanostructures Group  
Josep Nogués

### One UK patent (UK) application:

- *A method for tuning the magnetic coercivity of a nanoporous film*  
Magnetic Nanostructures Group  
Josep Nogués

### Three granted patents:

- *Coating with photochromic properties, method for producing said coating and use thereof applicable to optical articles and glazed surfaces*, granted in Japan
- *Biogas Production*, granted in Europe
- *Graphene-based electroactive nanofluids as liquid electrodes in flow cells*, granted in Spain

### Five international PCT extensions filed:

- *Synthesis of UiO-66 by Spray Drying combined with continuous flow*
- *Ceria nanoparticles for use in the treatment of hepatocellular carcinoma*
- *Película de material polimérico con propiedades termo-fotocrómicas para regulación del color de superficies acristaladas y materiales plásticos*
- *A hybrid hyperthermia device, and methods using the same*
- *A process for the post-synthetic modification of metal organic frameworks*

### Four patent/know-how licensing agreements:

- For the patent *Method of forming an electronic device on a flexible substrate*, signed with ICN2 spin-off Graphenicalab, S.L.
- For the patent *Liposome-based immunotherapy*, signed with the ICN2 spin-off company Ahead Therapeutics, S.L.
- For the know-how related to *paper-based biosensors* co-owned by the ICN2 and ICREA, a licensing agreement was signed with ICN2 spin-off Paperdrop Diagnostics, S.L.
- For the know-how related to *iron encapsulation*, an agreement was signed with the company Lubrizol Advanced Materials, Inc.

### One new spin-off company:

- Ahead Therapeutics, S.L.



## OTHER HIGHLIGHTS

Other technology transfer activities include new contacts and meetings with more than 79 companies, 39 signed NDAs, 5 patent licence discussions, 11 new invention disclosures, 7 signed R&D contracts, 33 R&D services, 15 technology assessments, 2 in-house IP training sessions, 1 new product on the market, 6 new valorisation projects and the evaluation of 6 spin-off companies.

# Research Groups



The ICN2 currently has 17 research groups which together cover much of the breadth of nanoresearch. Each group pursues its own clear lines, while also working towards joint research objectives.

- > Advanced Electron Nanoscopy **p.26**
- > Advanced Electronic Materials and Devices **p.32**
- > Atomic Manipulation and Spectroscopy **p.38**
- > Force Probe Microscopy and Surface Nanoengineering **p.44**
- > Inorganic Nanoparticles **p.50**
- > Magnetic Nanostructures **p.56**
- > NanoBioelectronics and Biosensors **p.64**
- > NanoBiosensors and Bioanalytical Applications **p.70**
- > Nanostructured Functional Materials **p.80**
- > Nanostructured Materials for Photovoltaic Energy **p.88**
- > Novel Energy-Oriented Materials **p.94**
- > Oxide Nanophysics **p.100**
- > Phononic and Photonic Nanostructures **p.104**
- > Physics and Engineering of Nanodevices **p.112**
- > Supramolecular NanoChemistry and Materials **p.118**
- > Theoretical and Computational Nanoscience **p.124**
- > Theory and Simulation **p.128**

# Advanced Electron Nanoscopy Group

## Main Research Lines

- Exploring the limits of physical resolution in advanced electron microscopy and related spectroscopies down to the atomic scale
- Understanding the behaviour of materials at the nano and atomic scales, from their growth mechanisms to their physical and chemical properties
- Design and study of new nanostructures for energy applications at the atomic scale, including the development of in-situ and in-operando TEM experiments to understand the physical and chemical phenomena underlying energy generation
- Analysis of the strain, relaxation and growth mechanisms in semiconductor/superconductor nanowire-based hybrid heterostructures for quantum technologies



## GROUP MEMBERS

**Arbiol Cobos, Jordi**, ICREA Research Professor and Group Leader

**David, Jeremy**, Postdoctoral Researcher

**González Febles, Ana**, Visiting Undergraduate Student

**Grau Carbonell, Albert**, Visiting Master's Student

**Infante Carrió, María Francisca**, Visiting Undergraduate Student

**Koch, Christian**, Undergraduate Fellowship Student

**Martí Sánchez, Sara**, PhD Student,

**Nasiou, Déspina**, Visiting Master's Student

**Samat, Gaël**, Visiting Undergraduate Student

**Tang, Pengyi**, Visiting PhD Student

**Zhang, Ting**, PhD Fellowship Student

## GROUP LEADER



ICREA Research Prof.  
Jordi Arbiol

Prof. Jordi Arbiol was born in Molins de Rei (Catalonia) in 1975. Having graduated in physics from the Universitat de Barcelona (UB) in 1997, he went on to obtain his PhD in transmission electron microscopy as applied to nanostructured materials from this same university in 2001, earning the "European Doctorate" label in recognition of the project's European dimension, as well as the university's extraordinary doctorate award. He then held the position of assistant professor at the UB, before becoming a group leader at the Institut de Ciència de Materials de Barcelona in 2009, as well as the scientific supervisor of this institute's electron microscopy facility. It was here that Prof. Arbiol began his

personal and professional mission to improve Barcelona's baseline electron microscopy infrastructure, a goal he has continued to pursue at the ICN2, which he joined in 2015 as the leader of the Advanced Electron Nanoscopy Group.

In 2017 he became the president of the Spanish Microscopy Society (SME), having been its vice-president from 2013 to 2017 and board member since 2009. He was also appointed by the Barcelona Institute of Science and Technology (BIST) as the scientific supervisor of its strategic multidisciplinary area of Electron Microscopy.

Other recognitions include the 2014 EU40 Materials Prize (E-MRS), the 2014 EMS Outstanding Paper Award and being listed in the Top 40 under 40 Power List (2014) by *The Analytical Scientist*. He currently has more than 295 peer-reviewed publications and more than 11000 citations.



## NEW PROJECTS & MILESTONES

The broad aim of this group is to develop expertise in advanced electron microscopy and related spectroscopies to meet the increasing demand for tools able to observe and analyse the behaviour and properties of materials at the atomic scale.

In 2017 the group established new lines in the design and study of nanostructures for exploitation in energy generation and storage. Specifically it is developing in-situ and in-operando experiments that will offer a window onto the physical and chemical phenomena underlying different energy mechanisms with unprecedented resolution. Through the BIST collaborative project InWOC awarded in 2017 it is already co-developing (with ICIQ) correlative in-situ experiments to characterise heterogeneous water oxidation catalysts for use in water splitting and solar fuels. A similar goal was pursued in the framework of the e-TNT project with IREC and Repsol, which came to an end this year.

Meanwhile a new collaboration begun this year with Microsoft's Copenhagen Q-Station sees the group's expertise applied to the analysis of the structure and complex physical properties of semi/superconducting Majorana nanowires, nanostructures touted to make quantum computing a reality.

The group, through its leader ICREA Prof. Jordi Arbiol, is also significantly involved in efforts to strengthen Catalonia's electron microscopy infrastructure, most recently taking the scientific lead role in a BIST project (BIST MET-CELLS) to acquire two advanced electron microscopies for installation at the ALBA Synchrotron by the end of 2018.

The expansion of the group's capabilities that these synergies will allow, together with the high impact results (plus those not yet reported) in 2017 in the areas of earth-abundant nanomaterials for photoelectrochemical water splitting and hydrogen generation, and novel nanomaterials for quantum technologies leave the ICN2 Advanced Electron Nanoscopy Group well-positioned for a productive 2018.



## PUBLICATIONS

**A prototype reactor for highly selective solar-driven CO<sub>2</sub> reduction to synthesis gas using nanosized earth-abundant catalysts and silicon photovoltaics**, Urbain F., Tang P., Carretero N.M., Andreu T., Gerling L.G., Voz C., Arbiol J., Morante J.R., *Energy and Environmental Science*; **10 (10)**: 2256-2266. 2017. IF: 29.518

**A universal strategy for metal oxide anchored and binder-free carbon matrix electrode: A supercapacitor case with superior rate performance and high mass loading**, Zhang X., Luo J., Tang P., Ye X., Peng X., Tang H., Sun S.-G., Fransaer J., *Nano Energy*; **31**: 311-321. 2017. IF: 12.343

**Charge Transfer Characterization of ALD-Grown TiO<sub>2</sub> Protective Layers in Silicon Photocathodes**, Ros C., Andreu T., Hernández-Alonso M.D., Penelas-Pérez G., Arbiol J., Morante J.R., *ACS Applied Materials and Interfaces*; **9 (21)**: 17932-17941. 2017. IF: 7.504

**Cobalt boride modified with N-doped carbon nanotubes as a high-performance bifunctional oxygen electrocatalyst**, Elumeeva K., Masa J., Medina D., Ventosa E., Seisel S., Kayran Y.U., Genç A., Bobrowski T., Weide P., Arbiol J., Muhler M., Schuhmann W., *Journal of Materials Chemistry A*; **5 (40)**: 21122-21129. 2017. IF: 8.867

**Colloidal Silicon-Germanium Nanorod Heterostructures**, Lu X., De La Mata M., Arbiol J., Korgel B.A., *Chemistry of Materials*; **29 (22)**: 9786-9792. 2017. IF: 9.466

**Enhanced photoelectrochemical water splitting of hematite multilayer nanowire photoanodes by tuning the surface state via bottom-up interfacial engineering**, Tang P., Xie H., Ros C., Han L., Biset-Peiró M., He Y., Kramer W., Rodríguez A.P., Saucedo E., Galán-Mascarós J.R., Andreu T., Morante J.R., Arbiol J., *Energy and Environmental Science*; **10 (10)**: 2124-2136. 2017. IF: 29.518

**Hollow metal nanostructures for enhanced plasmonics: Synthesis, local plasmonic properties and applications**, Genç A., Patarroyo J., Sancho-Parramon J., Bastús N.G., Puentes V., Arbiol J., *Nanophotonics*; **6 (1)**: 193-213. 2017. IF: 4.492

**Inorganic photocatalytic enhancement: Activated RhB Photodegradation by surface modification of SnO<sub>2</sub> Nanocrystals with V<sub>2</sub>O<sub>5</sub>-like species**, Epifani M., Kaciulis S., Mezzi A., Altamura D., Giannini C., Díaz R., Force C., Genç A., Arbiol J., Siciliano P., Comini E., Concina I., *Scientific Reports*; **7**. 2017. IF: 4.259

**Insights into the Performance of Co<sub>x</sub>Ni<sub>1-x</sub>TiO<sub>3</sub> Solid Solutions as Photocatalysts for Sun-Driven Water Oxidation**, Murcia-López S., Moschogiannaki M., Binas V., Andreu T., Tang P., Arbiol J., Jacas Biendicho J., Kiriakidis G., Morante J.R., *ACS Applied Materials and Interfaces*; **9 (46)**: 40290-40297. 2017. IF: 7.504

**Low-Temperature Growth of Axial Si/Ge Nanowire Heterostructures Enabled by Trisilane**, Hui H.Y., De La Mata M., Arbiol J., Filler M.A., *Chemistry of Materials*; **29 (8)**: 3397-3402. 2017. IF: 9.466

**Polybenzoxazine-Derived N-doped Carbon as Matrix for Powder-Based Electrocatalysts**, Barwe S., Andronescu C., Masa J., Ventosa E., Klink S., Genç A., Arbiol J., Schuhmann W., *ChemSusChem*; **10 (12)**: 2653-2659. 2017. IF: 7.226

**Probing the surface reactivity of nanocrystals by the catalytic degradation of organic dyes: The effect of size, surface chemistry and composition**, Piella J., Merkoçi F., Genç A., Arbiol J., Bastús N.G., Puentes V., *Journal of Materials Chemistry A*; **5 (23)**: 11917-11929. 2017. IF: 8.867

**Solution-based synthesis and processing of Sn- and Bi-doped Cu<sub>3</sub>SbSe<sub>4</sub> nanocrystals, nanomaterials and ring-shaped thermoelectric generators**, Liu Y., García G., Ortega S., Cadavid D., Palacios P., Lu J., Ibáñez M., Xi L., De Roo J., López A.M., Martí-Sánchez S., Cabezas I., Mata M.D.L., Luo Z., Dun C., Dobrozhan O., Carroll D.L., Zhang W., Martins J., Kovalenko M.V., Arbiol J., Noriega G., Song J., Wahnón P., Cabot A., *Journal of Materials Chemistry A*; **5 (6)**: 2592-2602. 2017. IF: 8.867

**Solvothermal Synthesis, Gas-Sensing Properties, and Solar Cell-Aided Investigation of TiO<sub>2</sub>-MoO<sub>x</sub> Nanocrystals**, Epifani M., Kaciulis S., Mezzi A., Altamura D., Giannini C., Tang P., Morante J.R., Arbiol J., Siciliano P., Comini E., Concina I., *ChemNanoMat*; **3 (11)**: 798-807. 2017. IF: 2.937

**Surface-Guided Core-Shell ZnSe@ZnTe Nanowires as Radial p-n Heterojunctions with Photovoltaic Behavior**, Oksenberg E., Martí-Sánchez S., Popovitz-Biro R., Arbiol J., Joselevich E., *ACS Nano*; **11 (6)**: 6155-6166. 2017. IF: 13.942

**Ultrathin High Surface Area Nickel Boride (Ni<sub>3</sub>B) Nanosheets as Highly Efficient Electrocatalyst for Oxygen Evolution**, Masa J., Sinev I., Mistry H., Ventosa E., de la Mata M., Arbiol J., Muhler M., Roldan Cuenya B., Schuhmann W., *Advanced Energy Materials*; **7 (17)**. 2017. IF: 16.721

**Unveiling the nucleation & coarsening mechanisms of solution-derived self-Assembled epitaxial Ce<sub>0.9</sub>Gd<sub>0.1</sub>O<sub>2-y</sub> Nanostructures**, Queralto A., De La Mata M., Arbiol J., Hühne R., Obradors X., Puig T., *Crystal Growth and Design*; **17 (2)**: 504-516. 2017. IF: 4.055

## PROJECTS

*e-TNT, e-Nanoscopías y Hetero-Multicapas para Dispositivos y Sistemas Tandem Basados en Nanoestructuras para Transformación de la Energía Solar en Combustibles Solares*, funded by **MINECO**, 01/01/15 to 31/12/17, Jordi Arbiol

*InWoc, In-situ atomic resolution transmission electron microscopy of heterogeneous water oxidation catalysts*, funded by **BIST**, 01/04/17 to 31/12/17, Jordi Arbiol

*Materials characterization of hybrid semi-super Majorana nanowires*, funded by **Microsoft**, 15/10/16 to 30/06/18, Jordi Arbiol

## CONTRIBUTIONS

### Plenary

*Free-standing nanostructures at atomic scale: from growth mechanisms to local properties at the nanoscale*, **International Conference on Electron Microscopy & Allied Techniques & XXXVIII Annual Meeting of EMSI (EMSI 2017)**, Chennai, India, 19/07/17, J. Arbiol

*Semiconductor nanostructures at atomic scale*, **Applied Nanotechnology and Nanoscience International Conference 2017 (ANNIC 2017)**, Rome, Italy, 19/10/17, J. Arbiol

### Keynote

*Free-standing nanostructures at atomic scale: from growth mechanisms to local properties at the nanoscale*, **14<sup>th</sup> International Conference on Nanomaterials and Nanotechnology (Nanomaterials 2017)**, Madrid, Spain, 30/03/17, J. Arbiol

*Free-standing nanostructures at atomic scale: from structure to growth mechanisms and applications*, **Nanoscience & Nanotechnology 2017 (N&N 2017)**, Frascati, Italy, 18/10/17, J. Arbiol

*Free-standing nanostructures at atomic scale: from growth mechanisms to local properties at the nanoscale*, **22<sup>nd</sup> International Conference and Expo on Nanoscience and Molecular Nanotechnology (Nanoscience 2017)**, Frankfurt, Germany, 08/11/17, J. Arbiol

### Invited

*Free-standing nanostructures at atomic scale: from growth mechanisms to local properties at the nanoscale*, **21<sup>st</sup> International Conference on Solid State Ionics (SSI-21)**, Padua, Italy, 19/06/17, J. Arbiol

*Free-standing nanostructures at atomic scale: from growth mechanisms to local properties at the nanoscale*, **Microscience Microscopy Congress (mmc2017)**, Manchester, United Kingdom, 04/07/17, J. Arbiol

### Oral

*Strain Relaxation Mechanisms in ZnSe@ZnTe Core-Shell Nanowires Grown Horizontally from a Guided Growth Approach*, **Microscopy at the Frontiers of Science 2017 (MFS 2017)**, Zaragoza, Spain, 08/09/17, S. Martí-Sánchez, E. Oksenberg, E. Joselevich, J. Arbiol

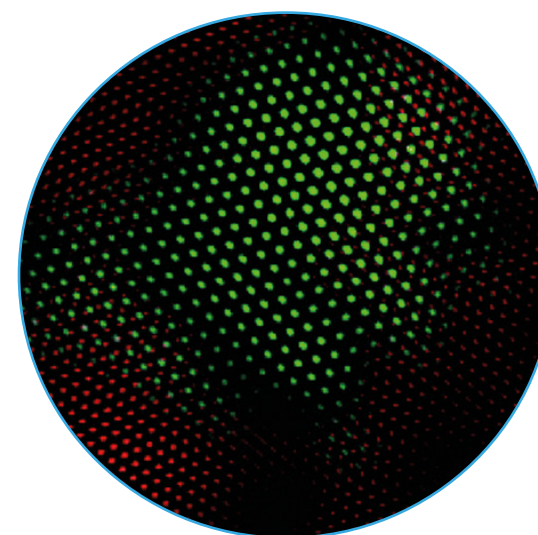
*Bottom-up Engineering of Nanoflake and Nanowire Heterostructures for Energy Storage and Conversion Applications*, **Microscopy at the Frontiers of Science 2017 (MFS 2017)**, Zaragoza, Spain, 08/09/17, P. Tang, H. Xie, C. Ros, L. Han, M. Biset-Peiro, A. Pérez, E. Saucedo, J.R. Galán-Mascarós, T. Andreu, J. Ramon Morante, J. Arbiol

*Strain Relaxation Mechanisms in ZnSe@ZnTe Core-Shell Nanowires Grown Horizontally from a Guided Growth Approach*, **E-MRS Fall Meeting 2017**, Warsaw, Poland, 19/09/17, S. Martí-Sánchez, E. Oksenberg, A. Grau-Carbonell, C. Koch, E. Joselevich, J. Arbiol

### Poster

*Cesium halide nanocrystals towards improved UV-stability solar cell systems*, **Microscopy at the Frontiers of Science 2017 (MFS 2017)**, Zaragoza, Spain, 08/09/17, A. Grau-Carbonell, S. Martí-Sánchez, M. Meyns, P. Shaw, A. Kanaras, A. Cabot, J. Arbiol

*Co-Cu-P and Ni-Co-Cu-P nanocrystals for hydrogen and oxygen evolution reactions*, **Microscopy at the Frontiers of Science 2017 (MFS 2017)**, Zaragoza, Spain, 08/09/17, D. Nasiou, J. Liu, M. Meyns, A. Cabot, J. Arbiol



## DISSEMINATION CONTRIBUTIONS

### Invited conference

*Dialogues on the boundaries of knowledge: Microscopy*, **BIST Founding Conference**, Barcelona, Spain, 31/03/17, J. Arbiol

*Veient els àtoms de prop: UN VIATGE AL NANOMÓN, II Festival of Nanoscience and Nanotechnology: 10alamos9*, Barcelona, Spain, 25/04/17, J. Arbiol

*Free-standing nanostructures at atomic scale: from growth mechanisms to local properties at the nanoscale*, **Universität Bremen**, Bremen, Germany, 02/11/17, J. Arbiol

*Veient els àtoms de prop: UN VIATGE AL NANOMÓN, 22<sup>a</sup> edició de la Setmana de la Ciència, Institut Cavall Bernat*, Terrassa, Spain, 02/11/17, J. Arbiol

*A close look to the atoms: a journey to the nanoworld through advanced electron microscopy*, **Universitat Rovira i Virgili (URV)**, Tarragona, Spain, 15/11/17, J. Arbiol

*Microscòpies Electròniques: com entendre i avançar en la ciència a partir de veure'n els petits detalls*, **Societat Catalana de Química (SCQ)**, Barcelona, Spain, 19/12/17, J. Arbiol

## AWARDS

Prof. Jordi Arbiol was **elected president of the Spanish Microscopy Society (SME)**

María de la Mata (one of the group's former PhD students) receives the **2015-2016 SME Award for the Best PhD in Materials Science**, from the Spanish Microscopy Society (SME)

PengYi Tang was awarded one of the prestigious **DAAD 2017 Scholarships** from the German Academic Exchange Service (DAAD) to perform an internship at the ER-C in Jülich



# Advanced Electronic Materials and Devices Group

## Main Research Lines

- Chemical vapor deposition (CVD) of high quality graphene and transition metal dichalcogenide (e.g. MoS<sub>2</sub>) films
- Fundamental electronic and electrochemical phenomena of 2D materials
- Technology and micro/nanofabrication for advanced electronic devices and systems based on 2D materials
- Bioelectronics and biomedical technologies: cell bioelectronics, flexible implant, neuroprosthetics
- Electronic and electrochemical biosensors



## GROUP LEADER



ICREA Research Prof.  
Jose A. Garrido

Jose A. Garrido is an ICREA research professor and leader of the ICN2 Advanced Electronic Materials and Devices Group, which explores novel electronic materials, such as graphene and other 2D materials, and their potential in electronic and bioelectronic applications.

He received his Master's and PhD degrees in telecommunication engineering from the Universidad Politécnica de Madrid in 1996 and 2000, respectively. From 2001 to 2004 he worked as a postdoc at the Walter Schottky Institute, Technische Universität München (Germany), before becoming the leader of its Functional Carbon Materials Group. He attained his habilitation in experimental physics at this university in 2010 and from 2011 to 2015 held a lecturer (privatdozent) position at its department of physics.

In 2015 Jose A. Garrido joined the ICN2 where, in addition to his role as group leader, he is vice-director and head of the Strategy Development Office. He is also co-leader of the Biomedical Technologies work package of the European Graphene Flagship initiative and coordinator of the EU FET-Proactive project BrainCom.



## GROUP MEMBERS

**Bonaccini Calia, Andrea Prieto**, PhD Student

**Bousquet, Jessica**, Postdoctoral Researcher

**Bullock, Christopher John**, Visiting PhD Student

**De la Cruz Sánchez, José Manuel**, PhD Student

**Del Corro García, Elena**, Postdoctoral Researcher

**Del Valle Macià, Jaume**, Postdoctoral Researcher

**García Cortadella, Ramón**, PhD Student

**Garrido, Jose Antonio**, ICREA Research Professor, Group Leader and Vice-Director

**Hebert, Clement**, Postdoctoral Researcher

**Kunze, Igor**, PhD Student

**Peña Díaz, Marina**, Visiting Master's Student

**Roche Carrasco, Gabriel**, Undergraduate Fellowship Student

**Schäfer, Christian Martin**, Research Assistant

**Schäfer, Nathan**, PhD Student

**Torralla Gombau, Ricard**, Visiting Undergraduate Student

**Viana Casals, Damià**, PhD Student

**Walston, Steven**, Postdoctoral Fellowship Researcher

## NEW PROJECTS & MILESTONES

The Advanced Electronic Materials and Devices team focuses on the study and application of novel electronic materials, with a strong emphasis on carbon materials such as graphene, though it also look as other 2D materials like MoS<sub>2</sub>.

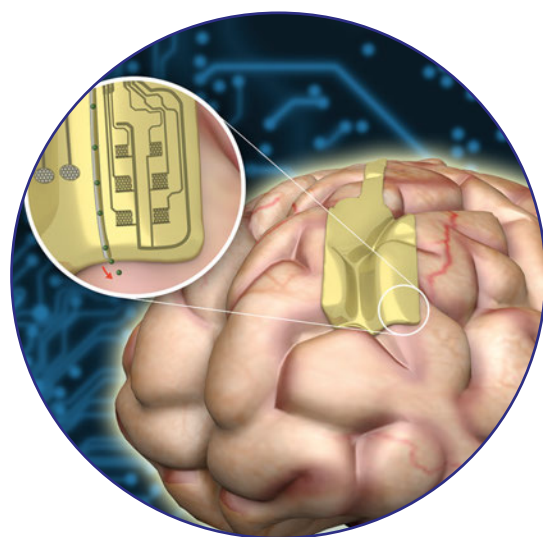
Where 2016 was a year devoted to setting-up our lab space, 2017 has seen the beginning of our scientific harvest. The labs have started to run at nearly full speed and, as a result, there has been significant scientific and technology progress.

2017 has also seen the kick-off of BrainCom, an EU FET Proactive project coordinated by our team with the ultimate goal of developing a new generation of neural prostheses able to restore communication in patients with severely impaired language processing abilities. During the course of this year, our team, together with colleagues at the IMB-CNM (teams led by Anton Guimerà and Rosa Villa), has designed, fabricated and tested the first prototypes of the flexible graphene-based sensors that will be at the core of future brain prostheses used to map brain activity over large areas of the cortex. We have also proposed and studied a very promising new multiplexing technique that aims to reduce the number of cables in high-channel count brain implants.

Within the EU Graphene Flagship project, significant efforts have been devoted to developing a new generation of graphene-based microelectrodes able to stimulate the central and peripheral nervous systems with unprecedented efficacy. The know-how and fabrication procedure related to this material will be protected by a patent shared with the University of Manchester (team led by Kostas Kostarelos).

Besides the two European projects mentioned above, in which our group plays a prominent role, we have also been awarded several new projects in 2017. Our efforts to develop new graphene-based technologies that can be used in retinal prostheses have been rewarded with a multidisciplinary BIST Ignite project (THEIA), developed in collaboration with ICFO, IFAE and the Barraquer Clinic. In addition, our team has received an award from the Fundación Ramon Areces for our project to develop novel flexible technologies to interface with the peripheral nervous system. This three-year project, to be developed alongside the team led by Xavier Navarro of the Universitat Autònoma de Barcelona, was selected in this foundation's eighteenth round of grants for research in the life and earth sciences. This year our group also received support from the Generalitat de Catalunya as a Consolidated Research Group.

At the individual level, Elena del Corro was awarded a Juan de la Cierva fellowship during 2017 – congratulations!



## PUBLICATIONS

**Electrochemical characterization of GaN surface states**, Winnerl A., Garrido J.A., Stutzmann M., *Journal of Applied Physics*; **122 (4)**: 45302. 2017. IF: 2.068

**Fine tuning of optical transition energy of twisted bilayer graphene via interlayer distance modulation**, Del Corro E., Peña-Alvarez M., Sato K., Morales-Garcia A., Bousa M., Mracko M., Kolman R., Pacakova B., Kavan L., Kalbac M., Frank O., *Physical Review B*; **95 (8)**: 85138. 2017. IF: 3.09

**Frequency response of electrolyte-gated graphene electrodes and transistors**, Drieschner S., Guimerà A., Cortadella R.G., Viana D., Makrygiannis E., Blaschke B.M., Vieten J., Garrido J.A., *Journal of Physics D: Applied Physics*; **50 (9)**. 2017. IF: 2.588

**GaN surface states investigated by electrochemical studies**, Winnerl A., Garrido J.A., Stutzmann M., *Applied Physics Letters*; **110 (10)**: 101602. 2017. IF: 3.411

**Graphene Field-Effect Transistors for In Vitro and Ex Vivo Recordings**, Kireev D., Zadorozhnyi I., Qiu T., Sarik D., Brings F., Wu T., Seyock S., Maybeck V., Lottner M., Blaschke B.M., Garrido J., Xie X., Vitusevich S., Wolfrum B., Offenhäusser A., *IEEE Transactions on Nanotechnology*; **16 (1)**: 140-147. 2017. IF: 2.485

**Graphene in the Design and Engineering of Next-Generation Neural Interfaces (review)**, Kostarelos K., Vincent M., Hebert, C., Garrido J.A., *Advanced Materials*; **29**: 1700909. 2017. IF: 15.78

**Interfacing neurons on carbon nanotubes covered with diamond**, Seyock S., Maybeck V., Scorsone E., Rousseau L., Hébert C., Lissorgues G., Bergonzo P., Offenhäusser A., *RSC Advances*; **7 (1)**: 153-160. 2017. IF: 3.108

**Mapping brain activity with flexible graphene micro-transistors**, Blaschke B.M., Tort-Colet N., Guimerà-Brunet A., Weinert J., Rousseau L., Heimann A., Drieschner S., Kempski O., Villa R., Sanchez-Vives M.V., Garrido J.A., *2D Materials*; **4 (2)**: 25040. 2017. IF: 6.937

**Protecting a Diamond Quantum Memory by Charge State Control**, Pfender M., Aslam N., Simon P., Antonov D., Thiering G., Burk S., Fávoro De Oliveira F., Denisenko A., Fedder H., Meijer J., Garrido J.A., Gali A., Teraji T., Isoya J., Doherty M.W., Alkauskas A., Gallo A., Grüneis A., Neumann P., Wrachtrup J., *Nano Letters*; **17 (10)**: 5931-5937. 2017. IF: 12.712

**Tuning the electronic properties of monolayer and bilayer transition metal dichalcogenide compounds under direct out-of-plane compression**, García Á.M., Corro E.D., Kalbac M., Frank O., *Physical Chemistry Chemical Physics*; **19 (20)**: 13333-13340. 2017. IF: 4.123

## PROJECTS

*BrainCom, High-density cortical implants for cognitive neuroscience and rehabilitation of speech using braincomputer interface, (H2020-FETPROACT-2016-2017), funded by EC, 01/12/16 to 30/11/21, Jose A. Garrido*

*Theia, Towards the implementation of micro-electrode array for retinal prosthesis, funded by BIST, 01/04/17 to 31/12/17, Jose A. Garrido*

*Graphene-based flexible neural interfaces for the peripheral nervous system, funded by Fundacion Ramón Areces, 02/03/17 to 01/03/20, Jose A. Garrido*

*GrapheneCore1, Graphene-based disruptive technologies (H2020-Adhoc-2014-20), funded by EC, 01/04/16 to 31/03/18, Jose A. Garrido*

### Keynote

*Graphene technologies for bioelectronics and neuroprosthetics*, **SPIE 2017 Microtechnologies**, Barcelona, Spain, 10/05/2017, J.A. Garrido

*Graphene technologies for bioelectronics and neuroprosthetics*, **Graphene Week 2017**, Athens, Greece, 27/09/2017, J.A. Garrido

### Invited

*Graphene technologies for bioelectronics and neuroprosthetics*, **Graphene 2017**, Barcelona, Spain, 28-31/03/17, J.A. Garrido

*Graphene technologies for bioelectronics and neuroprosthetics*, **Swiss NanoConvention 2017**, Fribourg, Switzerland, 30/05/2017, J.A. Garrido

*Graphene Bioelectronics*, talk at **Manchester University**, Manchester, United Kingdom, 16-18/10/17, J.A. Garrido

### Oral

*Flexible solution-gated graphene field-effect transistor arrays for in vivo recording of neural signals*, **Graphene 2017**, Barcelona, Spain, 28-31/03/17, C. Hébert

*Graphene flexible electronics for biomedical technologies*, **Severo Ochoa-BIST Visitors**, Bellaterra, Spain, 01/06/2017, A. Bonaccini

*Bidirectional cell interfacing with graphene electrodes*, **III Severo Ochoa Scientific Workshop**, Bellaterra, Spain, 13-14/06/17, D. Viana

*Integration of MoS<sub>2</sub> and graphene technologies for flexible electronics*, **III Severo Ochoa Scientific Workshop**, Bellaterra, Spain, 13-14/06/17, I. Kunze

*Optimization of S/N in Graphene SGFETs for Sensing of Neural Signals*, **III Severo Ochoa Scientific Workshop**, Bellaterra, Spain, 13-14/06/17, R. García

### Poster

*1/f noise characterization of graphene-based neural sensors*, **Graphene 2017**, Barcelona, Spain, 28-31/03/17, B. Bonaccini, R.García, C. Hébert, E. Del Corro, D. Viana, A. Guimerà, X. Illa, E. Masvidal, R. Villa, J.A. Garrido

*1/f noise characterization of graphene-based neural sensors*, **III Severo Ochoa Scientific Workshop**, Bellaterra, Spain, 13-14/06/17, A. Bonaccini, R.García, C. Hébert, E. Del Corro, D. Viana, A. Guimerà, X. Illa, E. Masvidal, R. Villa, J.A. Garrido

*Bidirectional cell interfacing with graphene electrodes*, **III Severo Ochoa Scientific Workshop**, Bellaterra, Spain, 13-14/06/17, D. Viana, C. Bullock, S. Walston, X. Illa, C. Hébert, J. del Valle, A. Bonaccini, A. Suárez, A. Guimerà, J. A. Garrido

*Integration of MoS<sub>2</sub> and graphene technologies for flexible electronics*, **III Severo Ochoa Scientific Workshop**, Bellaterra, Spain, 13-14/06/17, I. Kunze, E. del Corro, J.M. Caceido, C. Hébert, J. Santiso, J.A. Garrido

*Metalorganic Chemical Vapour Deposition of MoS<sub>2</sub>*, **Graphene 2017**, Barcelona, Spain, 28-31/3/17, I. Kunze, E. Del Corro, J.M Caicedo, J. Bousquet, C. Hébert, J. Santiso, J.A. Garrido

*Next-Generation Brain Computer Interfaces based on Graphene*, **2017 Annual Whitaker Grantee Enrichment Seminar**, Lisbon, Portugal, 24-28/4/17, S. Walston, D. Viana, C. Bullock, X. Illa, J.A. Garrido

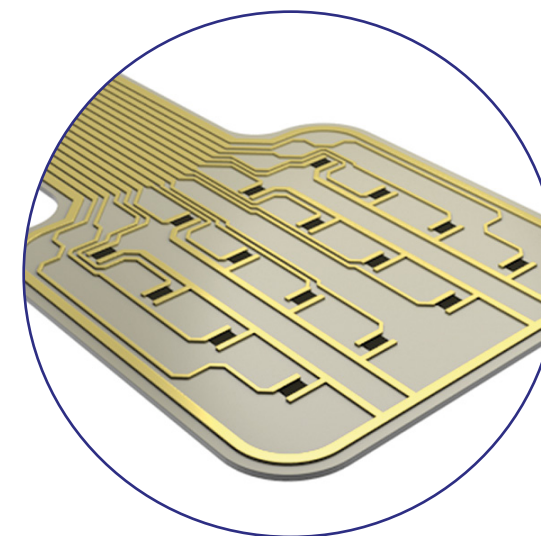
*Optimization of S/N in Graphene SGFETs for Sensing of Neural Signals*, **III Severo Ochoa Scientific Workshop**, Bellaterra, Spain, 13-14/06/17 R. Garcia, A. Bonaccini, E. Masvidal, A. Guimerà, J.A. Garrido

*Transparent array of graphene SGFETs for in vitro electrophysiology*, **Graphene 2017**, Barcelona, Spain, 28-31/3/17, J. De la Cruz, X. Illa, E. del Corro, C. Hébert, J.A. Garrido



### PARTICIPATED CONGRESSES

**3<sup>rd</sup> Scientific Meeting of BNC-b PhD students in nanoscience**, Bellaterra, Spain, 07-09/11/17, Organising Committee, J.A. Garrido



# Atomic Manipulation and Spectroscopy Group

## Main Research Lines

- Metal-organic hybrid interfaces
- Graphene nanostructures
- Topological insulators



## GROUP LEADER



ICREA Research Prof.  
Aitor Mugarza

Prof. Aitor Mugarza graduated in physics in 1997, before earning his PhD in the same field in 2002, both at the Euskal Herriko Unibertsitatea (University of the Basque Country). He was awarded a Marie Curie Fellowship to work as a postdoctoral scientist at the Lawrence Berkeley National Laboratory (USA) and the Institut de Ciència de Materials de Barcelona (ICMAB). He joined the former Catalan Institute of Nanotechnology in 2007 with a Ramon y Cajal Fellowship. In 2013 he became group leader of the Atomic Manipulation and Spectroscopy Group at the ICN2. He has been an ICREA Research Professor since 2015.

His research activity is based on the study of quantum electronic and magnetic phenomena at the nanoscale and the development of strategies for their manipulation with atomic precision. By combining scanning tunnelling microscopy techniques with spectroscopy using synchrotron radiation, he correlates microscopic phenomena to macroscopic observables for the characterisation and design of new materials and devices. He is currently focused on novel materials including molecular and graphene nanostructures, topological insulators and other 2D materials with strong spin-orbit interactions.



## GROUP MEMBERS

**Carbonell Sanromà, Eduard**, Visiting PhD Student

**Gastaldo, Michele**, PhD Student

**González Cuxart, Marc**, Severo Ochoa PhD Student

**Kimouche, Amina**, Postdoctoral Researcher

**Moreno Sierra, César**, Senior Researcher

**Mugarza Ezpeleta, Aitor**, ICREA Research Professor and Group Leader

**Paradinas Aranjuelo, Markos**, Laboratory Engineer

**Schirone, Stefano**, PhD Student

**Tenorio Tuñas, María**, Visiting Undergraduate Student

**Valbuena Martínez, Miguel Angel**, Postdoctoral Researcher

## NEW PROJECTS & MILESTONES

The work carried out by the Atomic Manipulation and Spectroscopy Group in 2017 has focused mainly on the synthesis and characterisation of carbon-based nanostructures, hybrid metal-organic networks and ferromagnetic impurities on topological insulators.

As part of our ongoing research on the synthesis of graphene nanoislands, we have developed a method to heal ill-defined polycrystalline structures into shape-selected single nanocrystals. We have also been exploring methods to tune the structural and electronic properties of these nanoislands by intercalating noble metals between the island and the nickel catalyst substrate, with the aim of exploring edge magnetism and electron confinement phenomena. Within the framework of the FUNMOLDEV project funded by the Spanish Ministry of Economy, Industry and Competitiveness (MINECO), we have been exploring methods for the on-surface synthesis of one- and two-dimensional graphene-based structures (nanoribbons and nanoporous membranes, respectively). We are currently studying the transfer of these structures onto gateable insulating substrates, fabricating and characterising three-terminal devices in collaboration with the ICN2 Physics and Engineering of Nanodevices Group. In 2017 we also began to explore the potential application of graphene nanoribbons in gate-controlled plasmonic devices through a collaborative BIST Ignite project with ICFO. Last but not least, we have also devoted some attention to the magnetic phenomena occurring at the surface of topological insulators, with a view to achieving its control using ligand chemistry to tune interfacial interactions.

## PUBLICATIONS

**Electronic Structure of Titanylphthalocyanine Layers on Ag(111)**, Lerch A., Fernandez L., Ilyn M., Gastaldo M., Paradinas M., Valbuena M.A., Mugarza A., Ibrahim A.B.M., Sundermeyer J., Höfer U., Schiller F., *Journal of Physical Chemistry C*; **121 (45)**: 25353-25363. 2017. IF: 4.46

**Growth of Twin-Free and Low-Doped Topological Insulators on BaF<sub>2</sub>(111)**, Bonell F., Cuxart M.G., Song K., Robles R., Ordejón P., Roche S., Mugarza A., Valenzuela S.O., *Crystal Growth and Design*; **17 (9)**: 4655-4660. 2017. IF: 4.055

**Inductively coupled remote plasma-enhanced chemical vapor deposition (rPE-CVD) as a versatile route for the deposition of graphene micro- and nanostructures**, Cuxart M.G., Šics I., Goñi A.R., Pach E., Sauthier G., Paradinas M., Foerster M., Aballe L., Fernandez H.M., Carlino V., Pellegrin E., *Carbon*; **117**: 331-342. 2017. IF: 6.337

**Kondo screening of the spin and orbital magnetic moments of Fe impurities in Cu**, Joly L., Kappler J.-P., Ohresser P., Saintavit P., Henry Y., Gautier F., Schmerber G., Kim D.J., Goyhenex C., Bulou H., Bengone O., Kavich J., Gambardella P., Scheurer F., *Physical Review B*; **95 (4)**. 2017. IF: 3.836

**Partial oxidation in a dense phase sub-monolayer of Fe-phthalocyanine on Ag(110)**, Bartolomé E., Bartolomé J., Sedona F., Herrero-Albillos J., Lobo J., Piantek M., García L.M., Panighel M., Mugarza A., Sambì M., Bartolomé F., *Solid State Phenomena*; **257**: 219-222. 2017. IF: 0.493

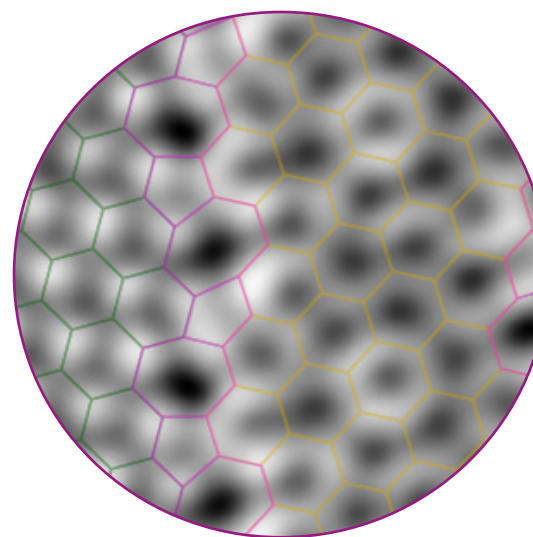
**Symmetry forbidden morphologies and domain boundaries in nanoscale graphene islands**, Parreiras S.O., Gastaldo M., Moreno C., Martins M.D., Garcia-Lekue A., Ceballos G., Paniago R., Mugarza A., *2D Materials*; **4 (2)**. 2017. IF: 6.937

## PROJECTS

2014 SGR AMU, funded by **AGAUR**, 01/01/14 to 30/04/17, Aitor Mugarza

*FunMolDev, Nanoestructuras Moleculares Funcionales para Dispositivos Optoelectrónicos: Hacia dispositivos de 3 terminales*, funded by **MINECO**, Ref. MAT2016-78293-C6-2-R, 30/12/16 to 29/12/19, Aitor Mugarza

*Nirgraph, Near-infrared Graphene Optoelectronic Devices with Atomically Controlled Nanoestructures*, funded by **BIST**, 01/04/17 to 31/12/17, Aitor Mugarza



## CONTRIBUTIONS

### Invited

*Spin-dependent electron scattering in 2D electron systems*, **Nanospain**, San Sebastian, Spain, 07-10/03/17, A. Mugarza

*Manipulating the charge and spin of single molecules by chemical doping*, **Operating Quantum States in Atoms and Molecules at Surfaces (QMol)**, Ascona, Switzerland, 10-14/09/17, A. Mugarza

*Magnetic dopants on the surface of Rashba alloys and topological insulators*, **2D Materials and Interfaces for Spintronics, First Taiwan-Spain Workshop**, Bellaterra, Spain, 21-23/10/17, M. A. Valbuena

*Charge and spin manipulation at hybrid organic/metal and organic/topological insulator interfaces*, **Technical University of Dortmund**, Dortmund, Germany, 16/11/17, A. Mugarza

### Oral

*Combining surface-guiding and functionalization for the self-assembly of graphene nanoribbon superstructures*, **Workshop on SPM & On-Surface Chemistry**, Prague, Czech Republic, 22-23/05/17, C. Moreno, M. Panighel, M. Vilas, D. Peña, G. Ceballos, A. Mugarza

*Electronic and Magnetic Properties of Atoms and Organic Molecules on Strong Spin-Orbit Coupling Surfaces*, **III Severo Ochoa Scientific Workshop**, Bellaterra, Spain, 12-13/06/17, M. A. Valbuena

*Topological defect boundaries in graphene nanoislands*, **13<sup>th</sup> European Conference on Surface Crystallography and Dynamics (ECSCD - 13)**, Donostia-San Sebastian, Spain 19-21/06/17, S.O. Parreiras, M. Gastaldo, C. Moreno, M.D. Martins, G. Ceballos, R. Paniago, A. Mugarza

*Magnetic anisotropy and electronic structure of molecular networks on topological insulators*, **Magnetic Frontiers: Topological Insulators**, Nancy, France, 18-21/09/17, M.G. Cuxart, M.A. Valbuena, F. Bonell, C. Moreno, J. Cruz, H. Xu, I. Imaz, D. MasPOCH, C. Nistor, P. Gargiani, P. Gambardella, S.O. Valenzuela, A. Mugarza

*Magnetic anisotropy of 3d individual atoms on a surface with strong Rashba spin-orbit interaction*, **VIII AUSE Congress and III Alba User's Meeting**, Madrid, Spain, 9-11/10/17, M. A. Valbuena, R. Robles, S. Schirone, S. Godey, A. Barla, C. Nistor, L. Persichetti, P. Gargiani, P. Gambardella, A. Mugarza

### Poster

*Topological defect boundaries in graphene nanoislands*, **Graphene and 2D Materials 2017**, Barcelona, Spain, 29-31/03/17, S.O. Parreiras, M. Gastaldo, C. Moreno, M.D. Martins, G. Ceballos, R. Paniago, A. Mugarza

*Superlattices of ultra-long graphene nanoribbons by on-surface synthesis*, **Graphene 2017**, Barcelona, Spain, 28-31/03/17, C. Moreno, M. Panighel, M. Vilas, D. Peña, G. Ceballos, A. Mugarza

*Electronic and Magnetic Properties of Atoms and Organic Molecules on Strong Spin-Orbit Coupling Surfaces*, **III Severo Ochoa Scientific Workshop**, Bellaterra, Spain, 12-13/06/17, M.A. Valbuena

*Magnetic properties of transition metal atoms on a surface with strong Rashba spin-orbit interaction*, **Operating Quantum States in Atoms and Molecules at Surfaces Q-Mol**, Ascona, Switzerland, 10-14/09/17, M.A. Valbuena, R. Robles, S. Schirone, A. Barla, S. Godey, C. Nistor, L. Persichetti, P. Gargiani, P. Gambardella, A. Mugarza

*Magnetic anisotropy and electronic structure of molecular networks on topological insulators*, **Operating Quantum States in Atoms and Molecules at Surfaces (QMol)**, Ascona, Switzerland, 10-14/09/17, M.G. Cuxart, M.A. Valbuena, F. Bonell, C. Moreno, J. Cruz, H. Xu, I. Imaz, D. MasPOCH, C. Nistor, P. Gargiani, P. Gambardella, S.O. Valenzuela, A. Mugarza

*Twin-free  $\text{Bi}_2\text{Te}_3$  thin films grown by molecular beam epitaxy*, **Magnetic Frontiers: Topological Insulators**, Nancy, France, 18-21/09/17, F. Bonell, M.G. Cuxart, G. Ceballos, A. Mugarza, S.O. Valenzuela

*Controlling size and self-assembly of graphene nanoribbons by templating and functionalization*, **FISMAT 2017**, Trieste, Italy, 01-05/10/17, M. Panighel, C. Moreno, S. Quiroga, M. Vilas, E. Guitián, D. Pérez, A. Garcia-Lekue, D. Peña, G. Ceballos, A. Mugarza

*Engineering edge structure and electronic properties of graphene nanoislands*, **Workshop on 2D Materials and Interfaces for Spintronics**, Barcelona, Spain, 23-27/10/17, M. Gastaldo, G. Ceballos, A. Mugarza

*Magnetic anisotropy and electronic structure of molecular networks on topological insulators*, **Taiwan-Spain Workshop on 2D Materials and Interfaces for Spintronics**, Bellaterra, Spain, 23-25/10/17, M.G. Cuxart, M.A. Valbuena, F. Bonell, C. Moreno, J. Cruz, H. Xu, I. Imaz, D. MasPOCH, C. Nistor, P. Gargiani, P. Gambardella, S.O. Valenzuela, A. Mugarza

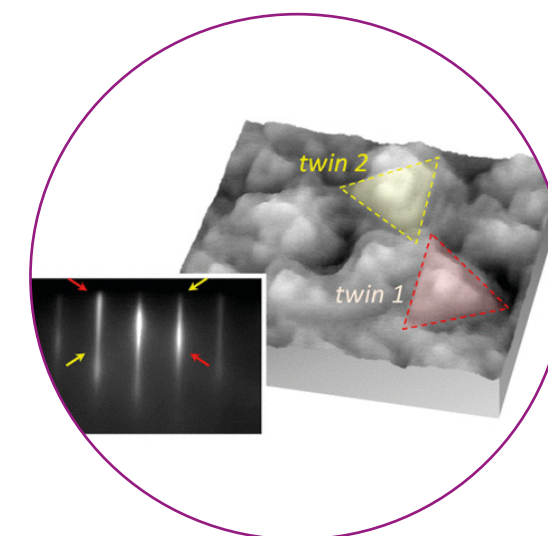
## DISSEMINATION CONTRIBUTIONS

*Somos Científicos, Sácanos de aquí. (EDUCAIXA)*, Spain, 01/11/17, M.G. Cuxart

*¿Qué es nanotecnología?*, **Escola Progrés**, Barcelona, Spain, 11/17, C. Moreno

## COURSES

Aitor Mugarza, *Local Probe Microscopies*. **Master's in Advanced Nanoscience and Nanotechnology**, Universitat Autònoma de Barcelona



# Force Probe Microscopy and Surface Nanoengineering Group

## Main Research Lines

- Force probe spectroscopy and metrology
- Self-sustained motion and catalytic micropumps
- Interfacial water
- Polymer-based interfaces
- Nanoparticles of organic superconductors



## GROUP LEADER



CSIC Scientific Researcher Dr Jordi Fraxedas

Jordi Fraxedas (Tarragona, 1962) graduated in physics from the University of Zaragoza in 1985 and obtained his PhD (Dr rer. nat.) in 1990 from the Universität Stuttgart (Germany). His thesis work was performed at the Max Planck Institut for Solid State Research and at the Berliner Speicherring für Synchrotronstrahlung (BESSY), under the supervision of Prof. M. Cardona.

After holding a postdoctoral position at the European Synchrotron Radiation Facility (ESRF) in Grenoble (France) and an established researcher position at the European Laboratory for Particle Physics (CERN) in Geneva (Switzerland), he joined the Institut de Ciència de Materials de Barcelona (ICMAB-CSIC) in 1995. He later worked as a research associate at the Centre National de la Recherche Scientifique (CNRS) in 2002.

His research activity is focused on interfacial phenomena and surface science. He has co-authored more than 130 peer-reviewed scientific articles and published the books *Molecular Organic Materials: From Molecules to Crystalline Solids* (Cambridge University Press, 2006), *Water at Interfaces: A Molecular Approach* (Taylor and Francis CRC, 2014) and *Molecular Materials: Preparation, Characterization, and Applications* (Taylor and Francis/CRC 2017).



## GROUP MEMBERS

**Bastos Arrieta, Julio**, Visiting Postdoctoral Researcher

**Colás Ortiz, Oriol**, Visiting Master's Student

**Contreras Encinas, M<sup>o</sup> Carmen**, Visiting Undergraduate Student

**Esplandiu Egido, María José**, CSIC Tenured Scientist

**Evangelio Araujo, Laura**, Visiting PhD Student

**Fraxedas Calduch, Jordi**, CSIC Scientific Researcher and Group Leader

**Gramazio, Federico**, PhD Student

**Latorre Lázaro, Núria**, Visiting Undergraduate Student

**Lorenzoni Galizia, Matteo**, Postdoctoral Researcher

**Martínez García, Pedro**, Visiting Master's Student

**Pach, Elzbieta**, Technician

**Sarrià Pascual, Alba**, Visiting Undergraduate Student

**Seco Guix, Marc**, Visiting Master's Student

**Tiemann, Daniel**, Research Engineer

**Verdaguer Prats, Albert**, CSIC Tenured Scientist



## NEW PROJECTS & MILESTONES

The group has participated in the European project Nanoscience Foundries and Fine Analysis (NFFA-EUROPE), where a prototype of a fast-scan AFM is being developed and successfully tested for scan frequencies above two frames per second. At the Spanish level, the group has participated in the project entitled Light-induced motion of micro-nano/objects in water, supported by the Spanish Ministry of Economy, Industry and Competitiveness (MINECO), to study the mass transport of water induced via electro-kinetic and diffusion-osmotic processes.



## PUBLICATIONS

**A statistical analysis of nanocavities replication applied to injection moulding**, Pina-Estany J., Colominas C., Fraxedas J., Llobet J., Perez-Murano F., Puigoriol-Forcada J.M., Ruso D., Garcia-Granada A.A., *International Communications in Heat and Mass Transfer*; **81**: 131-140. 2017. IF: 3.718

**Encapsulation of two-dimensional materials inside carbon nanotubes: Towards an enhanced synthesis of single-layered metal halides**, Sandoval S., Pach E., Ballesteros B., Tobias G., *Carbon*; **123**: 129-134. 2017. IF: 6.337

**Evaluation of the immunological profile of antibody-functionalized metal-filled single-walled carbon nanocapsules for targeted radiotherapy**, Perez Ruiz De Garibay A., Spinato C., Klippstein R., Bourgoignon M., Martincic M., Pach E., Ballesteros B., Ménard-Moyon C., Al-Jamal K.T., Tobias G., Bianco A., *Scientific Reports*; **7**. 2017. IF: 4.259

**Filling Single-Walled Carbon Nanotubes with Lutetium Chloride: A Sustainable Production of Nanocapsules Free of Nonencapsulated Material**, Kierkowicz M., González-Domínguez J.M., Pach E., Sandoval S., Ballesteros B., Da Ros T., Tobias G., *ACS Sustainable Chemistry and Engineering*; **5 (3)**: 2501-2508. 2017. IF: 5.951

**Functional dependence of resonant harmonics on nanomechanical parameters in dynamic mode atomic force microscopy**, Gramazio F., Lorenzoni M., Pérez-Murano F., Trinidad E.R., Staufer U., Fraxedas J., Beilstein *Journal of Nanotechnology*; **8 (1)**. 2017. IF: 3.127

**Identifying the nature of surface chemical modification for directed self-assembly of block copolymers**, Evangelio L., Gramazio F., Lorenzoni M., Gorgoi M., Espinosa F.M., García R., Pérez-Murano F., Fraxedas J., *Beilstein Journal of Nanotechnology*; **8 (1)**. 2017. IF: 3.127

**In Situ Determination of the Water Condensation Mechanisms on Superhydrophobic and Superhydrophilic Titanium Dioxide Nanotubes**, Macias-Montero M., Lopez-Santos C., Filippin A.N., Rico V.J., Espinos J.P., Fraxedas J., Perez-Dieste V., Escudero C., Gonzalez-Elipe A.R., Borrás A., *Langmuir*; **33 (26)**: 6449-6456. 2017. IF: 3.833

**Inductively coupled remote plasma-enhanced chemical vapor deposition (rPE-CVD) as a versatile route for the deposition of graphene micro- and nanostructures**, Cuxart M.G., Šics I., Goñi A.R., Pach E., Sauthier G., Paradinas M., Foerster M., Aballe L., Fernandez H.M., Carlino V., Pellegrin E., *Carbon*; **117**: 331-342. 2017. IF: 6.337

**Leucine zipper motif inspiration: A two-dimensional leucine Velcro-like array in peptide coordination polymers generates hydrophobicity**, Rodríguez-Hermida S., Evangelio E., Rubio-Martínez M., Imaz I., Verdaguer A., Juanhuix J., Maspoch D., *Dalton Transactions*; **46 (34)**: 11166-11170. 2017. IF: 4.029

**Petrographic and geochemical evidence for multiphase formation of carbonates in the Martian orthopyroxenite Allan Hills 84001**, Moyano-Camero C.E., Trigo-Rodríguez J.M., Benito M.I., Alonso-Azcárate J., Lee M.R., Mestres N., Martínez-Jiménez M., Martín-Torres F.J., Fraxedas J., *Meteoritics and Planetary Science*; **52 (6)**: 1030-1047. 2017. IF: 2.391

**Photochemically Activated Motors: From Electrokinetic to Diffusion Motion Control**, Zhang K., Fraxedas J., Sepulveda B., Esplandiú M.J., *ACS Applied Materials and Interfaces*; **9 (51)**: 44948-44953. 2017. IF: 7.504

**Special Issue European Conference on Surface Science 2015**, J. Fraxedas, *Appl. Surf. Sci.*; **391**: 1-2. 2017



## BOOKS

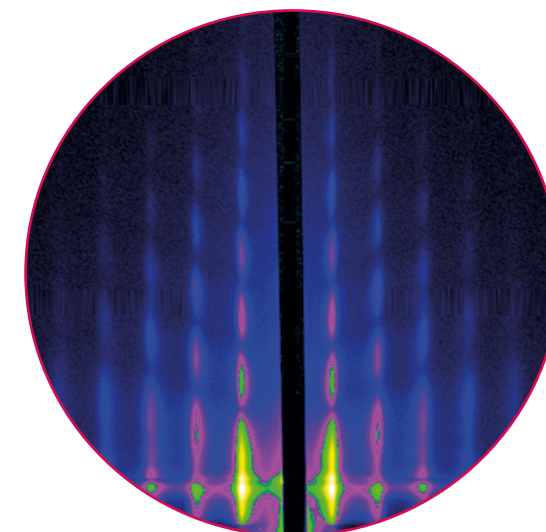
**Molecular Materials: Preparation, Characterization, and Applications**, S. V. Malhotra, B. L. V. Prasad and J. Fraxedas (Eds.), 316p. Ed. CRC Press / Taylor and Francis, FL, USA (2017). ISBN: 978-1-4822-4595-0



## PROJECTS

*Nanoscòpia i Nanoenginyeria de Superfícies*, funded by **AGAUR**, 01/01/14 to 30/04/17, Jordi Fraxedas

*Simuove, Movimiento de Micro/nano-objetos de agua inducido por luz*, funded by **MINECO**, 01/01/16 to 31/12/18, Jordi Fraxedas and María José Esplandiú





## CONTRIBUTIONS

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### Invited

*Experimental characterization of dimensionality-based functional polymer films*, **SurfCoat Korea 2017**, Seoul, Republic of Korea, 29-31/03/17, J. Fraxedas

*Determination of nanomechanical properties of surfaces using higher harmonics of AFM cantilevers*, **14<sup>th</sup> International Conference on Nanosciences & Nanotechnologies**, Thessaloniki, Greece, 04-07/07/17, J. Fraxedas, F. Gramazio, M. Lorenzoni, L. Evangelio, M. Fernández-Regúlez, F. Pérez-Murano, E. Rull Trinidad, U. Staufer

### Oral

*Micro/Nanomachines self-propelled by chemical gradients: from electrokinetics to diffusion control*, **International Conference on Micro and Nanomachines (MNM2017)**, Wuhan, China, 01/08/2017, K. Zhang, J. Fraxedas, B. Sepulveda, M.J. Esplandiu

*Self-assembly of block copolymer thin films as revealed by GISAXS*, **VIII Ause Congress And III Alba User's Meeting**, Madrid, Spain, 09-11/10/17, J. Fraxedas, L. Evangelio, M. Fernández-Regúlez, S. Gottlieb, G. Rius, F. PérezMurano, H. Amenitsch, E. Gutiérrez, A. Nogales, M. C. García-Gutiérrez, T. Ezquerro

## Poster

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*CVD Graphene shape evolution during growth: Impact of the in-situ increased hydrogen partial pressure*, **Graphene 2017 Conference, Barcelona**, Spain, 01/03/17, Z.M.Gebeyehu, M.V. Costache, M.J. Esplandiu, S.O. Valenzuela

*Simulations and testing of polymer replication on nanoscale*, **4<sup>th</sup> Polymer Replication on Nanoscale**, Aachen, Germany, 8-9/05/17, O. Muntada-Lopez, J.Pina-Estany, J.Fraxedas, C. Colominas, A.A. Garcia-Granada, F. Perez-Murano

*Chemomagnetooptically controlled nanomotors for (bio)contaminant removal in water*, **Micromotors Workshop and Summer School**, Dresden, Germany, 13-19/08/17, K. Zhang, M. J. Esplandiu, B. Sepúlveda



## THESES

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**Laura Evangelio**, *Directed self-assembly of block copolymers on chemically nano-patterned surfaces*, 11/05/17, supervised by Prof. Francesc Pérez Murano and Dr Jordi Fraxedas

## COURSES

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M.J. Esplandiu, **Official international teaching at the UAB: Introduction to Nanoscience and Nanotechnology. Summer course for foreign students with a degree in science or engineering**, 26/06/17 to 14/07/17, 60 hours (6 credits), organised by the Institute of Education Sciences, Autonomous University of Barcelona (UAB)

M.J. Esplandiu, **Summer course for high school students: Discovering the world of Nanoscience**, 26-30/06/17, 10 hours, organised by the Institute of Education Sciences, UAB

M.J. Esplandiu, **Official teaching in the degree of Nanoscience and Nanotechnology at the UAB. Subject: Introduction to Nanoscience and Nanotechnology**, academic years 2016/2017 and 2017/2018, 60 hours (6 credits) each, Faculty of Sciences, UAB

M.J. Esplandiu, **Master's in Industrial Chemistry and Introduction to Research. Subject: Microscopy**, 3 hours, Faculty of Sciences, UAB

M.J. Esplandiu, **Master's in Industrial Chemistry and Introduction to Research. Subject: Chemistry for specific materials of interest in industry and research**, 10 hours, Faculty of Sciences, UAB

M.J. Esplandiu, **Seminar: Chemically-Propelled Micro and Nanomotors, a course for secondary school teachers**, 11/17/17, organised by the Permanent Seminar of Physics and Chemistry

# Inorganic Nanoparticles Group

## Main Research Lines

- Design and development of synthetic strategies for the production of complex nanoparticles
- Functionalisation with specific relevant (bio)molecules
- Study of their physicochemical and fundamental properties
- Applicability of inorganic nanoparticles in biomedicine, energy harvesting and catalysis

## GROUP MEMBERS

Balsells Pàmies, Max, Visiting HS Student

Bamiduro, Faith, Visiting Postdoctoral Researcher

Barbero, Francesco, PhD Student

Castellví Corrons, Xavier, Research Assistant

Domenech García, Natalia, Visiting PhD Student

Ferrari, Eleonora, PhD Fellowship Student

Franco Puntès, Víctor, ICREA Research Professor and Group Leader

Girona Alarcón, Marta, Visiting Undergraduate Student

Gómez Bastus, Neus, Senior Researcher

Mayall, Craig, PhD Fellowship Student

Merkoçi Xhelo, Florindi, Technician

Michelini, Sara, Visiting PhD Student

Moriones Botero, Oscar Hernando, PhD Student

Oliveras Solà, Jana, Master's Fellowship Student

Patarroyo Rengifo, Javier, PhD Student

Pérez Brizuela, Sara, Visiting Undergraduate Student

Piella Bagaria, Jordi, PhD Student

Rovira Esteva, Muriel, Postdoctoral Researcher



## GROUP LEADER



ICREA Prof.  
Víctor F. Puntès

ICREA Research Prof. Víctor F. Puntès' work spans the full breadth of nanoparticle research: synthesis, conjugation and characterisation of inorganic nanoparticles; study of their physicochemical properties; nanotoxicology and nanosafety; and myriad applications for sectors including energy harvesting, catalysis, medicine and the environment.

Víctor Puntès completed his undergraduate studies in chemical engineering and materials science at the Université Louis Pasteur Strasbourg (France) and at the Universitat Autònoma de Barcelona (UAB). In 1998, he earned his PhD in physics from the Universitat de

Barcelona (UB), working with Prof. Xavier Batlle and Prof. Amílcar Labarta on giant magnetoresistance in granular alloys. He then spent over three years at the University of California, Berkeley (USA) and the Lawrence Berkeley National Laboratory (LBNL, USA) in the groups led by Prof. Paul Alivisatos and Prof. Kannan Krishnan, working on the synthesis and control of nanostructures. In 2003 he returned to Catalonia with a Ramón y Cajal research position at the UB. In 2005 he obtained an ICREA Professorship at the then ICN (now ICN2) to create the Inorganic Nanoparticles Group, which he currently leads.

By the end of 2017, Víctor Puntès had 195 peer-reviewed publications and over 12,500 citations.

Prof. Puentes is also well-known for his work in science communication to the general public, his industrial and commercial efforts, and for his endeavours linking science and art.

Nanoparticles are engineered and designed in view of their applicability in materials science, catalysis, energy harvesting, environmental remediation, and nanobiomedicine and nanotoxicology, among others. This is achieved by controlling the size, shape and structure of their inorganic core, and selectively linking active molecules to the nanoparticle surface, which allows them to selectively interact with specific systems (materials, biological, environmental, etc.).

In this regard, the main scientific objectives of the group include:

I. Design and development of synthetic strategies for the production of complex nanoparticles (focusing on complex multicomponent and hollow nanoparticles comprising different families of metal, metal oxides, semiconductor oxides and semiconductors). Nanoparticles are engineered and designed in view of their applicability in materials science, catalysis, energy harvesting, environmental remediation.

II. Functionalisation with specific relevant (bio) molecules and materials (core-shell NPs, heterodimers...) in order to interface the nanoparticle in the desired system and increase nanoparticle functionality.

III. The study of their physicochemical and fundamental properties. As a result, we design new drug-delivery platforms, advanced catalysts to improve energy chemical processes, optimise the features of nanoparticles to enhance the production of hydrogen or boost biogas production. We also focus on the precise characterisation of the obtained nanoparticles in terms of their reactivity (aggregation, corrosion and dissolution) and physicochemical properties as prepared, during and after use.



## NEW PROJECTS & MILESTONES

In 2017 the Inorganic Nanoparticles Group continued work on its several ongoing projects on the design and synthesis of inorganic nanoparticles for interaction with biological systems and energy harvesting (see list of projects). Among them: DANAE, a national project funded by the Spanish Ministry of Economy, Industry and Competitiveness (MINECO) for the design of advanced inorganic nanocrystal complexes for the transformation and storage of energy; HISENTS (High-level Integrated Sensor for NanoToxicity Screening), a European collaborative project funded under H2020; and PANDORA, a Marie Curie ITN project also funded under H2020, to promote the safety assessment of nano-objects by defining their impact on the immune and defensive response of organisms in the environment.



## PUBLICATIONS

**Assembly of Plasmonic Nanoparticles on Nanopatterns of Polymer Brushes Fabricated by Electrospin Nanolithography**, Kiremitler N.B., Pekdemir S., Patarroyo J., Karabel S., Torun I., Puentes V.F., Onses M.S., *ACS Macro Letters*; **6 (6)**: 603-608. 2017. IF: 6.185

**Bacterial endotoxin (lipopolysaccharide) binds to the surface of gold nanoparticles, interferes with biocorona formation and induces human monocyte inflammatory activation**, Li Y., Shi Z., Radauer-Preiml I., Andosch A., Casals E., Luetz-Meindl U., Cobaleda M., Lin Z., Jaber-Douraki M., Italiani P., Horejs-Hoeck J., Himly M., Monteiro-Riviere N.A., Duschl A., Puentes V.F., Boraschi D., *Nanotoxicology*; **11 (9-10)**: 1157-1175. 2017. IF: 6.428

**Cancer resistance to treatment and antiresistance tools offered by multimodal multifunctional nanoparticles**, Casals E., Gusta M.F., Cobaleda-Siles M., Garcia-Sanz A., Puentes V.F., *Cancer Nanotechnology*; **8 (1)**, 2017.

**Cationic liposomal vectors incorporating a bolaamphiphile for oligonucleotide antimicrobials**, Mamusa M., Sitia L., Barbero F., Ruyra A., Calvo T.D., Montis C., Gonzalez-Paredes A., Wheeler G.N., Morris C.J., McArthur M., Berti D., *Biochimica et Biophysica Acta - Biomembranes*; **1859 (10)**: 1767-1777. 2017. IF: 3.498

**Confining Functional Nanoparticles into Colloidal Imine-Based COF Spheres by a Sequential Encapsulation-Crystallization Method**, Rodríguez-San-Miguel D., Yazdi A., Guillerm V., Pérez-Carvajal J., Puentes V., Maspoch D., Zamora F., *Chemistry - A European Journal*; **23 (36)**: 8623-8627. 2017. IF: 5.317

**Conserved effects and altered trafficking of Cetuximab antibodies conjugated to gold nanoparticles with precise control of their number and orientation**, García-Fernández L., Garcia-Pardo J., Tort O., Prior I., Brust M., Casals E., Lorenzo J., Puentes V.F., *Nanoscale*; **9 (18)**: 6111-6121. 2017. IF: 7.367

**Core-shell Au/CeO<sub>2</sub> nanoparticles supported in UiO-66 beads exhibiting full CO conversion at 100 °C**, Yazdi A., Abo Markeb A., Garzón-Tovar L., Patarroyo J., Moral-Vico J., Alonso A., Sánchez A., Bastus N., Imaz I., Font X., Puentes V., Maspoch D., *Journal of Materials Chemistry A*; **5 (27)**: 13966-13970. 2017. IF: 8.867

**Critical review of existing nanomaterial adsorbents to capture carbon dioxide and methane**, Alonso A., Moral-Vico J., Abo Markeb A., Busquets-Fité M., Komilis D., Puentes V., Sánchez A., Font X., *Science of the Total Environment*; **595**: 51-62. 2017. IF: 4.9

**Diverse applications of nanomedicine**, B Pelaz, C Alexiou, RA Alvarez-Puebla, F Alves, AM Andrews, S Ashraf, et al., *ACS nano*; **11 (3)**: 2313-2381. 2017. IF: 13.942

**Domain Formation and Conformational Changes in Gold Nanoparticle Conjugates Studied Using DPD Simulations**, Raman A., Jaime C., Puentes V.F., *Langmuir*; **33 (50)**: 14502 - 14512. 2017. IF: 3.833

**Formation of the Protein Corona: The Interface between Nanoparticles and the Immune System**, Barbero F., Russo L., Vitali M., Piella J., Salvo I., Borrajo M.L., Busquets-Fité M., Grandori R., Bastús N.G., Casals E., Puentes V., *Seminars in Immunology*; **34**: 52-60. 2017. IF: 9.611

**Hollow metal nanostructures for enhanced plasmonics: Synthesis, local plasmonic properties and applications**, Genç A., Patarroyo J., Sancho-Parramon J., Bastús N.G., Puentes V., Arbiol J., *Nanophotonics*; **6 (1)**: 193-213. 2017. IF: 4.492

**Inclusion of oligonucleotide antimicrobials in biocompatible cationic liposomes: A structural study**, Mamusa M., Barbero F., Montis C., Cutillo L., Gonzalez-Paredes A., Berti D., *Journal of Colloid and Interface Science*; **508**: 476-487. 2017. IF: 4.233

**Intrinsic and extrinsic properties affecting innate immune responses to nanoparticles: The case of cerium oxide**, Casals E., Gusta M.F., Piella J., Casals G., Jiménez W., Puentes V., *Frontiers in Immunology*; **8 (AUG)**. 2017. IF: 6.429

**Modeling the Optical Responses of Noble Metal Nanoparticles Subjected to Physicochemical Transformations in Physiological Environments: Aggregation, Dissolution and Oxidation**, Piella J., Bastús N.G., Puentes V., *Zeitschrift für Physikalische Chemie*; **231 (1)**: 33-50. 2017. IF: 1.012

**Nanosafety: Towards Safer Nanoparticles by Design**, Bastus, N. G.; Puentes, V., *Current medicinal chemistry*; **24**: 1-15

**One-Pot Synthesis of Cationic Gold Nanoparticles by Differential Reduction**, Sperling R.A., Garcíá-Fernández L., Ojea-Jiménez I., Piella J., Bastús N.G., Puentes V., *Zeitschrift für Physikalische Chemie*; **231 (1)**: 7-18. 2017. IF: 1.012

**Probing the surface reactivity of nanocrystals by the catalytic degradation of organic dyes: The effect of size, surface chemistry and composition**, Piella J., Merkoçi F., Genç A., Arbiol J., Bastús N.G., Puentes V., *Journal of Materials Chemistry A*; **5 (23)**: 11917-11929. 2017. IF: 8.867

**Safer by design strategies**, Cobaleta-Siles M., Guillamon A.P., Delpivo C., Vázquez-Campos S., Puentes V.F., *Journal of Physics: Conference Series*; **838 (1)**, 2017.

**Seeded Growth Synthesis of Au-Fe<sub>3</sub>O<sub>4</sub> Heterostructured Nanocrystals: Rational Design and Mechanistic Insights**, Fantechi E., Roca A.G., Sepúlveda B., Torruella P., Estradé S., Peiró F., Coy E., Jurga S., Bastús N.G., Nogués J., Puentes V., *Chemistry of Materials*; **29 (9)**: 4022-4035. 2017. IF: 9.466

**Size-Dependent Protein-Nanoparticle Interactions in Citrate-Stabilized Gold Nanoparticles: The Emergence of the Protein Corona**, Piella J., Bastús N.G., Puentes V., *Bioconjugate Chemistry*; **28 (1)**: 88-97. 2017. IF: 4.818

## PROJECTS

2014 SGR 612, funded by **AGAUR**, 01/01/14 to 30/04/17, Víctor F. Puentes

*High level Integrated Sensor for NanoToxicity Screening (HISENTS)*, funded by **EC**, 01/04/16 31/03/19, Víctor F. Puentes

*Diseño de complejos nanocristales inorganicos avanzados para la transformación y el almacenamiento óptimo de energía (DANAE)*, funded by **MINECO**, 01/01/16 to 31/12/18, Víctor F. Puentes

## TECHNOLOGY TRANSFER

**Patent ICN2PAT\_07\_15 Ceria nanoparticles for use in the treatment of hepatocellular carcinoma**, with Ref. PCT/EP2017/057570 on 30/03/17.

Inventors: Víctor Puentes (ICREA-ICN2), Wladimiro Jiménez (UB-CIBER), Guillermo Fernández (UB-CIBER)

## CONTRIBUTIONS

### Invited

*The use of reactive inorganic nanoparticles in medicine*, **Nanotech**, Paris, France, 28-30/06/17, V.F. Puentes

*Pharmacokinetics aspects of the use of Nanoparticles*, **ICONAN**, Barcelona, Spain, 25-27/09/17, V.F. Puentes

*Nanoparticle interaction with biomolecules: how it shapes the nano-effects on immunity*, **Euronanotox**, Bratislava, Slovakia, 01/10/17, V.F. Puentes

### Oral

*A Coupled Redox Approach for the Synthesis of Au/CeO<sub>2</sub> Hybrid Nanostructures*, **II Workshop on Chemistry of Group 11 Elements**, Barcelona, Spain, 26/01/17, N. Bastús

*New Synthetic Strategies for the Production of Colloidal Pt Hollow Nanocatalysts*, **II Workshop on Chemistry of Group 11 Elements**, Barcelona, Spain, 26/01/17, F. Merkoçi

### Poster

*Size-Controlled Synthesis of Sub-10-nanometer Citrate-Stabilized Gold Nanoparticles and Related Optical Properties*, **II Workshop on Chemistry of Group 11 Elements**, Barcelona, Spain, 26/01/17, J. Piella

*One-pot polyol synthesis of highly monodisperse short green silver nanorods*, **II Workshop on Chemistry of Group 11 Elements**, Barcelona, Spain, 26/01/17, J. Patarroyo

## PARTICIPATED CONGRESSES

**Pharmacokinetics aspects of the use of Nanoparticles**, Barcelona, Spain, 25-27/09/17, Chairman, V.F. Puentes

## AWARDS

PhD student Jordi Piella wins **Best Poster Award** at the II Workshop on Chemistry of Group 11 Elements.

PhD Student Javier Patarroyo wins **2<sup>nd</sup> prize** at the *Premio Bienal de Fotografía Científica de la IUNAN*.

# Magnetic Nanostructures Group

## Main Research Lines

- Exchange coupling in bi-magnetic core/shell nanoparticles and nanostructures
- Magnetic nanostructures for biomedical applications
- Magnetoplasmonic effects
- Novel magnetic and structural characterisation tools for nanoparticles
- Innovative fabrication approaches

## GROUP MEMBERS

Aranda Ramos, Antonio, Visiting PhD Student

Contreras Encinas, María del Carmen, Technician

Del Valle Benedi, Núria, Postdoctoral Researcher

Fantechi, Elvira, Postdoctoral Researcher

Gómez Roca, Alejandro, Postdoctoral Researcher

Güell Grau, Pau, Visiting PhD Student

Li, Zhi, PhD Fellowship Student

López-Barberá Martín, José Francisco, Postdoctoral Researcher

## GROUP LEADER



ICREA Research Prof.  
Josep Nogués

ICREA Research Professor Josep Nogués earned his degree from the Universitat Autònoma de Barcelona (UAB) in 1986. After obtaining his PhD at the Kungliga Tekniska Högskolan (Royal Institute of Technology) in Stockholm (Sweden) in 1993, he moved to the University of California San Diego (USA) to complete his postdoctoral studies. Four years later he returned to the UAB as associate researcher, becoming an ICREA research professor in 2001 and a founding member of the former Catalan Institute of Nanotechnology (ICN) shortly thereafter. His group on Magnetic Nanostructures was formally integrated into the ICN structure in 2006.

Prof. Nogués has published 225 articles (including eight reviews), with over 15,300 citations and an H-index of 54. He is the author of three patents and has given over 215 invited talks at international conferences and workshops.



Menéndez Dalmau, Enric, Visiting Senior Researcher

Muro Cruces, Javier, PhD Student

Navarro, Cristina, Visiting PhD Student

Nogués Sanmiquel, Josep, ICREA Research Professor and Group Leader

Pou Macayo, Laia, Visiting Master's Student

Quintana, Alberto, Visiting PhD Student

Robbenolt, Shauna, Visiting Postdoctoral Researcher

Sepúlveda Martínez, Borja, CSIC Tenured Scientist

Sort, Jordi, Visiting Senior Researcher

Zhang, Kuan, Severo Ochoa PhD Student

Zhang, Yue, PhD Fellowship Student

## NEW PROJECTS & MILESTONES

In 2017 the group started work on the MAGOAPP project funded by the Spanish Ministry of Economy, Industry and Competitiveness (MINECO) to develop novel nanoparticles for use in diverse biomedical applications. Jointly led by Prof. Nogués and group member Dr. Borja Sepúlveda, the specific aim of this project is to develop bottom-up and top-down designs for multifunctional magnetic

and magnetoplasmonic nanostructures for use in such as hyperthermia therapies and multimode imaging.

The group has also continued to work on the M-ERA-NET project PAIRED, which aims to develop magnetically and photochemically active drug carriers for controlled drug delivery.



## PUBLICATIONS

**Lateral Magnetically Modulated Multilayers by Combining Ion Implantation and Lithography**, Menéndez E., Modarresi H., Petermann C., Nogués J., Domingo N., Liu H., Kirby B.J., Mohd A.S., Salhi Z., Babcock E., Mattauch S., Van Haesendonck C., Vantomme A., Temst K., *Small*; **13 (11)**: 1603465, 2017. IF: 8.643

**Magnetically-actuated mesoporous nanowires for enhanced heterogeneous catalysis**, Serrà A., Grau S., Gimbert-Suriñach C., Sort J., Nogués J., Vallés E., *Applied Catalysis B: Environmental*; **217**: 81-91. 2017. IF: 9.446

**Maximizing Exchange Bias in Co/CoO Core/Shell Nanoparticles by Lattice Matching between the Shell and the Embedding Matrix**, González J.A., Andrés J.P., López Antón R., De Toro J.A., Normile P.S., Muniz P., Riveiro J.M., Nogués J., *Chemistry of Materials*; **29 (12)**: 5200-5206. 2017. IF: 9.466

**Metamirrors Based on Arrays of Silicon Nanowires with Height Gradients**, Otte M.A., Garcia-Martin A., Borrise X., Sepulveda B., *Advanced Optical Materials*; **5 (4)**: 1600933, 2017. IF: 6.875

**Novel Ba-hexaferrite structural variations stabilized on the nanoscale as building blocks for epitaxial bi-magnetic hard/soft sandwiched maghemite/hexaferrite/maghemite nanoplatelets with out-of-plane easy axis and enhanced magnetization**, Belec B., Dražić G., Gyergyek S., Podmiljšak B., Goršak T., Komelj M., Nogués J., Makovec D., *Nanoscale*; **9 (44)**: 17551-17560. 2017. IF: 7.367

**Photochemically Activated Motors: From Electrokinetic to Diffusion Motion Control**, Zhang K., Fraxedas J., Sepulveda B., Esplandiu M.J., *ACS Applied Materials and Interfaces*; **9 (51)**: 44948-44953. 2017. IF: 7.504

**Remanence plots as a probe of spin disorder in magnetic nanoparticles**, De Toro J.A., Vasilakaki M., Lee S.S., Andersson M.S., Normile P.S., Yaacoub N., Murray P., Sánchez E.H., Muñiz P., Peddis D., Mathieu R., Liu K., Geshev J., Trohidou K.N., Nogués J., *Chemistry of Materials*; **29 (19)**: 8258-8268. 2017. IF: 9.466

**Seeded Growth Synthesis of Au-Fe<sub>3</sub>O<sub>4</sub> Heterostructured Nanocrystals: Rational Design and Mechanistic Insights**, Fantechi E., Roca A.G., Sepúlveda B., Torruella P., Estradé S., Peiró F., Coy E., Jurga S., Bastús N.G., Nogués J., Puentes V., *Chemistry of Materials*; **29 (9)**: 4022-4035. 2017. IF: 9.466

**Unveiling a New High-Temperature Ordered Magnetic Phase in  $\epsilon$ -Fe<sub>2</sub>O<sub>3</sub>**, García-Muñoz J.L., Romaguera A., Fauth F., Nogués J., Gich M., *Chemistry of Materials*; **29 (22)**: 9705-9713. 2017. IF: 9.466

**Voltage-Induced Coercivity Reduction in Nanoporous Alloy Films: A Boost toward Energy-Efficient Magnetic Actuation**, Quintana A., Zhang J., Isarain-Chávez E., Menéndez E., Cuadrado R., Robles R., Baró M.D., Guerrero M., Pané S., Nelson B.J., Müller C.M., Ordejón P., Nogués J., Pellicer E., Sort J., *Advanced Functional Materials*; **27 (32)**: 1701904, 2017. IF: 12.124



## PROJECTS

*PAIRED*, Magnetically and photochemically actuated bioactive nanowires for remotely controlled drug delivery, funded by **MINECO-EU**, 01/05/16 to 30/04/19, Borja Sepúlveda

*THERANANO*, Multifunctional magnetic and magnetoplasmonic theranostic nanostructures, funded by **MINECO**, 01/01/14 to 31/03/17, Josep Nogués, Borja Sepúlveda

*MAGOAPP*, Nanomateriales magneto-fotónicos multifuncionales para aplicaciones biomédicas: fabricación top-down, bottom-up e híbridas, funded by **MINECO**, 30/12/16 to 29/12/19, Josep Nogués, Borja Sepúlveda



## TECHNOLOGY TRANSFER

**Patent ICN2PAT\_01\_17** A method for tuning the magnetic coercivity of a nanoporous film. A device and uses thereof has been filed in Spain, EU and UK, on 10/05/17.

Inventors: Jordi Sort (ICREA-UAB), Eva Pellicer (UAB), Josep Nogués (ICREA-ICN2), Alberto Quintana (UAB), Isaraín Chávez (UAB)

**Patent ICN2PAT\_10\_15** A hybrid hyperthermia device, and methods using the same, with Ref. PCT/EP2017/065842 on 27/06/17.

Inventors: Josep Nogués (ICREA-ICN2), Borja Sepúlveda (CSIC), Alejandro Gómez (ICN2), José Luis Tajada (ICN2), Elvira Fantechi (ICN2).



## CONTRIBUTIONS

### Keynote

*Formation of Mn<sub>3</sub>O<sub>4</sub>/Fe<sub>3</sub>O<sub>4</sub> hollow oxide nanoparticles by galvanic replacement*, **International Union of Materials Research Societies – International Conference of Advanced Materials**, Kyoto, Japan, 27/08/17 to 01/09/17, A. Lopez-Ortega, A.G. Roca, P. Torruella, M. Petrecca, S. Estarde, F. Peiro, V. Puentes, J. Nogués

*Multifunctional magneto-plasmonic nanostructures for nanotherapies and imaging*, **Conference on Molecular Nanoscience and Nanotechnology**, Frankfurt, Germany, 6-8/11/17, B. Sepúlveda

### Invited

*Synthesis of Hybrid magnetic nanoparticles for NMR imaging*, **ICMM-CNIC Workshop on Chemistry and Molecular Imaging**, Madrid, Spain, 21/04/17, A.G. Roca

*Tri-segmented magnetic nanowires with antiparallel alignment: suitable platforms for biomedical applications with minimized agglomeration*, **International Conference on Magnetism (INTERMAG)**, Dublin, Ireland, 24-28/04/17, J. Sort, J. Zhang, S. Agramunt, N. Del Valle, C. Navau, S. Estrade, F. Peiro, S. Pane, A. Sanchez, E. Pellicer, J. Nogués

*Formation of Mn<sub>3</sub>O<sub>4</sub>/Fe<sub>3</sub>O<sub>4</sub> hollow oxide nanoparticles by galvanic replacement*, **International Conference on Small Science and Energy Materials Nanotechnology Nanoparticles Meeting**, San Sebastián, Spain, 9-13/05/17, A. Lopez-Ortega, A.G. Roca, P. Torruella, S. Estarde, F. Peiro, V. Puentes, J. Nogués

*Combined photo-thermal therapy and multimodal imaging with magneto-plasmonic nanodomains*, **International Conference on Small Science and Energy Materials Nanotechnology Nanoparticles Meeting**, San Sebastián, Spain, 9-13/05/17, Z. Li, A. Aranda-Ramos, P. Guell-Grau, J.L. Tajada, L. Pou-Macayo, S. Lope-Piedrafita, F. Pi, M.D. Baro, J. Sort, C. Nogués, J. Nogués, B. Sepulveda

*Controlled formation of Mn<sub>3</sub>O<sub>4</sub>/Fe<sub>3</sub>O<sub>4</sub> hollow oxide nanoparticles, with possible biomedical applications, by galvanic replacement*, **Symposium on Magnetic Nanoparticles and SuperSpinGlasses**, Uppsala, Sweden, 01/06/17, J. Nogués

*Multifunctional magneto-plasmonic nanodomains for combines magnetic manipulation multi-modal imaging and photo-thermal therapies*, **Collaborative Conference on Materials Research**, Jeju Island, Korea, 26-30/06/17, Z. Li, A. Aranda-Ramos, P. Guell-Grau, J.L. Tajada, L. Pou-Macayo, S. Lope-Piedrafita, F. Pi, M.D. Baro, J. Sort, C. Nogués, J. Nogués, B. Sepulveda

*Exchange bias in thin Co-CoO films: inner secrets revealed by polarized neutron reflectometry*, **Moskow International Symposium on Magnetism**, Moskow, Russia, 1-5/07/17, K.

Temst, E. Menedez, J. Demeter, R. Steitz, A.R. Wildes, A.S. Mohd, A. Koutsoumpanis, E. Babcock, S. Mattauch, J. Nogués, A. Vantomme

*Structure, composition and magnetism in FeAl alloys*, **Frontiers in Materials Processing Applications and Technology**, Bordeaux, France, 09-12/07/17, E. Menedez, S. Suriñach, M.D. Baro, M.O. Liedke, J. Fassbender, J. Nogués, J. Sort

*Spatio-temporal patterns formation in Co-In system: films vs nanodisks*, **Frontiers in Materials Processing Applications and Technology**, Bordeaux, France, 9-12/07/17, I. Golvano-Escobal, J.C. Gonzalez-Rosillo, N. Domingo, X. Illa, J.F. Lopez-Barbera, J. Fornell, P. Solsona, L. Aballe, M. Foerster, S. Suriñach, M.D. Baro, T. Puig, S. Pane, J. Nogués, E. Pellicer, J. Sort

*Controlled formation of  $Mn_3O_4/Fe_3O_4$  hollow oxide nanoparticles, with possible biomedical applications, by galvanic replacement*, **International Conference on Composites/Nano Engineering**, Rome, Italy, 16-22/07/17, A. Lopez-Ortega, A.G. Roca, P. Torruella, M. Petrecca, S. Estarde, F. Peiro, V. Puentes, J. Nogués

*Synthesis of  $Fe_3O_4$  nanorods using different approaches and their potential biomedical applications*, **International Conference on Composites/Nano Engineering**, Rome, Italy, 16-22/07/17, J. Muro-Cruces, A.G. Roca, A. Lopez-Ortega, J. Nogués

*Remanence plots are sensitive to surface spin disorder in oxide nanoparticles*, **International Conference on Composites/Nano Engineering**, Rome, Italy, 16-22/07/17, J.A. De Toro, M. Vasilakaki, S.S. Lee, M.S. Andersson, P.S. Normile, N. Yaacoub, P. Murray, E.H. Sanchez, P. Muñoz, D. Peddis, R. Mathieu, K. Liu, J. Geshev, K.N. Trohidou, J. Nogués

*Seeded growth synthesis of  $Au-Fe_3O_4$  heterostructured nanocrystals for potential biomedical applications*, **International Conference on Composites/Nano Engineering**, Rome, Italy, 16-22/07/17, E. Fantechi, A.G. Roca, B. Sepulveda, P. Torruella, S. Estarde, F. Peiro, E. Coy, S. Jurga, F. Pineider, N. Bastús, V. Puentes, J. Nogués

*Correlative transmission electron microscopy of highly perfect  $Fe_3O_4$  nanocubes*, **Microscopy and Microanalysis Conference**, St. Louis, USA, 06-10/08/17, A. Kovacs, P. Diehle, T. Maeda, J. Caron, J. Muro-Cruces, A.G. Roca, J. Arbiol, J. Nogués, K. Kaneko, R. Dunin-Borowski

*Revealing magnetic core-shell nanoparticles structure at the nanoscale*, **International Union of Materials Research Societies – International Conference of Advanced Materials**, Kyoto, Japan, 27/08/17 to 01/09/17, A. Ruiz-Caridad, M.G. Walls, A. Gomez-Roca, J. Nogués, P. Torruella, L. Lopez-Conesa, S. Estarde, F. Peiro

*Multifunctional iron-oxide based magnetic and magneto-plasmonic nanoparticles for biomedical applications*, **International Union of Materials Research Societies – International Conference of Advanced Materials**, Kyoto, Japan, 27/08/17 to 01/09/17, E. Fantechi, A.G. Roca, C. Innocent, B. Sepulveda, P. Torruella, S. Estarde, F. Peiro, E. Coy, S. Jurga, F. Pineider, C. Sangregorio, N. Bastús, V. Puentes, J. Nogués

*Multifunctional magneto-plasmonic nanodomains for combined magnetic manipulation multi-modal imaging and photo-thermal therapies*, **International Union of Materials Research Societies – International conference of Advanced Materials**, Kyoto, Japan, 27/08/17 - 01/09/17, Z. Li, A. Aranda-Ramos, P. Guell-Grau, J.L. Tajada, L. Pou-Macayo, S. Lopez-Piedrafita, F. Pi, M.D. Baro, J. Sort, C. Nogués, J. Nogués, B. Sepulveda

*Understanding the synthesis of  $Au-Fe_3O_4$  heterostructures*, **Autumn Japanese Society of Applied Physics**, Fukuoka, Japan, 5-8/09/17, A.G. Roca, E. Fantechi, A. López-Ortega, N. G. Bastus, S. Estrade, P. Torruella, F. Peiro, V. Puentes, J. Nogués

*Unveiling the secrets of  $Mn_xO_y/Fe_xO_y$  core/shell nanoparticles through electron microscopy techniques*, **Conference on Analytical Science and Technology**, Cheongju, Korea, 23-24/10/17, P. Torruella, L. Lopez-Conesa, A. Ruiz-Caridad, M.G. Walls, A.G. Roca, A. Lopez-Ortega, J. Nogués, S. Estarde, F. Peiro

*Remanence plots as a probe of spin disorder in magnetic nanoparticles*, **Symposium on Magnetic Coupling in Nanostructures Materials**, Rome, Italy, 23-24/10/17, J.A. De Toro, M. Vasilakaki, S.S. Lee, M.S. Andersson, P.S. Normile, N. Yaacoub, P. Murray, E.H. Sanchez, P. Muñoz, D. Peddis, R. Mathieu, K. Liu, J. Geshev, K.N. Trohidou, J. Nogués

*Antiferromagnetic coupling in ferrimagnetic hard-soft core/shell nanoparticles and possible biomedical applications*, **Symposium on Magnetic Coupling in Nanostructures Materials**, Rome, Italy, 23-24/10/17, M. Estrader, A. López-Ortega, A. Juhin, S. Estradé, I. Golosovsky, M. Sikora, C. Carvallo, G. Salazar-Alvarez, M. Vasilakaki, K.N. Trohidou, M. Varela, D.C. Stanley, M.J. Pechan, P. Saintcavit, P. Galtzel, D. J. Keavney, F. Peiro, S. Suriñach, M.D. Baró, J. Nogués

### Oral

*Controlled synthesis of  $Fe_3O_4$  nanorods using a solvothermal approach*, **International Conference on Small Science and Energy Materials Nanotechnology Nanoparticles Meeting**, San Sebastián, Spain, 9-13/05/17, J. Muro-Cruces, A.G. Roca, J. Nogués

*Magneto-plasmonic nanodomains for photothermal treatments*, **NanoBioMed 2017**, Alghero, Italy, 24-27/06/17, C. Nogués, A. Aranda-Ramos, Z. Li, L. Pou-Macayo, J. Sort, J. Nogués, B. Sepulveda

*Incommensurate magnetic order in CoO nanoparticles revealed by neutron diffraction*, **International Baltic Conference on Magnetism**, Svetlogorsk, Russia, 20-24/08/17, I.V. Golosovsky, M. Estrader, A. Lopez-Ortega, A.G. Roca, I. Puente-Orench, J. Nogués

### Poster

*Drastic enhancement of the catalytic activity of both water remediation and hydrogen production using magnetically-actuated mesoporous CoPt nanowires*, **World Congress of Chemical Engineering**, Barcelona, Spain, 1-5/10/17, A. Serra, S. Grau, C. Gimbert, J. Sort, J. Nogués, E. Valles

*Exchange bias revisited: unusual field-dependent effects*, **Conference on Magnetism and Magnetic Materials**, Pittsburg, USA, 6-10/11/17, J.L. Fernandez-Cuñado, P. Perna, A. Bollero, N.S. Sokolov, S. Gastev, S. Suturin, A. Banskikof, V. Fedorov, D. Baranov, K. Koshmak, L. Pascual, J. Nogués, R. Miranda, J. Camarero

# NanoBioelectronics and Biosensors Group

## Main Research Lines

- **Catalytic/carrier nanomaterials:** nanoparticles as electrocatalysts, nanoparticles as biomolecule carriers, and nanowires/nanotubes for non-enzymatic and enzyme mimic sensors
- **Nanomicrofluidics and lab-on-a-chip technologies**
- **Paper- or nanopaper-based nanobiosensors**
- **Nanochannels:** nanoporous membranes as electrical sensing platforms
- **Graphene:** biosensors based on graphene-related materials
- **Nanomotors:** self-propelled micro/nanomotors for biosensing and other applications



## GROUP MEMBERS

**Abdulhadee, Yakoh**, Visiting PhD Student

**Alarcón Angeles, Georgina**, Visiting Senior Researcher

**Álvarez Diduk, Ruslan Raulevich**, Postdoctoral Researcher

**Balsells Vives, Marc**, Severo Ochoa Technician on INK Development

**Bergua Canudo, José Francisco**, PhD Student

**Botifoll Moral, Marc**, Visiting Degree Student

**Calabretta, Maria Maddalena**, Visiting PhD Student

**Calucho Palma, Enric**, Master's Fellowship Student

**Cañamero Núñez, Alba** Visiting TFG Student

**Capoferri, Denise**, Visiting Undergraduate Student

**Chalupniak, Andrzej**, PhD Student

**Cheeveewattanag, Nopchulee**, Visiting PhD Student

**Cladera Cladera, Adrià**, Visiting Undergraduate Student

**De la Escosura Muniz, Alfredo**, Senior Postdoctoral Researcher

**Guardia Giros, Pablo**, Severo Ochoa Postdoctoral Researcher

**Hassan, Abdel-Rahim**, Visiting Postdoctoral

Researcher

**Jakubec, Petr**, Visiting Postdoctoral Researcher

**Khater, Mohga**, PhD Fellowship Student

**Leva Bueno, Juan**, Visiting Master's Student

**Liu, Jie**, Visiting PhD Student

**Martínez Domingo, Carme**, Visiting PhD Student

**Martos De la Torre, Andrea Ascensión**, Visiting Undergraduate Student

## GROUP LEADER



ICREA Research Prof.  
Arben Merkoçi

ICREA research professor and leader of the ICN2 Nanobioelectronics and Biosensors Group, Arben Merkoçi obtained his PhD at the Universiteti i Tiranës (Albania) in ion selective electrodes. Since 1992 he has carried out research as postdoctoral fellow and research professor at the Polytechnic University of Budapest (Hungary), University of Ioannina (Greece), Università degli Studi di Padova (Italy), Universitat

Politécnica de Catalunya, Universitat Autònoma de Barcelona and New Mexico State University (USA). His research is focused on the integration of biological molecules and other species with micro- and nanostructures of interest in the design of novel (bio)sensors.

Prof. Merkoçi is the co-founder of two spin-off companies: GraphenicaLab, devoted to graphene patterning, and PaperDrop, to clinical diagnostics. He has published 270 articles and supervised 25 PhD theses.



Merkoçi Hyka, Arben, ICREA Research Professor and Group Leader

Miani Bonilla, Sonia, Undergraduate Fellowship Student

Müller, Mark Alexander, Visiting Master's Student

Nagar, Bhawna, Severo Ochoa PhD Student

Ngu, Mark Angelo, Visiting PhD Student

Patella, Bernardo, Visiting PhD Student

Pérez Toma, Luz Agueda, Visiting PhD Student

Puig Font, Anna, Project Manager and Group Administrator

Quesada Gonzalez, Daniel, PhD Student

Romero Gil, Javier, Visiting Undergraduate Student

Russo, Lorenzo, Severo Ochoa PhD Student

Sena Torralba, Amadeo, PhD Student

Yang, Qiuyue, PhD Fellowship Student

Zamora Gálvez, Alejandro, PhD Student

Zhao, Lei, PhD Fellowship Student

## NEW PROJECTS & MILESTONES

In 2017 the group has continued to work on two large ongoing projects. The first, INTCATCH, is a project to develop nanobiosensors for pollutant monitoring funded under the European H2020 research and innovation framework programme. The second, NANCANCEL, is a EuroNanoMed II project coordinated by Prof. Merkoçi to develop a nanodiagnosics platform for monitoring cancer cell-secreted proteins.

The group also continued to make progress in paper- and nanopaper-based platforms, as well as in graphene-based platforms of interest for biosensing and other device fabrication.

This year four students defended their PhD theses: Alejandro Zamora, Andrzej Chalupniak, Bentolhoda Heli and Jie Liu.

## PUBLICATIONS

**Biosensors for plant pathogen detection**, Khater M., de la Escosura-Muñiz A., Merkoçi A., *Biosensors and Bioelectronics*; **93**: 72-86. 2017. IF: 7.78

**Electrochemically reduced graphene and iridium oxide nanoparticles for inhibition-based angiotensin-converting enzyme inhibitor detection**, Kurbanoglu S., Rivas L., Ozkan S.A., Merkoçi A., *Biosensors and Bioelectronics*; **88**: 122-129. 2017. IF: 7.78

**Graphene-Based Biosensors: Going Simple**, Morales-Narváez E., Baptista-Pires L., Zamora-Gálvez A., Merkoçi A., *Advanced Materials*; **29 (7)**. 2017. IF: 19.791

**Graphene-based hybrid for enantioselective sensing applications**, Zor E., Morales-Narváez E., Alpaydin S., Bingol H., Ersoz M., Merkoçi A., *Biosensors and Bioelectronics*; **87**: 410-416. 2017. IF: 7.78

**Graphene-encapsulated materials: Synthesis, applications and trends**, Morales-Narváez E., Sgobbi L.F., Machado S.A.S., Merkoçi A., *Progress in Materials Science*; **86**: 1-24. 2017. IF: 31.14

**Graphene Oxide-Poly(dimethylsiloxane)-Based Lab-on-a-Chip Platform for Heavy-Metals Preconcentration and Electrochemical Detection**, Chalupniak A., Merkoçi A., *ACS Applied Materials and Interfaces*; **9 (51)**: 44766-44775. 2017

**Magnetic nanoparticle-molecular imprinted polymer: A new impedimetric sensor for tributyltin detection**, Zamora-Gálvez A., Mayorga-Matinez C.C., Parolo C., Pons J., Merkoçi A., *Electrochemistry Communications*; **82**: 6-11. 2017. IF: 4.396

**Mobile phone-based biosensing: An emerging "diagnostic and communication" technology**, Quesada-González D., Merkoçi A., *Biosensors and Bioelectronics*; **92**: 549-562. 2017. IF: 7.78

**Nanocellulose in Sensing and Biosensing**, Golmohammadi H., Morales-Narváez E., Naghdi T., Merkoçi A., *Chemistry of Materials*; **29 (13)**: 5426-5446. 2017. IF: 9.466

**Nanomaterials-based enzyme electrochemical biosensors operating through inhibition for biosensing applications**, Kurbanoglu S., Ozkan S.A., Merkoçi A., *Biosensors and Bioelectronics*; **89**: 886-898. 2017. IF: 7.78

**Nanomaterials connected to antibodies and molecularly imprinted polymers as bio/receptors for bio/sensor applications**, Zamora-Gálvez A., Morales-Narváez E., Mayorga-Martinez C.C., Merkoçi A., *Applied Materials Today*; **9**: 387-401. 2017

**Paper strip-embedded graphene quantum dots: A screening device with a smartphone readout**, Álvarez-Diduk R., Orozco J., Merkoçi A., *Scientific Reports*; **7 (1)**. 2017. IF: 4.259

**Production of biofunctionalized MoS<sub>2</sub> flakes with rationally modified lysozyme: A biocompatible 2D hybrid material**, Siepi M., Morales-Narváez E., Domingo N., Monti D.M., Notomista E., Merkoçi A., *2D Materials*; **4 (3)**. 2017. IF: 6.937

**Rapid on-chip apoptosis assay on human carcinoma cells based on annexin-V/quantum dot probes**, Montón H., Medina-Sánchez M., Soler J.A., Chalupniak A., Nogués C., Merkoçi A., *Biosensors and Bioelectronics*; **94**: 408-414. 2017. IF: 7.78

**Straightforward Immunosensing Platform Based on Graphene Oxide-Decorated Nanopaper: A Highly Sensitive and Fast Biosensing Approach**, Cheeveewattanagul N., Morales-Narváez E., Hassan A.-R.H.A., Bergua J.F., Surareungchai W., Somasundrum M., Merkoçi A., *Advanced Functional Materials*; **27 (38)**. 2017. IF: 12.124

**Toward integrated detection and graphene-based removal of contaminants in a lab-on-a-chip platform**, Chalupniak A., Merkoçi A., *Nano Research*; **10 (7)**: 2296-2310. 2017. IF: 7.354

## PROJECTS

*INTCATCH*, Development and application of Novel, Integrated Tools for monitoring and managing Catchments (H2020-WATER-2015-two-stage), funded by EC, 01/06/16 to 31/01/20, Arben Merkoçi

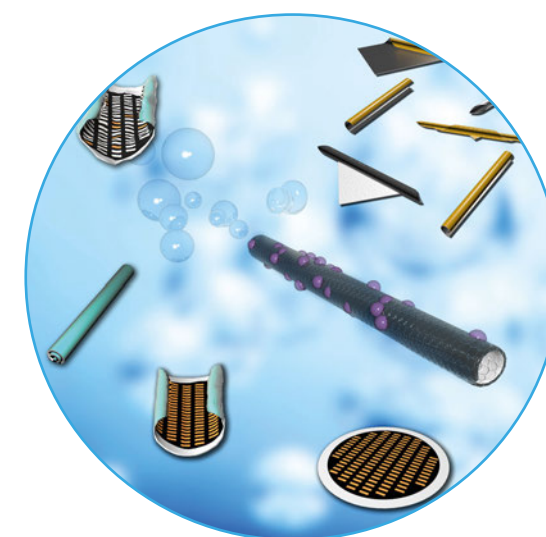
*NANCANCEL*, Development of a Nanodiagnostic platform for monitoring of Cancer cell secreted proteins, funded by MINECO, 01/06/16 to 31/01/20, Arben Merkoçi

*NAP2DIAGNOSTICS*, Nanobioconjugated paper/plastic platforms for improved diagnostics applications, funded by MINECO, 01/01/15 to 31/12/17, Arben Merkoçi

*ELECTROBIONET, RED DE SENSORES Y BIOSENSORES ELECTROQUÍMICOS*, funded by MINECO, 01/12/15 to 30/11/17, Arben Merkoçi

*SMS, Sensing toxicants in Marine waters makes Sense using biosensors (FP7-OCEAN-2013-1)*, funded by EC, 01/12/13 to 31/08/17, Arben Merkoçi

*SMART PRINTED PAPER, Printed Electronics para nuevas funcionalidades en papel*, funded by MINECO, 01/02/14 to 30/06/17, Arben Merkoçi





## TECHNOLOGY TRANSFER

**European patent (EP) application ICN2PAT\_10\_16** *A system for detecting an analyte from a sample in an analytical test substrate and a portable device for carrying out said detection*, with ref. EP17382091 and priority date 24/02/17  
Inventors: Arben Mekoçi (ICREA-ICN2), Ruslan Álvarez (ICN2), Jahir Orozco (ICN2)

**Industry collaboration** to develop biosensors, (*University of Santo Tomas*), with project ref. ICN2PRJ\_04\_17\_MANILA and signing date 01/03/17



## CONTRIBUTIONS

### Keynote

*Nanobiosensors based on printing onto paper or plastic platforms*, **General Assembly of ESMA 2017**, Lisbon, Portugal, 24/03/17, A. Merkoçi

*Diagnostics with paper-based sensors using nanomaterials as signalling tools*, **NanoBioSensor Conference**, Dresden, Germany, 4-5/09/17, A. Merkoçi

*Paper-based Nanobiosensors: Diagnostics Going Simple*, **Lab-on-a-Chip & Microfluidics World Congress 2017**, California, USA, 2-4/10/17, A. Merkoçi

*Health and environment diagnostics using paper-based nanobiosensors*, **NanoBioMed Conference**, Barcelona, Spain, 22-24/11/17, A. Merkoçi

### Invited

*Graphene-based platforms for biosensing applications*, **Graphene Connect Workshop - Biomedical Technologies**, Dusseldorf, Germany, 16/11/17, A. Merkoçi

### Invited panel discussion

*Promoting the establishment of Centres of Excellence in Albania and the impacts on promoting Albanian young scientists*, **Capacity Building and Knowledge Transfer in Albania**, Tirana, Albania, 16-17/02/17, A. Merkoçi

### Oral

*Toward integrated detection and graphene-based removal of contaminants in a lab-on-a-chip platform*, **Graphene 2017**, Barcelona, Spain, 28-31/03/17, A. Chalupniak, A. Merkoçi

*Toward integrated detection and graphene-based removal of contaminants in a lab-on-a-chip platform*, **TNT 2017**, Dresden, Germany, 5-9/06/17, A. Chalupniak, A. Merkoçi

*Nanoparticle/nanochannel based sensing systems for neuroblastoma biomarkers detection on plastic and paper platforms*, **VIII International Congress on Analytical Nanoscience and Nanotechnology (NyNA 2017)**, Barcelona, Spain, 03-05/07/17, A. de la Escosura, M. Espinoza, A. Chamorro, C. J. Rodríguez, C. de Torres, A. Merkoçi

*Toward integrated detection and graphene-based removal of contaminants in a lab-on-a-chip platform*, **VIII International Congress on Analytical Nanoscience and Nanotechnology (NyNA 2017)**, Barcelona, Spain, 3-5/07/17, A. Chalupniak, A. Merkoçi

### Poster

*Molecular imprinted polymer for hazard compounds detection*, **VIII International Congress on Analytical Nanoscience and Nanotechnology (NyNA 2017)**, Barcelona, Spain, 03-05/07/17, A. Zamora, A. Merkoçi

*Bioluminescent Nanopaper for the Fast Screening of Toxic Substances*, **VIII International Congress on Analytical Nanoscience and Nanotechnology (NyNA 2017)**, Barcelona, Spain, 3-5/07/17, J. Liu, J. Francisco, E. Morales, J. Orozco, R. Álvarez, T. Vincent, G. Zhong, A. Merkoçi

*Paper strip-embedded graphene quantum dots: a screening device with a smartphone*, **VIII International Congress on Analytical Nanoscience and Nanotechnology (NyNA 2017)**, Barcelona, Spain, 3-5/07/17, R. Álvarez, J. Orozco, A. Merkoçi

*Heavy Metals Detection using Screen printed Carbon electrodes*, **GLOBAQUA WORKSHOP**, Barcelona, Spain, 09/11/17, B. Nagar, M. Balsells, A. de la Escosura, A. Merkoçi

*Bioluminescent Nanopaper for the Fast Screening of Toxic Substances*, **GLOBAQUA WORKSHOP**, Barcelona, Spain, 09/11/17, J. Liu, J. F. Bergua, E. Morales, J. Orozco, R. Álvarez, T. Vincent, G. Zhong, A. Merkoçi



## DISSEMINATION CONTRIBUTIONS

### Invited seminar

*Diagnostics using nanobiosensors*, **School of Biological Sciences & SynthSys, University of Edinburgh**, Edinburgh, United Kingdom, 23/02/17, A. Merkoçi

*Diagnostics using nanobiosensors*, **Beijing Institute of Technology**, Beijing, China, 15/03/17, A. Merkoçi

*Nanomaterials-based sensors for diagnostics*, **Instituto de Química Orgánica General, CSIC**, Madrid, Spain, 31/05/17, A. Merkoçi

*Nanobiosensors for diagnostics*, **European Foundation for the Study of Chronic Liver Failure - EF Clif**, Barcelona, Spain, 28/11/17, A. Merkoçi

*Nanobiosensors for diagnostics*, **BioSystems S.A.**, Barcelona, Spain, 29/11/17, A. Merkoçi

### Invited lecture

*Nanobiosensors for diagnostics: from plastic to simple paper-based platforms*, **Department of Information Engineering, Università degli Studi di Padova**, Padova, Italy, 19/01/17, A. Merkoçi

*Nanobiosensors for diagnostics*, **Universidad de Alicante, Departamento de Química Física, Instituto Universitario de Materiales**, Alicante, Spain, 21/02/17, A. Merkoçi



## COURSES

A. Merkoçi, **Master's in Nanoscience and Nanotechnology. Subject: Nanodiagnosics**, (6 hours). Universitat Autònoma de Barcelona, Nov/Dec 2017



## AWARDS

Daniel Quesada entered the *Somos Científicos* competition to promote science communication to high school students, receiving the **Winning Scientist "Ne Zone"** award for the creation of a YouTube channel (*El Nanomundo de Daniel / Daniel's Nanoworld*)

# Nanobiosensors and Bioanalytical Applications Group

## Main Research Lines

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



## GROUP LEADER



CSIC Research Prof.  
Laura Lechuga Gómez

Prof. Laura M. Lechuga received her PhD in chemistry from the Universidad Complutense de Madrid in 1992. From 2012 to 2015 she was an adjunct professor at the department of Physics and Technology at the Arctic University of Norway (Tromsø, Norway). Since 2013 she has been a distinguished visiting professor at the School of Electrical and Computer Sciences of the Universidade Estadual de Campinas (Brazil). She has been a fellow of the Optical Society since 2014.

Prof. Lechuga is the leader of the ICN2 Nanobiosensors and Bioanalytical Applications Group. The main focus of her group lies in the technological development of nanophotonic (nanoplasmonics and silicon-based) biosensors, their integration into portable lab-on-a-chip platforms and their application in clinical and environmental diagnostics.

She has published over 200 articles, book chapters and conference proceedings and delivered more than 350 invited presentations. She also has eight families of patents at the European, US and international levels. She was the driving force behind the founding of spin-off company SENSIA, SL in 2004 and the co-founder of BIOD, SL in 2010.

Prof. Lechuga is an associate editor of the *IEEE Photonics and Optics and Laser Technology* (Elsevier) journals, and is on the editorial board of the *Journal of Sensors*. She is a member of the international society for optics and photonics (SPIE), as well as of the European Optical Society (EOS), the Spanish Optical Society and the Real Sociedad Española de la Física (RSEF). She is a member of permanent steering committees for the Advanced Study Course on Optical Chemical Sensors (ASCOS) and for the Europt(r)ode Conference Series.

She has often served on the scientific committees of major international conferences and is regularly involved in the organisation of international conferences and workshops. She is a member of the scientific advisory boards of the Andalusian Centre for Nanomedicine (BIONAND), the Biomedical Research Institute of the Universidade de Vigo (CINBIO), the Micro and Nano Research Facility (RMIT, Melbourne, Australia) and the Centro de Investigaciones en Óptica (CIO, Mexico). She is regularly called upon as an expert evaluator and expert reviewer for the European Commission (FP5, FP6, FP7, H2020), as well as for high level panel evaluations at worldwide level.

She has received several prizes and recognitions over the years, including the 2016 Physics, Innovation and Technology Prize from the RSEF and the Fundación BBVA. In 2017 she was selected for inclusion in AcademiaNet: The Portal to Excellent Women Academics.

## GROUP MEMBERS

**Aviñó Andrés, Ana María**, Visiting Senior Researcher

**Calvo Lozano, Olalla**, Technician

**Chocarro Ruiz, Blanca**, Severo Ochoa PhD Student

**Dey, Priyanka**, Research Engineer

**Díaz Luis-Ravelo, Heriberto J.**, Technician

**Diéguez Gonzalez, Rebeca**, Scientific Project Manager

**Estévez Alberola, Maria Carmen**, Senior Researcher

**Fabri Faja, Núria**, PhD Student

**García Fox, Mario Alejandro**, Visiting Research Assistant

**Grajales García, Daniel**, PhD Fellowship Student

**Guiu Tort, Roger**, Technician

**Homs Corbera, Antoni de Padua**, Severo Ochoa Senior Researcher

**Kurachi, Cristina**, Visiting Postdoctoral Researcher

**Lechuga Gómez, Laura**, CSIC Research Professor and Group Leader

**Llop Castellbou, Jessica**, Scientific Group Administrator

**López Muñoz, Gerardo Arturo**, PhD Fellowship Student

**Maldonado Vázquez, Jesús Manuel**, PhD Fellowship Student

**Nieves Paniagua, Óscar**, Visiting Master's Student

**Ortiz Pérez, Ana**, Visiting Undergraduate Student

**Peláez Gutiérrez, Enelia Cristina**, PhD Student

**Portela Otaño, Alejandro Ernesto**, Postdoctoral Researcher

**Ramírez Priego, Patricia**, Technician

**Robles, Denise**, PhD Fellowship Student

**Sánchez Huertas, César**, Postdoctoral Researcher

**Sierra Montoya, Miquel**, Visiting Undergraduate Student

**Vázquez García, Marc**, Visiting Undergraduate Student

## NEW PROJECTS & MILESTONES

The activities of the Nanobiosensors and Bionalytical Applications Group are focused on the development of novel nanobiosensor devices based on the principles of nanoplasmonics and silicon-based photonics, including surface biofunctionalisation, microfluidics for automatic fluid delivery and complete lab-on-a-chip integration for point-of-care devices. The application of nanobiosensor devices in real clinical diagnostics and environmental control is one of the group's main objectives. Its research

activities range from basic research to the technological operation of working sensing platforms, as well as the transfer of its research outcomes to industry. The group is at the forefront of developments in photonic biosensors at the international level, with such as its bimodal waveguide interferometric device. Since 2006 the group has been associated to the ISCIII Biomedical Research Networking Centre (CIBER) as part of its Centre for Bioengineering, Biomaterials and Nanomedicine (CIBER-BBN).

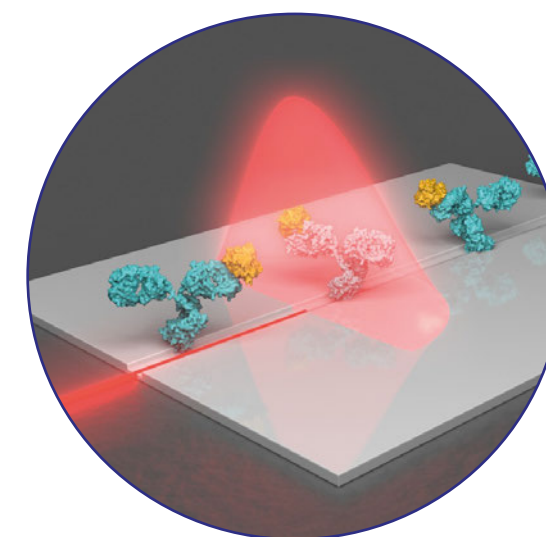
In 2017 the group has made significant progress in the development of integrated and multiplexed devices with interferometric nanophotonic and (nano)plasmonic biosensors, with the end goal of achieving sensitive, affordable, handheld and portable point-of-care devices. New multiplexed nanoplasmonics sensor devices have been implemented based on flexible substrates using blue-ray disc for further integration in portable platforms. New solutions based on vertical adiabatic tapers for light incoupling in the nanometric structures of the bimodal waveguide biosensor have been successfully implemented, allowing incoupling with the tolerances required for a multiplexed point-of-care. New designs of the nanointerferometric sensors have further expanded the capabilities of this ultrasensitive technology.

In parallel to the technological developments, we have demonstrated the feasibility of our nanophotonic biosensor technology in several fields of application. We have maintained our focus on applications of clinical interest, including the early detection of colorectal cancer biomarkers with a simple test in serum (i.e. autoantibodies, as part of the RETOS COLONTEST project), the specific detection of infectious diseases like tuberculosis via a simple biosensor test in urine (European project POCKET and additional collaborations), and the early detection of sepsis (European project RAIS).

In the research line to evaluate the dysregulation of cellular pathways, we have used our nanobiosensor technologies as alternative analytical techniques for the evaluation of different gene regulating pathways in a bid to obtain more informative and accurate cancer diagnoses and follow-up therapies. They also allow for a fast, direct and highly-sensitive analysis of these regulating routes without the need for labelling or amplification. We have completed the

quantitative evaluation of alternatively-spliced mRNA isoforms with label-free, real-time sensing. We have also successfully demonstrated miRNA detection in biological media at exceptionally low detection limits (aM range), which has allowed us to stratify between healthy patients and those with bladder cancer with a simple urine analysis.

In addition, we have continued work on point-of-care nanoplasmonic biosensor prototypes, via national projects URINETEST (RETOS-Colaboración, RTC-2016-5452-1) for the monitoring of a gluten-free diet through the detection of gluten toxic peptides in urine, and PreDICT (RETOS-Investigación, TEC-2016-78515-R) for the design and fabrication of an advanced multiplexed device for disease detection, progression and therapeutic follow-up of lung cancer. We have also been working on the NANOFOTOSENS project (Fundación Domingo Martínez) for the development of a novel ultrasensitive photonic nanosensor that integrates a new class of porous materials –metal-organic frameworks or MOFs– as specific receptors and nanointerferometers for the fast and specific detection of minute concentrations of gas pollutants for environmental quality control.





## PUBLICATIONS

**Metamirrors Based on Arrays of Silicon Nanowires with Height Gradients**, Otte M.A., Garcia-Martin A., Borrisse X., Sepulveda B., *Advanced Optical Materials*; **5 (4)**, 2017. IF: 6.875

**Analysis of alternative splicing events for cancer diagnosis using a multiplexing nanophotonic biosensor**, Huertas C.S., Domínguez-Zotes S., Lechuga L.M., *Scientific Reports*; **7**, 2017. IF: 4.259

**Direct and label-free detection of the human growth hormone in urine by an ultrasensitive bimodal waveguide biosensor**, González-Guerrero A.B., Maldonado J., Dante S., Grajales D., Lechuga L.M., *Journal of Biophotonics*; **10 (1)**: 61-67, 2017. IF: 4.328

**A label-free nanostructured plasmonic biosensor based on Blu-ray discs with integrated microfluidics for sensitive biodetection**, López-Muñoz G.A., Estevez M.-C., Peláez-Gutierrez E.C., Homs-Corbera A., García-Hernandez M.C., Imbaud J.I., Lechuga L.M., *Biosensors and Bioelectronics*; **96**: 260-267, 2017. IF: 7.78

**Nanophotonic interferometric immunosensors for label-free and real-time monitoring of chemical contaminants in marine environment**, Chocarro-Ruiz B., Herranz S., Fernández Gavela A., Lechuga L.M., *Proceedings of SPIE - The International Society for Optical Engineering*; **10215**, 2017

**An automated optofluidic biosensor platform combining interferometric sensors and injection moulded microfluidics**, Szydzik C., Gavela A.F., Herranz S., Roccisano J., Knoerzer M., Thurgood P., Khoshmanesh K., Mitchell A., Lechuga L.M., *Lab on a Chip*; **17 (16)**: 2793-2804, 2017. IF: 6.045

**Asymmetrically coupled resonators for mass sensing**, Marquez S., Alvarez M., Plaza J.A., Villanueva L.G., Dominguez C., Lechuga L.M., *Applied Physics Letters*; **111 (11)**, 2017. IF: 3.411

**Species-specific modulation of food-search behavior by respiration and chemosensation in Drosophila larvae**, Kim D., Alvarez M., Lechuga L.M., Louis M., *eLife*; **6**, 2017. IF: 7.725

**Array of Microfluidic Beam Resonators for Density and Viscosity Analysis of Liquids**, Marquez S., Álvarez M., Fariña Santana D., Homs-Corbera A., Domínguez C., Lechuga L.M., *Journal of Microelectromechanical Systems*; **26 (4)**: 749-757, 2017. IF: 2.124

**Nanophotonic label-free biosensors for environmental monitoring**, Chocarro-Ruiz B., Fernández-Gavela A., Herranz S., Lechuga L.M., *Current Opinion in Biotechnology*; **45**: 175-183, 2017. IF: 9.294

**Recent advances in nanoplasmonic biosensors: Applications and lab-on-a-chip integration**, Lopez G.A., Estevez M.-C., Soler M., Lechuga L.M., *Nanophotonics*; **6 (1)**: 123-136, 2017. IF: 4.492

**Simple, low-cost and timely optical biosensors for the detection of epigenetics biomarkers: the future of cancer diagnosis**, C. S. Huertas and L. M. Lechuga, *European Medical Journal*; **5**: 54-61, 2017

**Cryptophane-cladded interferometric waveguide sensor for aqueous methane detection**, Jágerská J., Dullo F.T., Lindecrantz S.M., Börgers J.M., Hansen J.H., Lechuga L.M., Hellesø O.G., *Optics InfoBase Conference Papers; Part F43-CLEO\_AT 2017*, 2017



## PROJECTS

*Nanobiosensors and Bioanalytical Applications, Suport a grups de recerca (SGR 2014-2016)*, funded by **AGAUR**, 01/01/2014 to 30/04/2017, Laura Lechuga

*POCKET, Development of a low-cost point-of-care test for tuberculosis detection (FP7-ICT-2013-10)*, funded by **EC**, 01/11/2013 to 30/04/2017, Laura Lechuga

*RAIS, Scalable, point-of-care and label free mecroarray platform for rapid detection of Sepsis (H2020-ICT-2014-1)*, funded by **EC**, 01/01/2015 to 31/03/2018, Laura Lechuga

*NANOFOTOLENS, Implementación de novedosos nanosensores fotónicos para la detección de ínfimas concentraciones de gases contaminantes*, funded by **FDM**, 21/03/2016 to 21/09/2017, Laura Lechuga

*URINETEST, Métodos Rápidos de análisis de péptidos inmunogénicos alimenticios en orina*, funded by **MINECO**, 01/04/2016 to 31/12/2018, Laura Lechuga

*PreDICT, Point-of-care Nanoplasmonic Platforms for Novel High-Value Diagnostics and Therapy Follow-Up*, funded by **MINECO**, 30/12/2016 to 29/12/2019, Laura Lechuga



## TECHNOLOGY TRANSFER

**European patent (EP) application ICN2PAT\_06\_16** *Sensors for translocating analytes comprising nanometer or sub-nanometer thick heterostructured functional layers and a method for sensing translocating analytes*, with Ref. EP17382015 and priority date 16/01/2017. Inventor: Antoni Homs (ICN2)



## CONTRIBUTIONS

### Keynote

*Nanophotonic point-of-care interferometric biosensors for high-value diagnostics*, **VIII International Congress on Analytical Nanoscience and Nanotechnology (NyNA 2017)**, Barcelona, Spain, 03-05/07/17, L.M. Lechuga

*Novel and versatile approaches for DNA-based nanosensing based on nucleic acid triplex formation*, **VIII International Congress on Analytical Nanoscience and Nanotechnology (NyNA 2017)**, Barcelona, Spain, 03-05/07/17, Eritja, L.M. Lechuga, C.S. Huertas, A. Aviñó.

*The potential of nanophotonic lab-on-chip biosensors for high-value portable diagnosis*, Euroanalysis 2017. **XIX European Conference in Analytical Chemistry**, Stockholm, Sweden, 28/08/17-01/09/17, L.M. Lechuga

*The potential of photonic point-of-care nanobiosensors for high-value diagnostics*, **NanoBio&Med2017**, Barcelona, Spain, 22-24/11/17, L.M. Lechuga

### Invited

*Nanophotonic point-of-care interferometric biosensors for high-value diagnostics*, **Workshop in New Concepts in Biosensing**, Dead Sea, Israel, 12-16/02/17, L.M. Lechuga

*Nanophotonic point-of-care devices for ultrasensitive label-free analysis*, **PITTCON 2017**. Session of Point-of-care and wearable sensors, Chicago, USA, 05-09/03/17, L.M. Lechuga

*Photonic lab-on-a-chip nanobiosensors for early diagnostics at the point-of-care*, **European Conference on Integrated Optics (ECIO´ 2017)**, Eindhoven, Netherlands, 03-05/04/17, L.M. Lechuga

*Ultrasensitive and portable lab-on-a-chip biosensors for environmental in-situ control, Advanced Environmental, Chemical, and Biological Sensing Technologies XIII. SPIE Symposium on Defense + Commercial Sensing*, Anaheim, California, USA, 09-13/04/17, L.M. Lechuga

*The potential of nanophotonic lab-on-chip biosensors for high-value diagnostics, Conference on Lasers and Electro-Optics Europe (CLEO/Europe) and the European Quantum Electronics Conference (EQEC) 2017. Symposium Optical Sensing and Metrology (CH)*, Munich, Germany, 25-29/06/17, L.M. Lechuga

*The potential of nanophotonic lab-on-chip biosensors for high-value point-of-care diagnostics, Workshop Dpto de Nanotecnología Química y Biomolecular*, 50 años del CID, Barcelona, Spain, 14/09/17, L.M. Lechuga

*Del laboratorio al mercado: creación de empresas en Nanobiotecnología, SCIENCE+ 2017*, Bilbao, Spain, 18-20/09/17, L.M. Lechuga

*Decoding the epigenome for cancer diagnosis with label-free biosensor devices, ESNAM Summer School in Nanomedicine*, Barcelona, Spain, 28-29/09/17, L.M. Lechuga

*Nanophotonic lab-on-chip biosensor platforms for ultrasensitive analysis at the point-of-care, MicroNanoConference*, Amsterdam, Netherlands, 12-13/12/17, L.M. Lechuga

### Oral

*Nanophotonic interferometric immunosensor for label-free and real-time monitoring of chemical contaminants in marine environment, SPIE Defense + Commercial Sensing (DCS) 2017*, Anaheim, USA, 09-13/04/17, B. Chocarro, S. Herranz, A. Fernández, M.P. Marco, J. Sanchís, M. Farre, L.M. Lechuga

*Vertical Adiabatic Taper for Efficient In-coupling in Nano-interferometric Waveguide Biosensors, CLEO Europe 2017*, Munich, Germany, 25-29/06/17, D. Grajales, A. Fernández-Gavela, C. Domínguez, L.M. Lechuga

*Metallic nanostructures based on Blu-ray discs for multiplexed Plasmonic biodetection, VIII International Congress on Analytical Nanoscience and Nanotechnology (NyNA 2017)*, Barcelona, Spain, 03-05/07/17, G.A. López-Muñoz, M. C. Estevez, A. Homs-Corbera, M. Berenguel-Alonso, J. Alonso-Chamarro, L.M. Lechuga

*Novel interferometric nanosensor for CO<sub>2</sub> detection using nanoZIF-8 MOFs as specific receptors, VIII International Congress on Analytical Nanoscience and Nanotechnology (NyNA 2017)*, Barcelona, Spain, 03-05/07/17, B. Chocarro, D. MasPOCH, L.M. Lechuga

### Poster

*Simulation and Experimental Evaluation of Optical Chirp Modulation for Bimodal Waveguide Interferometer Biosensors, ECIO 2017*, Eindhoven, Netherlands, 03-05/04/17, D. Grajales, J.R. Sendra, L.M. Lechuga

*Cryptophane-Cladded Interferometric Waveguide Sensor for Aqueous Methane Detection, CLEO 2017*, San Jose, California, USA, 14-19/05/17, J. Jágerská, F.T. Dullo, S.M. Lindecrantz, J.M. Börgers, J.H. Hansen, L.M. Lechuga, O.G. Hellesø

*Multiplexed detection of alternative spliced mrna isoforms for cancer detection using a Bimodal Waveguide interferometer biosensor, VIII International Congress on Analytical Nanoscience and Nanotechnology (NyNA 2017)*, Barcelona, Spain, 03-05/07/17, D. Grajales, C.S. Huertas, L.M. Lechuga

*Rapid detection of Sepsis with a Point-of care and label free microarray platform, VIII International Congress on Analytical Nanoscience and Nanotechnology (NyNA 2017)*, Barcelona, Spain, 03-05/07/17, N. Fabri-Faja, O. Calvo, M.-C. Estévez, J. Pello, R.A. Terborg, F. Yesilköy, P. Soetaert, M. Rabaey, H. Altug, V. Pruneri, L.M. Lechuga

*Development of a low-cost Point-of-care test for Tuberculosis detection, VIII International Congress on Analytical Nanoscience and Nanotechnology (NyNA 2017)*, Barcelona, Spain, 03-05/07/17, P. Ramírez, D. Martens, P. Bienstman, M. Singh, A.A. Elamin, W. Van Roy, R. Vos, P. Soetaert, B. Anton, H. Becker, L.M. Lechuga

*Localised Surface Plasmon Resonance biosensor for the monitoring of Sintrom® therapeutic drug in plasma, VIII International Congress on Analytical Nanoscience and Nanotechnology (NyNA 2017)*, Barcelona, Spain, 03-05/07/17, E.C. Peláez, M-C. Estevez, J-P. Salvador, M-P. Marco, L.M. Lechuga

*Development of a low-cost Point-of-care test for Tuberculosis detection, µTAS2017. 21<sup>st</sup> International Conference on Miniaturized Systems for Chemistry and Life Sciences*, Savannah, Georgia, USA, 22-26/10/17, B. Anton, P. Ramírez, D. Martens, P. Bienstman, M. Singh, A.A. Elamin, W. Van Roy, R. Vos, P. Soetaert, L.M. Lechuga, H. Becker

*Novel photonic nanosensor integrating MOFs as specific receptors for gas sensing, 2<sup>nd</sup> European Conference on Metal- Organic Frameworks and Porous Polymers (EuroMOF)*, Delft, Netherlands, 29/10/17-1/10/17, B. Chocarro-Ruiz, J. Pérez, C. Avci, D. MasPOCH, L.M. Lechuga



### Invited seminar

*Nanophotonics Point-of-Care Biosensors for ultrasensitive diagnosis, Universitat de Barcelona*, Barcelona, Spain, 31/01/17, L.M. Lechuga

*Nanophotonics "Lab-on-a-chip" biosensors for portable diagnostics, RMIT University*, Melbourne, Australia, 23/02/17, L.M. Lechuga

*Nanophotonics Point-of-Care Biosensors for ultrasensitive diagnosis, University of Cincinnati*, Cincinnati, USA, 09/03/17, L.M. Lechuga

*Portable Optical Biosensors as the Next Diagnostics Generation for Environmental Protection, Institut Català de Recerca de l'Aigua (ICRA)*, Girona, Spain, 23/05/17, L.M. Lechuga

*Ultrasensitive "Lab-on-a-chip" nanophotonic biosensors for point-of-care diagnostics, Mackenzie University*, Sao Paulo, Brazil, 07/08/17, L.M. Lechuga

*Nanophotonic lab-on-chip biosensors for point-of-care diagnosis, School of Electrical and Computer Science*, University of Campinas, Campinas, Brazil, 10/08/17, L.M. Lechuga

*Nanophotonic lab-on-chip biosensors for point-of-care diagnosis, University of São Paulo*, São Carlos, Brazil, 18/08/17, L.M. Lechuga

*Nanophotonic lab-on-chip biosensors for point-of-care diagnosis, Centro de Tecnologia da Informação Renato Archer-CTI*, Campinas, Brazil, 24/08/17, L.M. Lechuga

*The future of the clinical diagnostics: point-of-care nanobiosensor devices, BioForum, series of Seminars on Molecular Biology at the University of the Basque Country*, Bilbao, Spain, 20/09/17, L.M. Lechuga

TEDx UPValència. **Imagine That**, Valencia, Spain, 17/02/17, L.M. Lechuga

### **Invited lecture**

*Silicon Photonics Biosensors*, **1<sup>st</sup> Photonic Integration Week**, Valencia, Spain, 16-18/01/17, L.M. Lechuga

*Nanomedicine: the Future of Health Care*, **Seminar V Anniversary SRUK: Tiny science, the science and applications behind nanotechnology**. Instituto Cervantes, Manchester, United Kingdom, 08/05/17, L.M. Lechuga

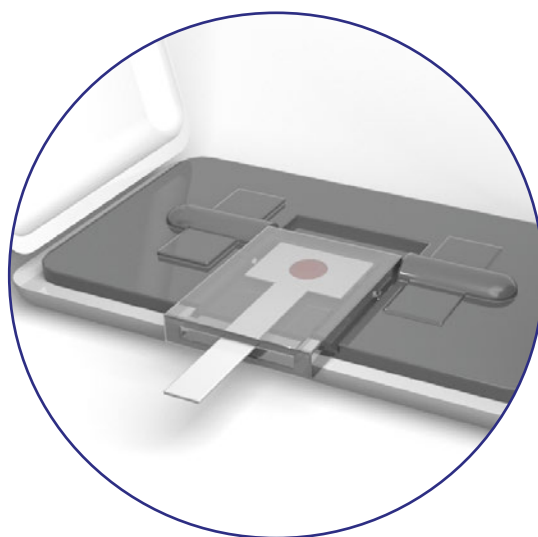
*Nanodispositivos biosensores como herramientas avanzadas en el diagnóstico clínico*, **Foro Científico “Aplicaciones Científicas en Nanomedicina”**. Ilustre Colegio de Médicos de Zaragoza, Zaragoza, Spain, 30/05/17, L.M. Lechuga

*Photonic lab-on-a-chip sensor technologies*, **Advanced Study Course on Optical Chemical Sensors (ASCOS 2017). Biochemical sensors in medicine**, Castle Trest, Czech Republic, 20-27/07/17, L.M. Lechuga

*El futuro del diagnóstico clínico: nanodispositivos biosensores point-of-care*, **Ciclo de Conferencias: “Desafíos y oportunidades de la NANOTECNOLOGÍA”**. Real Academia Galega de Ciencia, Santiago de Compostela, Spain, 21/11/17, L.M. Lechuga

*Nanomedicine: combining Nanotechnology and Medicine for the Future Health Care*, **Taller Internacional: Tuberculosis como modelo de integración de ciencias ómicas y nanotecnología**, Universidad Libre, Barranquilla, Colombia, L.M. Lechuga

*Nanophotonic biosensors for the direct and label-free detection of miRNAs in untreated clinical samples*, **Workshop NANOPLASMIRNA “The promise of miRNA profiling in medical diagnostics: clinical, analytical and technological challenges**, Milan, Italy, 15/12/17, L.M. Lechuga



### PARTICIPATED CONGRESSES

**Advanced Environmental, Chemical, and Biological Sensing Technologies XIII. SPIE Symposium on Defense + Commercial Sensing**, Anaheim, California, USA, 09-13/04/17, *Co-Chair*, L.M. Lechuga

**VIII International Congress on Analytical Nanoscience and Nanotechnology (NyNA 2017)**, Barcelona, Spain, 03-05/07/17, *Co-Chair*, L.M. Lechuga

**5<sup>th</sup> International Conference on Photonics, Optics and Laser Technology - PHOTOPTICS 2017**, Porto, Portugal, 27/02/17 - 01/03/17, *International Scientific Programme Committee*, L.M. Lechuga

**META´ 2017. the 8<sup>th</sup> International Conference on Metamaterials, Photonic Crystals and Plasmonics**, Incheon-Seoul, Korea, 25-28/07/17, *Scientific Technical Programme*, L.M. Lechuga

**14<sup>th</sup> IEEE International Conference on Group IV Photonics 2017 (GFP2017)**, Berlin, Germany, 23-25/08/17, *Scientific Programme Committee and Technical Programme Subcommittee “Sensing and Instrumentation”*, L.M. Lechuga

### COURSES

Laura Lechuga, **Organiser** of *10<sup>th</sup> Advanced Study Course on Optical Chemical Sensors (ASCOS) 2017*, 20-27/07/17, Trest, Czech Republic

Enelia Cristina Pélaez Gutiérrez, **Speaker** in the *Biosensors Specialisation Course*, 3/12/17, Bogotá, Colombia

MCarmen Estévez, **Speaker** at the *Poseidon Summer School 2017 - Photonics for Health*, 18-22/06/17, San Martino di Castrozza, Italy

### AWARDS

Laura M. Lechuga **was selected for inclusion in AcademiaNet: The Portal to Excellent Women Academics**.

Blanca Chocarro, **won the Best Poster Award** at the 2<sup>nd</sup> European Conference on Metal-Organic Frameworks and Porous Polymers (EuroMOF), 29/10/17 – 01/11/17, Delft University of Technology, Delft, Netherlands

Blanca Chocarro, **Best Poster Award**, III Severo Ochoa Scientific Workshop, 12-13/06/2017, Bellaterra, Barcelona

Daniel Grajales, **Best Poster Award**, 19<sup>th</sup> edition of the European Conference on Integrated Optics (ECIO), 3-5/04/17, Eindhoven University of Technology, Netherlands

Nuria Fabri, **first prize of the Student Project Competition**, 10<sup>th</sup> Advanced Study Course on Optical Chemical Sensors (ASCOS) 20-27/07/17, Trest, Czech Republic

Patricia Ramirez, **Best Poster Award**, VIII International Congress on Analytical Nanoscience and Nanotechnology (NyNA 2017), 3-5/07/17 Barcelona, Spain

# Nanostructured Functional Materials Group

## Main Research Lines

- **Nanoscale functional polymers for health and social welfare:**
  - Catechol-based polymers
  - Engineering polymers for optimal micro/nanoencapsulation
  - Coordination polymers
- **Light harvesting and chromogenic nanomaterials for energy saving:**
  - Photochromism
  - Thermochromism
  - Fluorescence
  - Upconversion
- **Hybrid devices and 2D materials for emerging technologies:**
  - 2D coordination polymers
  - Active molecular nanostructures on surfaces



## GROUP MEMBERS

## GROUP LEADER



CSIC Research Scientist  
Dr Daniel Ruiz-Molina

Daniel Ruiz-Molina earned his PhD in polyradical dendrimers at the Institut de Ciència de Materials de Barcelona (ICMAB-CSIC) under Prof. Jaume Veciana. He then took a postdoctoral position at the University of California San Diego (USA), where he spent three years working on single molecule magnets and molecular switches.

Since 2001 he has held a permanent position as a Spanish National Research Council researcher, most recently at the ICN2, where he is the leader of the Nanostructured Functional Materials Group. His main research areas include the fabrication of hybrid colloids and surfaces, biomimetic functional nanostructures, and micro- or nanoparticles for smart applications and encapsulation and delivery systems.

Ayala García, Àlex, Visiting PhD Student  
Bellacanzone, Christian, Severo Ochoa PhD Student  
Casagualda Clapés, Carolina, Visiting PhD Student  
Chen, Jing, Visiting Undergraduate Student  
Contreras Pareda, Noemí, La Caixa PhD Student  
Frías, Carolina, Technician  
García Martínez, Beatriz, Specialised Technician  
García Pardo, Javier, Severo Ochoa Postdoctoral Researcher  
Giró, Roger, Visiting Master's Student  
González Monje, Pablo, Specialised Technician  
González Ros, Cristina, Visiting Undergraduate Student  
Hayati, Payam, Visiting Master's Student  
Julià Lopez, Àlex, PhD Student

Lorente Casado, Helena, Visiting Undergraduate Student  
Lorenzo Rivera, Julia, Researcher  
Magerramov, Ruslan, Visiting Master's Student  
Moghzi, Faezeh, Visiting PhD Student  
Montpeyó García-Moreno, David, PhD Student  
Moreno Villaécija, Miguel Angel, FPI PhD Student  
Nayarassery, Adarsh, CSIC Postdoctoral Researcher  
Novio, Fernando, Senior Scientist  
Otaegui Rabanal, Jaume, Visiting Master's Student  
Rivas Dapena, Anton, Internship Student  
Roscini, Claudio, Senior Scientist  
Ruiz-Molina, Daniel, CSIC Research Scientist and Group Leader  
Sedó Vergara, Josep, Senior Scientist



Lecina, Segura, Visiting Undergraduate Student

Serra Capdevila, Albert, Visiting Undergraduate Student

Solórzano Rodríguez, Rubén, Visiting PhD Student

Suárez García, Salvio, FPI-Severo Ochoa PhD Student

Tello Valero, Alexis, Visiting Undergraduate Student

Torrés Pierna, Hector, Visiting PhD Student

Vázquez Mera, Nuria Alexandra, Postdoctoral Researcher

Verdini, Emanuela, Master's Fellowship Student

Mao, Xiaoman, La Caixa-Severo Ochoa PhD Student



## NEW PROJECTS & MILESTONES

The goal of the Nanostructured Functional Materials or "NANOSFUN" group is to develop new routes to molecular nanostructures with properties inspired in nature and smart responses to external stimuli. As such work continued in 2017 on novel catechol-based coatings and wet adhesives that reproduce the sticking power of marine mussels, as well as the development of nanoencapsulation strategies for photoactive species with potential photophysical and chemical applications. The group also has a strong line in photo- and thermochromism. New this year are lines devoted to the development of coordination polymers for theranostic applications, and the synthesis of 2D coordination flakes for electronic applications.



## PUBLICATIONS

**Copolymerization of a catechol and a diamine as a versatile polydopamine-like platform for surface functionalization: The case of a hydrophobic coating.** S Suárez-García, J Sedó, J Saiz-Poseu, D Ruiz-Molina, *Biomimetics*; **2 (4)**: 221, 2017

**Dynamics of Novel Photoactive AgCl Microstars and Their Environmental Applications.** J. Simmchen, A. Baeza, A. Miguel-Lopez, M. M. Stanton, M. Vallet-Regí, D. Ruiz-Molina, S. Sánchez, *ChemNanoMat*; **3 (1)**: 65-71. 2017. IF: 2.937

**Ligand and solvent effects in the formation and self-assembly of a metallocupramacrocyclic cage.** Adarsh N.N., Chakraborty A., Tarrés M., Dey S., Novio F., Chattopadhyay B., Ribas X., Ruiz-Molina D., *New Journal of Chemistry*; **41 (3)**: 1179-1185. 2017. IF: 3.269

**Photochromism of dihydroazulene-based polymeric thin films,** Torres-Pierna H., Roscini C., Vlasceanu A., Broman S.L., Jevric M., Cacciarini M., Nielsen M.B., *Dyes and Pigments*; **145**: 359-364. 2017. IF: 3.473

**Polyamide-polyamine cryptand as dicarboxylate receptor: Dianion binding studies in the solid state, in solution, and in the gas phase.** Chakraborty S., Saha S., Lima L.M.P., Warzok U., Sarkar S., Akhuli B., Nandi M., Bej S., Adarsh N.N., Schalley C.A., Delgado R., Ghosh P., *Journal of Organic Chemistry*; **82 (19)**: 10007-10014. 2017

**Recent advances in porous nanoparticles for drug delivery in antitumoral applications: inorganic nanoparticles and nanoscale metal-organic frameworks,** Baeza A., Ruiz-Molina D., Vallet-Regí M., *Expert Opinion on Drug Delivery*; **14 (6)**: 783-796. 2017. IF: 5.434

**Replacing nitrogen by sulfur: From structurally disordered eumelanins to regioregular thiomelanin polymers,** Iacomino M., Mancebo-Aracil J., Guardingo M., Martín R., D'Errico G., Perfetti M., Manini P., Crescenzi O., Busqué F., Napolitano A., d'Ischia M., Sedó J., Ruiz-Molina D., *International Journal of Molecular Sciences*; **18 (10)**. 2017. IF: 3.226

**Sonochemical synthesis and characterization of a novel hetero-binuclear metal organic nano polymer based on picolinic acid ligand,** Hayati P., Sori B., Rezvani A.R., Morsali A., Gutierrez A., *Journal of Molecular Structure*; **1150**: 404-410. 2017. IF: 1.753

**Sonochemical synthesis, characterization, and effects of temperature, power ultrasound and reaction time on the morphological properties of two new nanostructured mercury(II) coordination supramolecular compounds,** Hayati P., Rezvani A.R., Morsali A., Molina D.R., Geravand S., Suarez-Garcia S., Villaecija M.A.M., García-Granda S., Mendoza-Meroño R., Retailleau P., *Ultrasonics Sonochemistry*; **37**: 382-393. 2017. IF: 4.218

**Surface Functionalization of Metal-Organic Framework Crystals with Catechol Coatings for Enhanced Moisture Tolerance,** Castells-Gil J., Novio F., Padial N.M., Tatay S., Ruiz-Molina D., Martí-Gastaldo C., *ACS Applied Materials and Interfaces*; **9 (51)**: 44641-44648. 2017. IF: 7.504

**Synthesis and characterization of a new nano lead(II) 0-D coordination supramolecular compound: A precursor to produce pure phase nano-sized lead(II) oxide,** Fard M.J.S., Hayati P., Naraghi H.S., Tabeie S.A., *Ultrasonics Sonochemistry*; **39**: 129-136. 2017. IF: 4.218

**Synthesis and Characterization of PtTe<sub>2</sub> Multi-Crystallite Nanoparticles using Organotellurium Nanocomposites,** Fernández-Lodeiro J., Rodríguez-González B., Novio F., Fernández-Lodeiro A., Ruiz-Molina D., Capelo J.L., Santos A.A.D., Lodeiro C., *Scientific Reports*; **7 (1)**. 2017. IF: 4.259

**Synthesis of Polydopamine-Like Nanocapsules via Removal of a Sacrificial Mesoporous Silica Template with Water,** Nador F., Guisasola E., Baeza A., Villaecija M.A.M., Vallet-Regí M., Ruiz-Molina D., *Chemistry - A European Journal*; **23 (12)**: 2753-2758. 2017. IF: 5.317

**Guest Editor - Bioinspired Catechol-Based Systems: Chemistry and Applications,** M d'Ischia, D Ruiz-Molina, *Biomimetics*; **2 (4)**: 25, 2017



## PROJECTS

*MICROREP, Microcápsulas inteligentes con repelentes de mosquitos y fragancias de aplicación en textiles que eviten la propagación de enfermedades tropicales,* funded by **MINECO**, 01/09/16 to 31/12/19, Daniel Ruiz-Molina

*NanoSVim, Materiales nanoestructurados de índice variable de aplicación en la industria óptica oftálmica,* funded by **MINECO**, 01/09/16 to 31/12/18, Daniel Ruiz-Molina

*TERACAT, Materiales Basados en Catecoles para Teranóstica de la Enfermedad de Parkinson,* funded by **MINECO**, 01/01/16 to 31/12/18, Daniel Ruiz-Molina



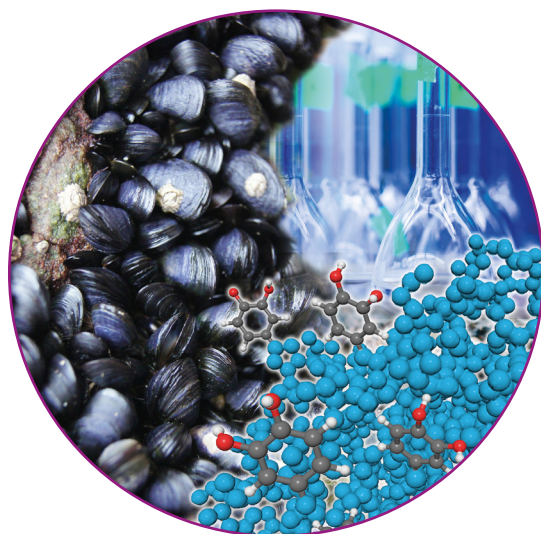
## TECHNOLOGY TRANSFER

**European patent (EP) application ICN2PAT\_07\_17, Chatecol derivatives and use thereof,** with Ref. EP17382539 and priority date 03/08/17  
Inventors: Daniel Ruiz-Molina (CSIC), Josep Sedó (ICN2), Juan Mancebo (ICN2)

**Patent ICN2PAT\_05\_16**, Película de material polimérico con propiedades termo-fotocrómicas para regulación del color de superficies acristaladas y materiales plásticos, with Ref. PCT/ES2017/070264 on 28/04/2017  
Inventors: Daniel Ruiz-Molina (CSIC), Claudio Roscini (ICN2), Alex Julià (ICN2)

**Industry collaboration** *Estudiar los efectos del veneno de abeja frente a enfermedades neurodegenerativas: microencapsulación, biodisponibilidad por vía oral y efectos neuroprotectores en peces cebrá y roedores*, with project ref. ICN2PRJ\_21\_17\_MICROVAN\_DR and signature date 17/03/17

**Industry collaboration** *Photochromes development*, with project ref. ICN2PRJ\_01\_17\_FUTURECHROMES\_RD2 and signature date 29/03/17



## CONTRIBUTIONS

### Plenary

*Novel (coordination) polymer nanoparticles for advanced theranostics*, **BioBilbao2017, X Reunión Científica de Bioinorgánica**, Bilbao, Spain, 9-12/07/17, D. Ruiz-Molina

*Plenary, Catechol-based adhesives and coatings: a biomimetic synthetic approach*, **XXI Simposio Nacional de Química Orgánica (Sociedad Argentina Química Orgánica)**, Potrero de los Funes, San Luis, Argentina, 8-11/11/17, D. Ruiz-Molina

### Invited

*Spin crossover on 2-D coordination polymer flakes*, **Chem2DMat**, Strasbourg, France, 22-26/08/17, D. Ruiz-Molina

*Functional coordination polymers at the nanoscale: old materials new tricks*, **9<sup>th</sup> Workshop of the Department of Chemical and Biomolecular Nanotechnology (IQAQ-CSIC) for the 50th anniversary of the Centre for Research and Development (CID)**, Barcelona, Spain, 14/09/2017, D. Ruiz-Molina

### Oral

*Spin Crossover in an Exfoliated 2D Coordination Polymer*, **Scientific Workshop ECOSTBio**, Madrid, Spain, 30/01/2017, S. Suarez

*Amorphous coordination polymer colloids: Looking for novel biomedical applications based on the metal-ligand interplay*, **7<sup>th</sup> International Colloids Conference**, Sitges, Spain, 18-21/06/17, F. Novio

*Sonochemical synthesis of new 2D coordination polymer compounds*, **XXXVI Biennial Meeting of the Spanish Royal Society of Chemistry**, Sitges, Spain, 25-29/06/17, P. Hayati

*Tunable optical properties in conjugated polymers nanoparticles*, **11<sup>th</sup> International Symposium on Flexible Organic Electronics (ISFOE 2017)**, Thessaloniki, Greece, 01-08/07/17, C. Bellacanzone

*Temperature Controlled Switchable Photochromism*, **28<sup>th</sup> International Conference on Photochemistry (ICP 2017)**, Strasbourg, France, 16-21/07/17, C. Roscini

*Crystal structure of human carboxypeptidase O, the missing player in dietary protein digestion*, **XIV Jornada Científica del Departament de Bioquímica i Biologia Molecular, UAB**, Bellaterra, Spain, 06/07/2017, J. Garcia-Pardo

*Thermally Switchable Upconversion Emission*, **28<sup>th</sup> International Conference on Photochemistry (ICP 2017)**, Strasbourg, France, 16-21/07/17, C. Roscini

*Dopamine-Based Coordination Polymer Nanoparticles For Biomedical Applications*, **European Congress and Exhibition on Advanced Materials and Processes (EUROMAT) 2017**, Thessaloniki, Greece, 17-22/09/17, J. Garcia-Pardo

*Polymerization of catechols with ammonia: a successful approach for biocompatible polydopamine-like coatings in health*, **EUROMAT 2017 (European Congress and Exhibition on Advanced Materials and Processes)**, Thessaloniki, Greece, 17-22/09/17, D. Ruiz-Molina

*Novel (coordination) polymer nanoparticles for advanced theranostics*, **EUROMAT 2017 (European Congress and Exhibition on Advanced Materials and Processes)**, Thessaloniki, Greece, 17-22/09/17, D. Ruiz-Molina

*Spectral shifts in waxes*, **Shift 2017**, Tenerife, Spain, 13-17/11/17, C. Roscini

### Poster

*Contrast agents for medical imaging based on Coordination Polymer Particles (CPP-CA)*, **First Young Spanish ESMI Group Meeting (ySMIN)**, Madrid, Spain, 30/01/2017, F. Novio

*Dual T1/T2 NCP-based novel contrast agents for brain tumor MRI: a preclinical study*, **XIV Jornada Científica del Departament de Bioquímica i Biologia Molecular, UAB**, Bellaterra, Spain, 06/06/2017, S. Suarez

*Nanoencapsulation of protein inhibitors. A novel strategy for gastric diseases therapy*, **7<sup>th</sup> International Colloids Conference**, Sitges, Spain, 18-21/06/17, D. Montpeyó

*Synthesis of two catechol-polyethylene glycol derivatives. Studies on a first approach for their polymerisation to construct new nanocarriers*, **XXXVI Biennial Meeting of the Spanish Royal Society of Chemistry**, Sitges, Spain, 25-29/06/17, D. Montpeyó, C. Casagualda

*New chromogenic materials with liquid-like behaviour based on microcapsules*, **9<sup>th</sup> Training School on Microencapsulation**, Berlin, Germany, 11-14/09/17, P. González

*Thin film deposition and growth of graphene-like 2-D Metal-Organic Frameworks (MOFs) for electronics applications*, **2D Materials and Interfaces for Spintronics**, Bellaterra, Spain, 23-25/10/17, N. Contreras

*Synthesis, characterization and ultrasound-assisted delamination of two 2-D cadmium-based coordination polymers*, **ECOSTBio: Seventh Scientific Workshop**, Dublin, Ireland, 14-15/12/17, N. Contreras

*Invited seminar*

*Novel (Coordination) Polymer Nanoparticles for Advanced Theranostics, NanoTech Poland International Conference & Exhibition, Poznan, Poland, 1-3/06/17, D. Ruiz-Molina*

*Bioinspired adhesives and coatings: the case of catechol chemistry, Training School: Chem2Nature, Porto, Portugal, 5-9/06/17, D. Ruiz-Molina*

*Catechol-based adhesives and coatings: a biomimetic synthetic approach, Univ. Tecnológica Metropolitana, Santiago de Chile, Chile, 02/11/17, D. Ruiz-Molina*

*Polímeros de coordinación: nuevas perspectivas y aplicaciones a la nanoescala, Departamento de Ingeniería Química, Biotecnología y Materiales, Universidad de Chile, Santiago de Chile, Chile, 03/11/17, D. Ruiz-Molina*

*Catechol-based adhesives and coatings: a biomimetic synthetic approach, POLYMAT, Donostia, Spain, 23/11/17, D. Ruiz-Molina*

*Novel nanocarriers for drug release and imaging: from nanoemulsions to out-of-equilibrium reactions, Institute for Research in Biomedicine, Barcelona, Spain, 14/12/17, D. Ruiz-Molina*

*Invited conference*

*Polymer Nanoparticles for Theranostic Applications, ALBA Synchrotron: Applied Nanotechnology, Cerdanyola, Barcelona, Spain, 21/01/17, F. Novio*

*Construeix el teu futur, Jornada de Orientació Profesional para alumnos de bachillerato, Viladecans, Barcelona, 06/02/17, M.A. Moreno*

*Recientes avances de la nanomedicina y su aplicación en terapia/diagnosis clínica, Consorci Sanitari de Terrassa - Hospital de Terrassa, Terrassa, Spain, 25/05/17, F. Novio*

*Biomimètica: La natura inspira els materials del futur, 11<sup>th</sup> Science Festival, Barcelona, Spain, 27/05/17, M.A. Moreno*

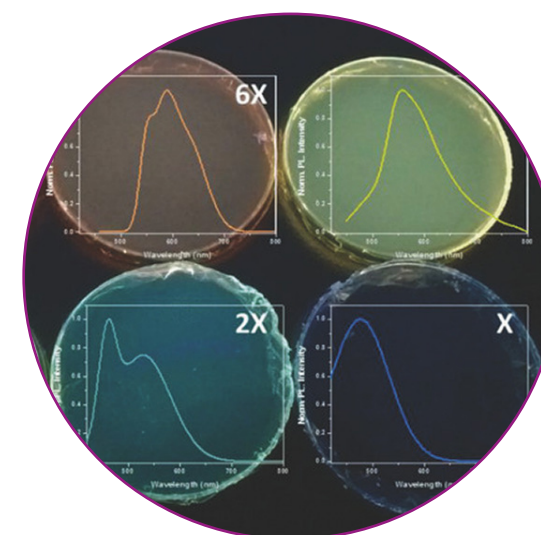
**EUROMAT 2017 - Session F3: Nanobiomaterials and nanotechnology for implants, devices and theranostics, Thessaloniki, Greece, 17-22/09/17, Co-organiser, D. Ruiz-Molina**

**MetDrugs Scientific Meeting "Metdrugs: At the frontier between coordination chemistry and nanotechnology", Bellaterra, Barcelona, 30/11/2017, Scientific Committee, F. Novio, D. Ruiz-Molina**

Dr F. Novio, **Associate Professor A3.5 in the Universitat Autònoma de Barcelona's Dept. Chemistry**, academic year 2016/17, 150 hours (15 credits), UAB

Dr F. Novio, **Master's in Advanced Nanoscience and Nanotechnology. Subject: Nanotechnology for Therapy and Remediation**, 6 hours, Faculty of Science, UAB

C. Roscini, **Master's in Industrial Chemistry and Introduction to Chemical Research. Subject: Micro- and Nanocapsules for Controlled Delivery of Functional Molecules**, 3 hours, Faculty of Sciences, UAB



# Nanostructured Materials for Photovoltaic Energy Group

## Main Research Lines

- **Photovoltaics: Next-generation thin film, organic, hybrid, dye-sensitised, halide perovskite and all-oxide solar cells**
- **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**



## GROUP MEMBERS

**Bénédicte Veronique, Saliba**, Master's Fellowship Student

**Echeverria Troya, Fernando**, PhD Fellowship Student

**Gallardo Ponce, Norma Janette**, Visiting Undergraduate Student

**Lira Cantu, Mónica**, CSIC Tenured Scientist and Group Leader

**Mergny, Loïs**, Visiting PhD Student

**Mingorance Ferrer, Alba**, Severo Ochoa PhD Student

**Morales Melgares, Anna**, Undergraduate Fellowship Student

**Pereyra Marina, Jose Carlos**, PhD Fellowship Student

**Perez-Tomas, Amador**, Severo Ochoa Senior Postdoctoral Researcher

**Reyna Velázquez, Yegraf**, PhD Fellowship Student

**Sánchez Sierras, Óscar**, Visiting Master's Student

**Santigosa Murillo, Elia**, PhD Fellowship Student

**Shirley, Ian**, PhD Fellowship Student

**Tanenbaum, David Michael**, Visiting Senior Researcher

**Xie, Haibing**, Severo Ochoa Postdoctoral Researcher

## GROUP LEADER



CSIC Tenured Scientist  
Dr Mónica Lira-Cantú

Mónica Lira-Cantú (Chemistry, 1992) obtained her Master's and PhD degrees in materials science at the Institut de Ciència de Materials de Barcelona (ICMAB) and the Universitat Autònoma de Barcelona in 1995 and 1997, respectively. She then completed her postdoctoral work in the form of a contract between Schneider Electric and ICMAB in 1998. From 1999 to 2001 she worked as a permanent senior staff chemist at ExxonMobil Research & Engineering (formerly Mobil Technology Co) in New Jersey (USA), establishing a group on energy-related applications.

Besides her role as group leader of the ICN2 Nanostructured Materials for Photovoltaic Energy Group, she is currently a visiting professor at the Laboratory of Photomolecular Science (LSPM) of the École Polytechnique Fédérale de Lausanne.

Dr Lira-Cantu has received different awards and fellowships as a visiting scientist at the following laboratories: Universitetet i Oslo (Norway) (ESF, 2003), Risø DTU Nationallaboratoriet (Denmark) (AGAUR, 2004/05) and the Center for Advanced Science and Innovation (Osaka University, Japan) (Canon Foundation in Europe, 2006). She obtained a permanent position in 2007 at the Consejo Superior de Investigaciones Científicas (CSIC), establishing the ICN2 Photovoltaic Energy Group in 2007.

Since then she has directly managed more than 50 researchers, including one visiting professor, five postdoctoral students, eight PhD students (four in progress), over 26 Master's and undergraduate students, two project managers and two technicians. She has been the principal investigator on several national, industrial and European projects, and is the main coordinator of a COST Action involving more than 470 partners from 35 countries and 22 companies to study the stability of organic and perovskite solar cells.

She has coordinated and organised more than 12 scientific conferences and is currently a scientific referee for more than 13 international and European research agencies, and 46 scientific journals. She is part of the editorial board of journals like *Frontiers in Energy Research* and the *Journal of Physics Energy*. She is a member of the advisory board for the Nanotechnology and Chemical Science degree (INCO) of the Instituto Tecnológico y de Estudios Superiores de Monterrey (Mexico).

Her research interests lie in the synthesis and application of nanostructured materials for stable next-generation thin-film solar cells: halide-perovskite, dye-sensitised, all-oxide and organic solar cells. Dr Lira-Cantú has more than 105 publications, among them 90 published papers, 7 patents and 10 book chapters, 1 edited book and several technical reports. Her h-index is 33.



## NEW PROJECTS & MILESTONES

The Nanostructured Materials for Photovoltaic Energy Group has several key objectives, all of them related to the **development of highly-efficient, highly-stable and low-cost solution processable photovoltaic and optoelectronic devices**.

A major goal is the **synthesis of nanostructured materials**, especially those involving transition metal oxides (TMOs) via the application of low-cost and solution processing methods. TMOs have many possible applications as main active materials or barrier layers, though they also find applications as materials for external light management. The application of **low-temperature synthesis methods** (sol-gel, hydrothermal, SILAR, among many others) permits tuning and control of 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. The **functionalisation** of these oxide surfaces is now carried out in our group by anchoring self-assembled monolayers with selected anchoring groups to interact simultaneously with the oxide and the active light harvesting material.

The **stability and lifetime** of optoelectronic devices, especially organic and perovskite solar cells, is a major limitation for these technologies. An important contribution of the group is the study and characterisation of solar cell stability following degradation and characterisation protocols. Prof. Lira-Cantu coordinates a COST Action with a consortium of more than 470 members, among them 60 internationally-recognised research laboratories and 22 companies from 35 countries. **StableNextSol, as the project is**

**known, is related to the stability of organic and perovskite solar cells**. Its goal is to take advantage of the multiple characterisation techniques available through the different partners to elucidate the degradation mechanism of these devices and propose disruptive solutions towards highly stable organic solar cells.

Other interests include the development of self-powered electronic and optoelectronic devices, and flexible and transparent devices for ICT and electronic applications.



## PUBLICATIONS

**Cryogenic characterisation and modelling of commercial SiC MOSFETs**, Woodend, L. J., Gammon, P. M., Shah, V. A., Pérez-Tomás, A., Li, F., Hamilton, D. P., Myronov, M., Mawby, P. A., *Materials Science Forum*; **897**: 557-560. 2017

**Effect of Cs-Incorporated NiO<sub>x</sub> on the Performance of Perovskite Solar Cells**, Kim, H.-S., Seo, J.-Y., Xie, H., Lira-Cantu, M., Zakeeruddin, S. M., Grätzel, M., Hagfeldt, A., *ACS Omega*; **2**: 9074-9079. 2017

**Facile and low cost oxidative conversion of MoS<sub>2</sub> in α-MoO<sub>3</sub>: Synthesis, characterization and application**, Bortoti A.A., Gavanski A.D.F., Velazquez Y.R., Galli A., de Castro E.G., *Journal of Solid State Chemistry*; **252**: 111-118. 2017. IF: 2.299

**Functional oxide as an extreme high-k dielectric towards 4H-SiC MOSFET incorporation**, Russell, S. A. O., Jennings, M. R., Dai, T., Li, F., Hamilton, D. P., Fisher, C. A., Sharma, Y. K., Mawby, P. A., Pérez-Tomás, A., *Materials Science Forum*; **897**: 155-158. 2017

**Heteroepitaxial Beta-Ga<sub>2</sub>O<sub>3</sub> on 4H-SiC for an FET with Reduced Self Heating**, Russell, S. A. O., Perez-Tomas, A., McConville, C. F., Fisher, C. A., Hamilton, D. P., Mawby, P. A., Jennings, M. R., *IEEE Journal of the Electron Devices Society*; **5**: 256-261. 2017

**High-Temperature Electrical and Thermal Aging Performance and Application Considerations for SiC Power DMOSFETs**, Hamilton, D. P., Jennings, M. R., Perez-Tomas, A., Russell, S. A. O., Hindmarsh, S. A., Fisher, C. A., Mawby, P. A., *IEEE Transactions on Power Electronics*; **32**: 7967-7979. 2017

**Incorporation of Counter Ions in Organic Molecules: New Strategy in Developing Dopant-Free Hole Transport Materials for Efficient Mixed-Ion Perovskite Solar Cells**, Zhang J., Xu B., Yang L., Mingorance A., Ruan C., Hua Y., Wang L., Vlachopoulos N., Lira-Cantú M., Boschloo G., Hagfeldt A., Sun L., Johansson E.M.J., *Advanced Energy Materials*; **7 (14)**. 2017. IF: 16.721

**Perovskite solar cells: Stability lies at interfaces**, Lira-Cantú M., *Nature Energy*; **2 (7)**. 2017. IF: 9.086

**Physical characterisation of 3C-SiC(001)/SiO<sub>2</sub> interface using XPS**, Li, F., Vavasour, O., Walker, M., Martin, D. M., Sharma, Y., Russell, S., Jennings, M., Pérez-Tomás, A., Mawby, P. A., *Materials Science Forum*; **897**: 151-154. 2017

**P-type β-gallium oxide: A new perspective for power and optoelectronic devices**, Chikoidze, E., Fellous, A., Perez-Tomas, A., Sauthier, G., Tchelidze, T., Ton-That, C., Thanh Huynh, T., Phillips, M., Russell, S., Jennings, M., Berini, B., Jomard, F., Dumont, Y., *Materials Today (Physics)*; **3**: 118-126. 2017

## BOOKS

**The future of semiconductor oxides in next generation solar cells**, Lira-Cantu, M., 566p, Ed. Elsevier (2017), ISBN: 9780128111659

## PROJECTS

*Nanostructured Materials for Photovoltaic Energy, SGR 2014-2016*, funded by **AGAUR**, 01/01/14 to 30/04/17, Monica Lira-Cantú

*Materiales avanzados y nanotecnologías para dispositivos y sistemas eléctricos, electrónicos y magnetoelectrónicos innovadores*, funded by **MINECO**, 01/12/15 to 30/11/17, Monica Lira-Cantú

*StableNextSol, Stable Next-Generation Photovoltaics: Unravelling Degradation Mechanisms of Organic Solar Cells by Complementary Characterization Techniques (COST ACTION)*, funded by **EC**, 20/03/14 to 19/03/18, Monica Lira-Cantú

*EFFECT, Expanding ferroelectric photovoltaics conventional playground*, funded by **MINECO**, 19/01/17 to 18/01/20, Amador Pérez

*GraPerOS\_PSC, Nanomateriales para celdas solares tipo perovskita de alta eficiencia y estabilidad*, funded by **MINECO**, 30/12/16 to 29/12/19, Monica Lira-Cantú

*ORGENERGY, Materiales orgánicos optoelectrónicos para la energía*, funded by **MINECO**, 01/07/17 to 30/06/19, Monica Lira-Cantú

## CONTRIBUTIONS

### Invited

*Nanostructured Metal Oxides for Organic Perovskite Solar Cells*, **4<sup>th</sup> World Congress and Expo on Nanotechnology and Materials Science**, Barcelona, Spain, 5-7/04/17, M. Lira-Cantú

*Stable Organic and Perovskite Solar Cells employing Oxide Interlayers*, **Thin Film Emerging Photovoltaic and Optoelectronic Technologies (EMETEC)**, Barcelona, Spain, 27-28/04/18, M. Lira-Cantú

*Oxide Interlayers for Stable Organic and Perovskite Solar Cells*, **IECS2017**, Nara, Japan, 14-15/05/17, M. Lira-Cantú

*Oxide Interlayers for Stable Organic and Perovskite Solar Cells*, **International Conference on Hybrid and Organic Photovoltaics (HOPV17)**, Lausanne, Switzerland, 21-24/05/17, M. Lira-Cantú

*Stable Next-Generation Photovoltaics: Unravelling Degradation Mechanisms of Organic Solar Cells by Complementary Characterisation Techniques (StableNextSol)*, **EURO NanoForum 2017 COST Workshop**, Valletta, Malta, 21-23/06/17, M. Lira-Cantú (presented by Dr Francesca Brunetti)

*Stable Organic and Perovskite Solar Cells Employing Oxide Interlayers*, **NATO/NANOAPP Conference 2017**, Bled, Slovenia, 14-18/06/17, M. Lira-Cantú

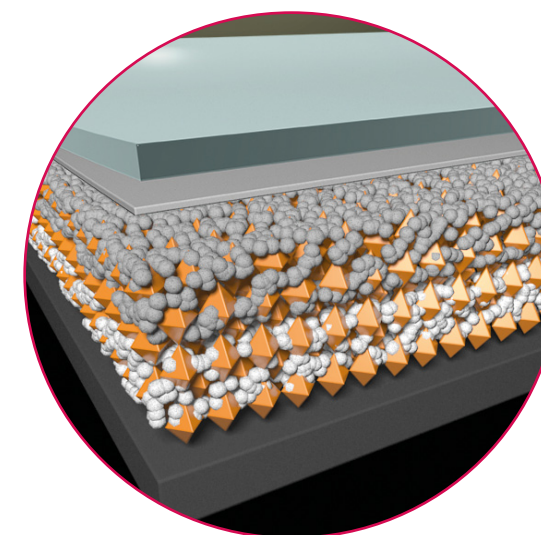
*Metal Oxide Interfaces for Stable Organic Solar Cells*, **14<sup>th</sup> International conference on Electrical and Related Properties of Organic Solids (ERPOS 17)**, Sant Andrews, United Kingdom, 9-13/07/17, M. Lira-Cantú

*Oxide Interlayers for Stable Organic and Perovskite Solar Cells*, **XXVI International Materials Research Congress (IMRC 2017)**, Cancún, Mexico, 20-25/08/17, M. Lira-Cantú

*Stable Next-Generation Photovoltaics: Unravelling Degradation Mechanisms of Organic Solar Cells by Complementary Characterisation Techniques (StableNextSol)* **COST Connect**, Brussels, Belgium, 24/11/17, M. Lira-Cantú

## PARTICIPATED CONGRESSES

**International Conference on Hybrid and Organic Photovoltaics (HOPV17)**, Lausanne, Switzerland, 21-24/05/17, *Session Chair*, M. Lira-Cantú



# Novel Energy-Oriented Materials Group

## Main Research Lines

- Hybrid electrode materials for supercapacitors and hybrid energy storage devices
- Graphene batteries. Nanocarbons for lithium-sulfur batteries
- Nanofluids. Thermal nanofluids for heat transfer in cooling and solar conversion
- Electroactive nanofluids for energy storage in flow cells. Redox flow batteries based on quinones
- Graphene production and development of secondary products (nanofluids, composites for 3D-printing, inks, etc.) for application in energy storage



## GROUP MEMBERS

**Benages Vilau, Raul**, Severo Ochoa Postdoctoral Researcher

**Caban Huertas, Zahilia**, Postdoctoral Researcher

**Fiuza Pérez, Iván Gabriel**, Undergraduate Student

**Gavalierová, Katarína**, Visiting PhD Student  
**Gómez Romero, Pedro**, CSIC Research Professor and Group Leader

**Hernández Cabello, Judith**, Undergraduate Student

**Hosseinzadeh, Batoul**, Visiting PhD Student

**Jiménez Lara, Mauricio**, Undergraduate Student

**Marchante Fernández, Carlos**, Research Engineer

**Nagar, Bhawna**, Severo Ochoa PhD Student

**Rodríguez Laguna, María del Rocío**, Severo Ochoa PhD Student

**Rueda García, Daniel**, PhD Student

**Sánchez Peña, Pilar**, Visiting Master's Student

**Zartenaar, Michael Ramón**, Undergraduate Student

## GROUP LEADER



CSIC Research Prof. Dr Pedro Gómez-Romero

Prof. Pedro Gómez-Romero completed his undergraduate and Master's degrees at the Universitat de València, before going on to earn his PhD in chemistry with distinction at Georgetown University (USA) in 1987. A CSIC researcher since 1990, he worked at the Institut de Ciència de Materials de Barcelona (ICMAB) from 1990 to 2007, spending a sabbatical year as a NATO Senior Research Fellow at the National Renewable Energy Laboratory (USA) in 1998-99. In 2007 he moved to the former Nanoscience and Nanotechnology Research Centre (CIN2) as group leader of the NEO-Energy lab. When CIN2 became the ICN2 in 2013, Prof. Gómez-Romero became group leader of the ICN2 Novel Energy-Oriented Materials Group, heading up projects on hybrid organic-inorganic nanostructures, nanocomposite materials for energy storage and conversion.

Becoming a CSIC Research Professor in 2006, Prof. Gómez-Romero has been a fellow of the Royal Society of Chemistry (UK) since 2014 and was the vice-director of MATGAS from 2010 to 2014. He has authored over 200 scientific publications in international peer-reviewed journals, and is the scientific editor of the books *Functional Hybrid Materials* (P. Gómez-Romero, C. Sánchez (Eds.) (Wiley-VCH 2004)) and *Metal Oxides in Supercapacitors* (D.P. Dubal, P. Gomez-Romero (Eds.) (Elsevier, 2017)). He is also the author of four award-winning popular science books (*Metaevolución. La Tierra en el espejo*, Celeste, 2001; *Un planeta en busca de energía*, Síntesis, 2007; *Creadors de futur*, Bromera, 2016; and *Nanomundo*, Materia/El País, 2016). In 2017 he received the CIDETEC prize for research in electrochemistry.

Group website: <http://www.neoenergy.cat>



## NEW PROJECTS & MILESTONES

This year the group was awarded the CIDETEC prize for scientific research in electrochemistry by the Spanish Royal Society of Chemistry for our contributions to energy storage materials and devices between 2013 and 2016. It should be noted that this time period corresponds precisely to the founding years of the ICN2, when our group consolidated research in the core field of hybrid materials for hybrid energy storage (batteries, supercapacitors, etc.). We are very proud and thankful for this recognition of our efforts.

Meanwhile, our work in graphene has also gone from strength to strength, especially as regards the development of secondary products like nanofluids (both thermal and electroactive) and inks for flexible device printing. We have also gone beyond graphene to develop our own nanocarbon materials. Namely, carbon nanotubes (45-50 nm inner diameter) have been prepared for the first time and are now being studied for many different applications, including as cathodes for Li-S batteries.

### Hybrid materials as improved electrodes for electrochemical supercapacitors

The boundaries between batteries and capacitors are now quickly blurring. Control over nanostructures is of great importance in the design of high-performance energy storage devices. We are developing materials with highly specific surfaces, as well as ultradispersed molecular materials for application in electrochemical supercapacitors with power densities greater than batteries. Examples of this type of electrode, prepared for the first time in our laboratory, include activated carbons or graphene with polyoxometalates or oxide nanoparticles (NANOCARHIBE MAT2012 National Project).

### Nanocarbon materials as cathodes for stable and safer Li-S batteries

The aforementioned carbon nanotubes are being tested to determine their capacity to encapsulate sulfur, act as cathodes in Li-S batteries and, by doing so, increase the stability of this very promising system for extra-high energy density batteries. This application is being pursued as part of an international project funded by NATO's Science for Peace and Security (SPS).

### Eco-friendly high-performance electrodes for rechargeable lithium batteries

This research line includes our work on the optimisation of the micro- and nanostructures of electroactive inorganic materials, such as LiFePO<sub>4</sub> with fractal granularity used in electrodes for lithium batteries. Here the goal is low-cost, safe batteries with faster recharge rates prepared under the mildest conditions in aqueous media (PhD Thesis Zahilia Caban-Huertas).

### Nanofluids

The development of nanofluids, including electroactive (NACARFLOW MAT2015 National Project) and heat transfer nanofluids for both cooling and thermal solar energy conversion is now at full thrust. This is an internationally emergent research line with implications in fundamental science and application in new technologies such as the load-levelling of renewable energies, electric vehicles and high temperature (concentration) solar power electricity generation.

### Graphene and graphene batteries

We are working on various large-scale methods (from mechanical to electrochemical) for the preparation of high-quality graphene and its use in the synthesis of nanohybrid materials. Our materials can be tailor-made for many different applications, but our favourite, and the one we are developing hard in our recent spin-off (EARTHIDAS), takes the form of fast-charging graphene batteries.



## PUBLICATIONS

**Functionalization of Polypyrrole Nanopipes with Redox-Active Polyoxometalates for High Energy Density Supercapacitors**, Dubal D.P., Ballesteros B., Mohite A.A., Gómez-Romero P., *ChemSusChem*; **10 (4)**: 731-737. IF: 7.226

**Mimics of microstructures of Ni substituted Mn<sub>1-x</sub>Ni<sub>x</sub>Co<sub>2</sub>O<sub>4</sub> for high energy density asymmetric capacitors**, Tamboli M.S., Dubal D.P., Patil S.S., Shaikh A.F., Deonikar V.G., Kulkarni M.V., Maldar N.N., Inamuddin, Asiri A.M., Gomez-Romero P., Kale B.B., Patil D.R., *Chemical Engineering Journal*; **307**: 300-310. IF: 6.216

**Influence of texture in hybrid carbon-phosphomolybdic acid materials on their performance as electrodes in supercapacitors**, Palomino P., Suarez-Guevara J., Olivares-Marín M., Ruiz V., Dubal D.P., Gómez-Romero P., Tonti D., Enciso E., *Carbon*; **111**: 74-82. IF: 6.337

**Hurdles to organic quinone flow cells. Electrode passivation by quinone reduction in acetonitrile Li electrolytes**, Rueda-García D., Dubal D.P., Hugenin F., Gómez-Romero P., *Journal of Power Sources*; **350**: 9-17. IF: 6.395

**Ultrathin Mesoporous RuCo<sub>2</sub>O<sub>4</sub> Nanoflakes: An Advanced Electrode for High-Performance Asymmetric Supercapacitors**, Dubal D.P., Chodankar N.R., Holze R., Kim D.-H., Gomez-Romero P., *ChemSusChem*; **10 (8)**: 1771-1782. IF: 7.226

**V<sub>2</sub>O<sub>5</sub> encapsulated MWCNTs in 2D surface architecture: Complete solid-state bendable highly stabilized energy efficient supercapacitor device**, Pandit B., Dubal D.P., Gómez-Romero P., Kale B.B., Sankapal B.R., *Scientific Reports*; **7**. IF: 4.259

**Nanostructured mixed transition metal oxides for high performance asymmetric supercapacitors: Facile synthetic strategy**, Tajik S., Dubal D.P., Gomez-Romero P., Yadegari A., Rashidi A., Nasernejad B., Inamuddin, Asiri A.M., *International Journal of Hydrogen Energy*; **42 (17)**: 12384-12395. IF: 3.582

**Capacitive vs Faradaic Energy Storage in a Hybrid Cell with LiFePO<sub>4</sub>/RGO Positive Electrode and Nanocarbon Negative Electrode**, Cabán-Huertas Z., Dubal D.P., Ayyad O., Gómez-Romero P., *Journal of the Electrochemical Society*; **164 (1)**: A6140-A6146. IF: 3.259

**Ultrahigh energy density supercapacitors through a double hybrid strategy**, Dubal D.P., Nagar B., Suarez-Guevara J., Tonti D., Enciso E., Palomino P., Gomez-Romero P., *Materials Today Energy*; **5**: 58-65

**Direct electrodeposition of imidazole modified poly(pyrrole) copolymers: synthesis, characterization and supercapacitive properties**, Wolfart F., Hryniewicz B.M., Marchesi L.F., Orth E.S., Dubal D.P., Gómez-Romero P., Vidotti M., *Electrochimica Acta*; **243**: 260-269. IF: 4.798

**Asymmetric Supercapacitors Based on Reduced Graphene Oxide with Different Polyoxometalates as Positive and Negative Electrodes**, Dubal D.P., Chodankar N.R., Vinu A., Kim D.-H., Gomez-Romero P., *ChemSusChem*; **10 (13)**: 2742-2750. IF: 7.226

**BiVO<sub>4</sub> Fern Architectures: A Competitive Anode for Lithium-Ion Batteries**, Dubal D.P., Patil D.R., Patil S.S., Munirathnam N.R., Gomez-Romero P., *ChemSusChem*; **10 (21)**: 4163-4169. IF: 7.226



## BOOKS

**Metal Oxides in Supercapacitors**, Deepak P. Dubal and Pedro Gómez-Romero, 292p. Ed. Elsevier, (2017). ISBN: 9780128111697

## PROJECTS

*NaCarFLOW, Nanofluidos basados en Carbones con micro-estructura optimizada y sus híbridos para almacenamiento de energía en celdas de flujo (Plan Nacional MAT2015-68394-R)*, funded by **MINECO**, 01/01/16 to 31/12/18, Pedro Gómez Romero

*NEO-Energy Group Recognized as a Quality Group by Generalitat de Catalunya, (2017\_SGR\_870)*, funded by **Generalitat de Catalunya**, 2018 to 2020, Pedro Gomez-Romero

*DeCaSUB, Development of New Cathodes for Stable and Safer Lithium-Sulfur Batteries.* Science for Peace and Security Program, funded by **NATO**, 15/11/16 to 15/11/19, Pedro Gómez-Romero

*NESTOR Nanomaterials for Energy STORAGE (2014\_SGR\_1505)*, funded by AGAUR, Generalitat de Catalunya, 2014-2016. Dino Tonti (ICMAB), Pedro Gomez-Romero

## TECHNOLOGY TRANSFER

### *Industry collaboration*

*Almacenamiento de Energía Mediante Baterías de Grafeno (Earthdas)*, with project ref. ICN2PRJ\_46\_16\_EARTHIDAS\_RD1 and signature date 04/04/17

## CONTRIBUTIONS

### *Invited*

*Hybrid energy storage. From graphite to graphene, from batteries to supercapacitors*, **International Conference on Advanced Rechargeable Batteries & Allied Materials (ICARBM)**, Pune, India, 8-10/03/17, P. Gomez-Romero, D.P. Dubal

*Nanofluids for energy applications*, **International Conference on Nanomaterials and Nanotechnology**, Madrid, Spain, 30/04/2017, P. Gómez-Romero

*Hybrid electrode materials for hybrid energy storage*, **Conferencia del premio CIDETEC 2016. 38 Reunion del Grupo Especializado de Electroquímica de la RSEQ**, Vitoria, Spain, 05/07/2017, P. Gómez-Romero

*Sustainable energy for a sustainable society. And vice versa Spain as a case study*, **Symposium on Energy, Water and Environmental Sciences. 46<sup>th</sup> World Chemistry Congress. IUPAC 49<sup>th</sup> General Assembly**, São Paulo, Brazil, 9-14/07/17, P. Gómez-Romero

*Graphene and other advanced materials. Materials in search of applications*, **BIT's 4<sup>th</sup> Annual Global Congress of Knowledge Economy**, Qingdao, China, 19-21/09/17, P. Gómez-Romero

*What could be better than graphene for energy storage?*, **GrpChina 2017**, Nanjing, China, 24-26/09/17, P. Gómez-Romero

### *Keynote*

*When Supercapacitors met Batteries. Hybrid Materials for Hybrid Energy Storage*, **Symposium on Energy, Water and Environmental Sciences. 46<sup>th</sup> World Chemistry Congress. IUPAC 49<sup>th</sup> General Assembly**, São Paulo, Brazil, 9-14/07/17, P. Gómez-Romero

### *Plenary*

*New old trends in electrochemical energy storage: From batteries to supercapacitors*, **VI Iberian Symposium on Hydrogen, Fuel Cells and Advanced Batteries (Hyceltec 2017)**, Porto, Portugal, 19-23/6/17, P. Gómez-Romero

### *Oral*

*What could be better than graphene for energy storage?*, **Graphene 2017**, Barcelona, Spain, 28-30/4/17, P. Gomez-Romero

## DISSEMINATION CONTRIBUTIONS

### *Invited conference*

*Energía verde para un planeta azul*, **Instituto IES El Cairat**, Esparreguera, Barcelona, 2/02/2017, P. Gómez-Romero

*Energía en transición: Hacia un modelo sostenible de producción y consumo de energía*, **Instituto Cervantes de Rabat**, Morocco, 23/02/2017, P. Gómez-Romero

*De los nanómetros a los teravatios. Nanomateriales para la energía*, **2<sup>nd</sup> Festival of Nanoscience and Nanotechnology: 10alamos9**, Cosmoaixa Barcelona, 26/04/2017, P. Gómez-Romero

*De los nanómetros a los teravatios. Nanotecnología para un modelo energético sostenible.* **2<sup>nd</sup> Festival of Nanoscience and Nanotechnology: 10alamos9**, Aula Magna de la Casa de Cultura, Girona, 15/11/2017, P. Gómez-Romero

*De las tierras raras al grafeno. Cerrando el círculo de los materiales avanzados*, **Aula d'Extensió Universitaria**, Sant Quirze del Vallés, Barcelona, 22/11/2017, P. Gómez-Romero

*Energía, Medio Ambiente y Economía Circular, Dilluns de Ciència al CSIC*, Residencia d'Investigadors del CSIC, Barcelona, 11/12/2017, P. Gómez-Romero

## COURSES

P. Gómez Romero, **Ponencia del Aula Ortega y Gasset de la Universidad Internacional Menéndez Pelayo, UIMP, Ciencia, Tecnología y Economía Circular**. Santander, 21-22/08/17

## THESES

**Zahilia Caban**, *Alternative approaches for the fabrication of electrodes based on LiFePO<sub>4</sub> as cathodes in LIBs*, 08/09/17, supervised by Prof. Pedro Gómez-Romero

## AWARDS

P. Gomez-Romero, awarded the **2016 CIDETEC Award for Scientific Research in Electrochemistry** for the work carried out by the Novel Energy-Oriented Materials between 2013 and 2016. Awarded in 2017.

# Oxide Nanophysics Group

## Main Research Lines

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



## GROUP MEMBERS

Braz Barroca, Nathalie, Postdoctoral Researcher

Catalán Bernabé, Gustau, ICREA Research Professor and Group Leader

Cordero Edwards, Rohini Kumara, PhD Student

Domingo Marimón, Neus, Senior Researcher

Núñez Toldrà, Raquel, Postdoctoral Researcher

Pach, Elzbieta, Technician

Pérez Tomás, Amador, Severo Ochoa Senior Postdoctoral Researcher

Rodríguez Dominguez, Laura, PhD Student

Sánchez Giménez, Irene, Technician

Senes, Nina, Visiting PhD Student

Spasojevic, Irena, Research Assistant

Stefani, Christina Georgia, Research Assistant

Vales Castro, Pablo, PhD Student

Vásquez Sancho, Fabián Norberto, PhD Student



## GROUP LEADER



ICREA Research Prof.  
Gustau Catalán

Prof. Gustau Catalán earned his degree in physics at the Universitat de Barcelona in 1997 and his PhD in physics at Queen's University of Belfast in 2001. He then took research positions at the Institut Mediterrani d'Estudis Avançats (2002-2004), the Rijksuniversiteit Groningen (University of Groningen, 2004-2005) and the University of Cambridge (2005-2009). In 2009 he was hired as an ICREA Research Professor, joining the former Nanoscience and Nanotechnology Research Centre (CIN2, now the ICN2) as leader of the Oxide Nanophysics Group. In 2012 he earned an ERC Starting Grant to set up the world's first laboratory devoted to nanoscale flexoelectricity.



## NEW PROJECTS & MILESTONES

This was the last financial year of our ERC project on flexoelectricity. This year's flexoelectric highlight has been the discovery that, thanks to flexoelectricity, the mechanical response of piezoelectric crystals to indentation changes when they are turned upside-down. In the case of ferroelectrics, which are switchable piezoelectrics, this means that their mechanical response can also be switched simply by applying a voltage. Interestingly, this implies that a ferroelectric memory "bit" can be read voltage-free, by touch alone. This work, led by Kumara Cordero-Edwards (now Dr Cordero-Edwards!), was published in *Advanced Materials*.

Meanwhile, we continue to look for practical applications for our discoveries, this time with the help of a project from the Government of Catalonia (*Indústria del Coneixement-Llabor*) to investigate the flexoelectric properties of textile materials. We have also continued our outreach and education activities, actively participating in the *Escolab* and *Bojos per la Física* programmes.

Finally, and to finish on a self-congratulatory note, our discovery of semiconductor flexoelectricity (published in *Nature* in 2016) was shortlisted among the top eight scientific highlights in the 2017 edition of the "La Vanguardia de la Ciencia" awards. We came fourth (first of the non-life sciences!) in the final popular vote.

**Departures:** Best wishes to James Zapata, who is now working at the Université de Toulouse (France).

**Arrivals:** Plenty of 'firsts' among our new arrivals: Dr Raquel Nuñez, the first-ever biologist in our group, who has worked on bioflexoelectricity; Irene Sanchez, our first-ever nanotechnologist, who is working on the flexoelectricity of fabrics; and Dr Elzbieta Pach, the first-ever chemist in our group, who has been working on surface adsorbates on ferroelectrics. We also welcome two new PhD candidates: Christina Stefani and Irena Spasojevic.

Just to note that all the new arrivals are women. This has not been a deliberate policy, but it is great that it is happening. We must be doing something right.



## PUBLICATIONS

**Cryogenic characterisation and modelling of commercial SiC MOSFETs**, Woodend L.J., Gammon P.M., Shah V.A., Pérez-Tomás A., Li F., Hamilton D.P., Myronov M., Mawby P.A., *Materials Science Forum*; **897 MSF**: 557-560, 2017. IF: 0.399

**Domain wall magnetoresistance in BiFeO<sub>3</sub> thin films measured by scanning probe microscopy**, Domingo N., Farokhipoor S., Santiso J., Noheda B., Catalán G., *Journal of Physics Condensed Matter*; **29 (33)**, 2017. IF: 2.678

**Epitaxial Growth of SrTiO<sub>3</sub> Films on Cube-Textured Cu-Clad Substrates by PLD at Low Temperature Under Reducing Atmosphere**, Padilla J.A., Xuriguera E., Rodríguez L., Vannozzi A., Segarra M., Celentano G., Varela M., *Nanoscale Research Letters*; **12 (1)**, 2017

**Ferroelectrics as Smart Mechanical Materials**, Cordero-Edwards K., Domingo N., Abdollahi A., Sort J., Catalán G., *Advanced Materials*; **29 (37)**, 2017. IF: 19.791

**Functional oxide as an extreme high-k dielectric towards 4H-SiC MOSFET incorporation**, Russell S.A.O., Jennings M.R., Dai T., Li F., Hamilton D.P., Fisher C.A., Sharma Y.K., Mawby P.A., Pérez-Tomás A., *Materials Science Forum*; **897 MSF**: 155-158, 2017. IF: 0.399

**Heteroepitaxial Beta-Ga<sub>2</sub>O<sub>3</sub> on 4H-SiC for an FET with Reduced Self Heating**, Russell S.A.O., Perez-Tomas A., McConville C.F., Fisher C.A., Hamilton D.P., Mawby P.A., Jennings M.R., *IEEE Journal of the Electron Devices Society*; **5 (4)**: 256-261, 2017. IF: 3.141

**Hidden Magnetic States Emergent under Electric Field, in A Room Temperature Composite Magnetolectric Multiferroic**, Clarkson J.D., Fina I., Liu Z.Q., Lee Y., Kim J., Frontera C., Cordero K., Wisotzki S., Sanchez F., Sort J., Hsu S.L., Ko C., Aballe L., Foerster M., Wu J., Christen H.M., Heron J.T., Schlom D.G., Salahuddin S., Kioussis N., Fontcuberta J., Marti X., Ramesh R., *Scientific Reports*; **7 (1)**, 2017.

**High-Temperature Electrical and Thermal Aging Performance and Application Considerations for SiC Power DMOSFETs**, Hamilton D.P., Jennings M.R., Perez-Tomas A., Russell S.A.O., Hindmarsh S.A., Fisher C.A., Mawby P.A., *IEEE Transactions on Power Electronics*; **32 (10)**: 7967-7979, 2017. IF: 7.151

**Lateral Magnetically Modulated Multilayers by Combining Ion Implantation and Lithography**, Menéndez E., Modarresi H., Petermann C., Nogués J., Domingo N., Liu H., Kirby B.J., Mohd A.S., Salhi Z., Babcock E., Mattauch S., Van Haesendonck C., Vantomme A., Temst K., *Small*; **13 (11)**, 2017. IF: 8.643

**On the persistence of polar domains in ultrathin ferroelectric capacitors**, Zubko P., Lu H., Bark C.-W., Martí X., Santiso J., Eom C.-B., Catalán G., Gruverman A., *Journal of Physics Condensed Matter*; **29 (28)**, 2017. IF: 2.678

**Physical characterisation of 3C-SiC(001)/SiO<sub>2</sub> interface using XPS**, Li F., Vavasour O., Walker M., Martin D.M., Sharma Y., Russell S., Jennings M., Pérez-Tomás A., Mawby P.A., *Materials Science Forum*; **897 MSF**: 151-154, 2017. IF: 0.399

**Production of biofunctionalized MoS<sub>2</sub> flakes with rationally modified lysozyme: A biocompatible 2D hybrid material**, Siepi M., Morales-Narváez E., Domingo N., Monti D.M., Notomista E., Merkoçi A., *2D Materials*; **4 (3)**, 2017. IF: 6.937



## PROJECTS

2014 SGR 1216, funded by **AGAUR**, 01/01/14 to 30/04/17, Gustau Catalán

*Flexoelectricity (ERC-2012-STG)*, funded by **EC**, 01/01/13 to 31/12/17, Gustau Catalán

*OSTRES, Estrestrónica de óxidos*, funded by **MINECO**, 01/01/14 to 30/04/17, Gustau Catalán

*ADVISE, Electromecánica de Superficies Avanzada*, funded by **MINECO**, 01/12/16 to 30/11/19, Neus Domingo

*Paredes de dominio, interfases y dominios de antifase en antiferroeléctricos*, funded by **MINECO**, 30/12/16 to 29/12/19, Gustau Catalán

*FLEXOFABRIC*, funded by **AGAUR**, 26/07/17 to 26/04/18, Gustau Catalán



## CONTRIBUTIONS

### Invited

*Cracking Flexoelectricity*, **Seoul National University**, South Korea, 04/12/2017, G. Catalán

*Bending Oxides*, **International Conference of Advanced Materials and Devices (ICAMD 2017)**, South Korea, 05/12/2017, G. Catalán

*Bending Oxides*, **XXXVI Bienal de Física, Grupo Español de Física del Estado Sólido (GEFES)**, Santiago de Compostela, Spain, 18/07/2017, G. Catalán

*Flexoelectricity: from semiconductors to memory devices*, **Transpyrenean Encounter on Advanced Materials (TEAM1)**, Sète, France, 05/07/2017, G. Catalán

### Oral

*Converse Flexoelectric Effects in PFM*, **ISAF/ECAPD/PFM Conference 2017**, Atlanta, USA, 7-11/05/17, N. Domingo

*Mechanically soft domain walls in hard ferroelectrics*, **2017 DPG General Meeting**, Dresden, Germany, 20-24/03/17, N. Domingo

### Tutorial

*Electromechanical Surface Properties by Force Microscopy*, **ISAF-PFM Joint Meeting**, Atlanta, USA, 7-11/05/17, N. Domingo

*Functional Oxides and their Properties*, **7th MANEP Winter School**, Saas Fee, Switzerland, 08-13/01/17, G. Catalán

# Phononic and Photonic Nanostructures Group

## Main Research Lines

- Nanophononics and nanophotonics
- Nanoscale thermal transport
- Optomechanics
- Nanofabrication
- Nanometrology
- Oxide-based nanostructures



## GROUP MEMBERS

**Alzina Sureda, Francesc**, Senior Researcher  
**Arregui Bravo, Guillermo**, BIST Doctoral Student  
**Arrighi, Alois**, Severo Ochoa PhD Student  
**Bericat Vadell, Robert**, Master's Student  
**Bhansali, Sweta**, PhD Student  
**Chatterjee, Arindom**, Severo Ochoa PhD Student

**Chávez Angel, Emigdio**, Severo Ochoa Postdoctoral Researcher  
**Colombano, Martín**, Severo Ochoa PhD Student  
**De Geer, Elsa**, Visiting Master's Student  
**El Sachat, Alexandros**, PhD Student & Postdoctoral Researcher  
**Fenoll Silvestre, Dídac Armand**, Visiting Undergraduate Student

**Fernández Estévez, Ariadna**, Postdoctoral Researcher  
**Francone, Achille Leo**, Postdoctoral Researcher  
**García Fernández, P. David**, Postdoctoral Fellow (BdP & MC)  
**Jaramillo Fernández, Juliana**, Postdoctoral Researcher  
**Kehagias, Nikolaos**, Senior Researcher

**Maire, Jeremie**, Postdoctoral Researcher  
**Morales Cuñado, Cristina**, Group Administrator & Project Manager  
**Morales Ferreiro, Jorge**, Visiting PhD Fellowship Student  
**Navarro Urrios, Daniel**, Ramón y Cajal Postdoctoral Fellow  
**Necio, Tomasz**, Visiting Undergraduate Fellowship Student

## GROUP LEADER



ICREA Research Prof. Dr Clivia M. Sotomayor Torres

ICREA Research Prof. Dr Clivia M. Sotomayor Torres was awarded her PhD in physics in 1984 by the University of Manchester (UK). She then held tenured academic appointments at the universities of St. Andrews and Glasgow universities in the UK, before becoming a C4 professor at Universität Wuppertal (Germany) in 1996. She was a research professor at the Tyndall National Institute, University College Cork (Ireland) from 2004 to 2008. Since May 2007 she has been an ICREA research professor based at the Catalan Institute of Nanoscience and Nanotechnology (formerly, the ICN).

She has received awards from the Royal Society of Edinburgh, the Nuffield Foundation and an Amelia Earhart Fellowship from Zonta International (USA). She has authored over 500 scientific publications, receiving over 7700 citations, and has edited/co-edited six books (Researcher ID: E-8418-2010, H-index 43).

She leads a strong team working on phonon engineering and is actively engaged in European research. She is a member of the Photonics21 Board of Stakeholders, represents the ICN2 in the Nanoelectronics AENEAS Joint Undertaking (Chamber B) and is a visiting professor at the Kungliga Tekniska Högskolan (Royal Institute of Technology, KTH) in Sweden.

During 2017 Prof. Sotomayor held the following commissions of trust:

- Coordinator of the EU FET Open project, PHENOMEN (full title: All-phononic circuits enabled by opto-mechanics)
- Member of the Expert Committee for the Excellence Strategy of German Universities
- Co-chair of the Advisory Group of the EC's Future and Emerging Technologies programme
- ERC panel member
- Evaluator for proposals submitted to the Swedish Research Council
- Member of the AENEAS Scientific Community Council

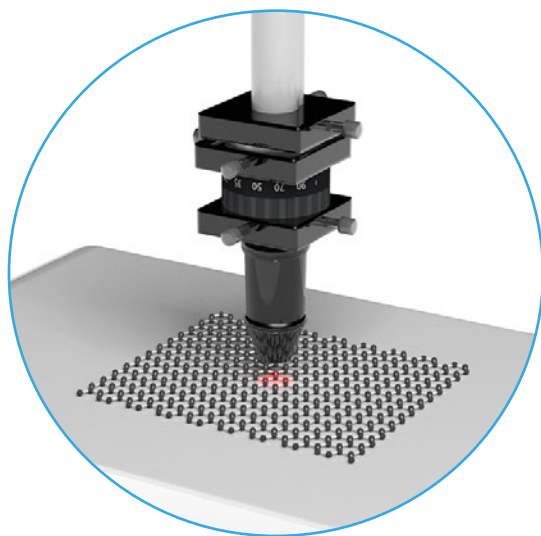
Nerantzaki, Maria, Visiting PhD Fellowship Student  
 Rodríguez, Rocío, Severo Ochoa PhD Student  
 Sánchez, Miguel Ángel, Severo Ochoa PhD Student  
 Singhal, Dhruv, Visiting PhD Fellowship Student  
 Sledzinska, Marianna, Laboratory Engineer  
 Sotomayor Torres, Clivia M., ICREA Research Professor & Group Leader  
 Whitworth, Guy Luke, Postdoctoral Researcher  
 Zoi Terzopoulou, Visiting PhD Fellowship Student

## NEW PROJECTS & MILESTONES

In 2017 the European FP7 project **QUANTIHEAT** (QUANTitative scanning probe microscopy techniques for HEAT transfer management in nanomaterials and nanodevices), in which the group participated, drew to a close. Meanwhile, the H2020 FET Open project **PHENOMEN** (All-phononics circuits enabled by opto-mechanics) coordinated by Prof. Sotomayor had its first successful periodic review, as did the Spanish National Plan project **PHENTOM** (Phonon Engineering for Advanced Thermal Management at the Nanoscale and Room Temperature optomechanics).

Group member Dr P.D. García Fernández, awarded the Marie Skłodowska-Curie Fellowship for the project **COPPOLa** (Complex Photon Phonon coupling) in 2016, terminated this project in favour of the Ramón y Cajal grant he was awarded in 2017.

In total, five projects were ongoing in 2017. Namely, the aforementioned FP7 project **QUANTIHEAT**, and four EU H2020 projects: **NANOARCHITECTONICS** (FET Open, CSA), **FLEXPOL** (Antimicrobial FLEXible POLymers for use in hospital environments, NBMP, PILOTS), **D-SPA** (Diamond-based nanomaterials and nanostructures for advanced electronic and photonic applications, MSCA, RISE), and **NEREID** (NanoElectronics Roadmap for Europe: Identification and Dissemination, ICT).



## PUBLICATIONS

**Angle-Dependent Photoluminescence Spectroscopy of Solution-Processed Organic Semiconducting Nanobelts**, Wang M., Gong Y., Alzina F., Sotomayor Torres C.M., Li H., Zhang Z., He J., *Journal of Physical Chemistry C*, **121 (22)**: 12441-12446, 2017. IF: 4.536

**Characterization of industrial Coolant Fluids and continuous ageing monitoring by wireless node-Enabled fiber optic sensors**, El Sachat A., Meristoudi A., Markos C., Sakellariou A., Papadopoulos A., Katsikas S., Riziotis C., *Sensors (Switzerland)*; **17 (3)**, 2017. IF: 2.677

**Design of Hierarchical Surfaces for Tuning Wetting Characteristics**, Fernández A., Francone A., Thamdrup L.H., Johansson A., Bilenberg B., Nielsen T., Guttmann M., Sotomayor Torres C.M., Kehagias N., *ACS Applied Materials and Interfaces*; **9 (8)**: 7701-7709, 2017. IF: 7.504

**Directional elastic wave propagation in high-aspect-ratio photoresist gratings: Liquid infiltration and aging**, Alonso-Redondo E., Gueddida A., Li J., Graczykowski B., Sotomayor Torres C.M., Pennec Y., Yang S., Djafari-Rouhani B., Fytas G., *Nanoscale*; **9 (8)**: 2739-2747, 2017. IF: 7.367

**Effect of the annealing on the power factor of un-doped cold-pressed SnSe**, Morales Ferreiro J.O., Diaz-Droguett D.E., Celentano D., Reparaz J.S., Sotomayor Torres C.M., Ganguli S., Luo T., *Applied Thermal Engineering*; **111**, 1426- 432, 2017. IF: 3.444

**Elastic Properties of Few Nanometers Thick Polycrystalline MoS<sub>2</sub> Membranes: A Nondestructive Study**, Graczykowski B., Sledzinska M., Placidi M., Saleta Reig D., Kasprzak M., Alzina F., Sotomayor Torres C.M., *Nano Letters*; **17 (12)**: 7647-7651, 2017

**Hierarchical surfaces for enhanced self-cleaning applications**, Fernández A., Francone A., Thamdrup L.H., Johansson A., Bilenberg B., Nielsen T., Guttmann M., Sotomayor Torres C.M., Kehagias N., *Journal of Micromechanics and Microengineering*; **27 (4)**, 2017. IF: 1.794

**Mechanical oscillations in lasing microspheres**, Toncelli A., Capuj N.E., Garrido B., Sledzinska M., Sotomayor-Torres C.M., Tredicucci A., Navarro-Urrios D., *Journal of Applied Physics*; **122 (5)**, 2017. IF: 2.068

**Nonlinear dynamics and chaos in an optomechanical beam**, Navarro-Urrios D., Capuj N.E., Colombano M.F., García P.D., Sledzinska M., Alzina F., Griol A., Martínez A., Sotomayor-Torres C.M., *Nature Communications*; **8**, 2017. IF: 12.124

**Optomechanical coupling in the Anderson-localization regime**, García P.D., Bericat-Vadell R., Arregui G., Navarro-Urrios D., Colombano M., Alzina F., Sotomayor-Torres C.M., *Physical Review B*; **95 (11)**, 2017. IF: 3.836

**Physics of Quantum Light Emitters in Disordered Photonic Nanostructures**, García P.D., Lodahl P., *Annalen der Physik*; 2017. IF: 3.039

**Raman antenna effect from exciton-phonon coupling in organic semiconducting nanobelts**, Wang M., Gong Y., Alzina F., Svoboda O., Ballesteros B., Sotomayor Torres C.M., Xiao S., Zhang Z., He J., *Nanoscale*; **9 (48)**: 19328-19336, 2017

**Record Low Thermal Conductivity of Polycrystalline MoS<sub>2</sub> Films: Tuning the Thermal Conductivity by Grain Orientation**, Sledzinska M., Quey R., Mortazavi B., Graczykowski B., Placidi M., Saleta Reig D., Navarro-Urrios D., Alzina F., Colombo L., Roche S., Sotomayor Torres C.M., *ACS Applied Materials and Interfaces*; **9 (43)**: 37905-37911, 2017. IF: 7.504

**Self-Assembled Nanofeatures in Complex Three-Dimensional Topographies via Nanoimprint and Block Copolymer Lithography Methods**, Cian Cummins, Dipu Borah, Sozaraj Rasappa, Ramsankar Senthamarakannan, Claudia Simao, Achille Francone, Nikolaos Kehagias, Clivia M. Sotomayor-Torres, Michael A. Morris, *ACS Omega*; **2 (2)**: 4417-4423, 2017

**Self-assembled three-dimensional inverted photonic crystals on a photonic chip**, Arpiainen S., Vynck K., Dekker J., Kapulainen M., Khunsin W., Aalto T., Mulot M., Kocher-Oberlehrer G., Zentel R., Torres C.M.S., Cassagne D., Ahopelto J., *Physica Status Solidi (A) Applications and Materials Science*; **214 (9)**, 2017. IF: 1.775

**Selfmix and optomechanics with silicon nitride membrane**, Baldacci L., Pitanti A., Masini L., Arcangeli A., Colangelo F., Navarro-Urrios D., Tredicucci A., *Optics InfoBase Conference Papers*; Part F43-CLEO\_AT 2017, 2017

**Synthesis and optical characterization of Er-doped bismuth titanate nanoparticles grown by sol-gel hydrothermal method**, Fuentes S., Muñoz P., Llanos J., Vega M., Martín I.R., Chavez-Angel E., *Ceramics International*; **43 (4)**: 3623-3630, 2017. IF: 2.986

**Thermal conductivity of epitaxially grown InP: experiment and simulation**, Jaramillo-Fernandez J., Chavez-Angel E., Sanatinia R., Kataria H., Anand S., Lourudoss S., Sotomayor-Torres C.M., *CrystEngComm*; **19 (14)**: 1879-1887, 2017. IF: 3.474

**Thermal conductivity and air-mediated losses in periodic porous silicon membranes at high temperatures**, Graczykowski B., El Sachat A., Reparaz J.S., Sledzinska M., Wagner M.R., Chavez-Angel E., Wu Y., Volz S., Wu Y., Alzina F., Sotomayor Torres C.M., *Nature Communications*; **8 (1)**, 2017. IF: 12.124

**Thermal transport in epitaxial Si<sub>1-x</sub>Ge<sub>x</sub> alloy nanowires with varying composition and morphology**, Sachat A.E., Reparaz J.S., Spiece J., Alonso M.I., Goñi A.R., Garriga M., Vaccaro P.O., Wagner M.R., Kolosov O.V., Sotomayor Torres C.M., Alzina F., *Nanotechnology*; **28 (50)**, 2017. IF: 3.44

**Unveiled electric profiles within hydrogen bonds suggest DNA base pairs with similar bond strengths**, Ruiz-Blanco Y.B., Almeida Y., Sotomayor-Torres C.M., García Y., *PLoS ONE*; **12 (10)**, 2017. IF: 2.806

**Comunicaciones seguras gracias al caos**, Navarro-Urrios, Daniel, Sotomayor Torres, Clivia M., *Investigacion y Ciencia*; **495**: 13 - 15, 2017

## PROJECTS

*D-SPA, Diamond-based nanomaterials and nanostructures for advanced electronic and photonic applications (H2020-MSCA-RISE-2016)*, funded by **EC**, 01/04/17 to 31/03/21, Clivia M. Sotomayor Torres

*2014 SGR 1238*, funded by **AGAUR**, 01/01/2014 to 30/04/2017, Clivia M. Sotomayor Torres

*NEREID, NanoElectronics Roadmap for Europe: Identification & Dissemination (H2020-ICT-2015)*, funded by **EC**, 16/11/2015 to 15/11/2018, Clivia M. Sotomayor Torres

*NANOARCHITECTONICS (H2020-FETOPEN-2016-2017)*, funded by **EC**, 01/01/2017 to 31/12/2018, Clivia M. Sotomayor Torres

*PHENOMEN, All-Phononic circuits Enabled by Opto-mechanics (H2020-FETOPEN-2014-2015-RIA)*, funded by **EC**, 01/09/16 to 31/08/19, Clivia M. Sotomayor Torres

*PHENTOM, Phonon engineering for advanced nanoscale thermal management and room temperature optomechanics*, funded by **MINECO**, 01/01/16 to 31/12/18, Clivia M. Sotomayor Torres

*Phonon Engineering in topological phononics for future fault-tolerant information technology*, funded by **MINECO**, 01/01/17 to 31/12/18, Clivia M. Sotomayor Torres

*QUANTIHEAT, QUANTitative scanning probe microscopy techniques for HEAT transfer management in nanomaterials and nanodevices (FP7-NMP-2013-LARGE-7)*, funded by **EC**, 01/12/2013 to 30/11/2017, Clivia M. Sotomayor Torres

## TECHNOLOGY TRANSFER

**Industry collaboration Thermoforming nanostructures (Germans Boada - Rubi)**, with contract ref. SRA17001 and signature date 31/01/17

## CONTRIBUTIONS

### Plenary talk

*Silicon-based optomechanics: Towards phononic components*, **Photonics Ireland**, Galway, Ireland, 13-15/09/17, C.M. Sotomayor Torres

### Invited

*Nanoscale thermal transport in 2D materials*, **Nanolito Workshop**, Salamanca, Spain, 25/01/17, M. Sledzinska

*Mechanics: an opto-mechanical and a hydrophobicity perspective*, **W3+FAIR. EPIC event**, Wetzlar, Germany, 21/02/17, C.M. Sotomayor Torres

*Thermal transport in Si phononic crystals*, **MRS (Material Research Society) 2017 Spring Meeting**, Phoenix, USA, 17-21/04/17, E. Chávez

*Thermal transport in Si phononic crystals*, **Heat Transfer Seminar**, Trondheim, Norway, 12/06/17, E. Chávez

*Dynamic surfaces: utilizing nanoimprint lithography for tailored functional plastic surfaces*, **PRN Conference 2017**, Aachen, Germany, 8-9/05/17, N. Kehagias

*Optomechanical interaction in complex dielectric media*, **Dinamo 2017**, Reykjavik, Finland, 14-19/05/17, D. García

*Advanced manufacturing techniques for high-rate replication and non-invasive monitoring of nano-enabled plastic surfaces*, **Euronanoforum**, Valeta, Malta, 20-23/06/17, N. Kehagias

*Design of hierarchical surfaces for tuning wetting characteristics*, **SMT31 Conference, University of Mons**, Mons, Belgium, 5-6/07/17, N. Kehagias

*GHz phonons in Si phononic crystals*, **Summer School SAWTrain Physics and Applications of GHz Vibrations**, Cargese, France, 10-21/07/17, C.M. Sotomayor Torres

*Probing Phonons with Inelastic light scattering: phonons in silicon nanostructures*, **Phonon Wave Phenomena and Phonon Thermal Transport School**, Oléron, France, 3-8/09/17, C.M. Sotomayor Torres

*Nanoimprint enabled dynamic surfaces: tailoring the wetting properties of amphiphobic surfaces*, **MNE Conference 2017**, Braga, Portugal, 18-22/09/17, N. Kehagias

*Nanoscale thermal transport in 2D materials*, **2D Materials and Interfaces for Spintronics**, Bellaterra, Spain, 25/10/17, M. Sledzinska

*Thermal Transport in Silicon Phononic Crystal*, **Physics Dept. Seminar, University of Oldenburg**, Oldenburg, Germany, 06/11/17, C.M. Sotomayor Torres

*Modification of thermal conductivity and phonon dispersion relation by means of phononic crystals*, **University of Birmingham**, Birmingham, United Kingdom, 06/12/17, M. Sledzinska

*Acoustic waves in freestanding silicon structures and applications to thermal engineering and optomechanics*, **ICU 2017**, Honolulu, Hawaii (USA), 18-20/12/17, J. Maire

## Oral

*Nanodevices based on graphene and 2D materials*, **Workshop Nanodevices 2017**, Salamanca, Spain, 25-26/01/17, M. Sledzinska

*Anderson localization to mediate the optomechanical coupling at the nanoscale*, **Combining Light and Sound at the nanoscale, Son et Lumière 2017**, Les Houches, France, 17-28/04/17, G. Arregui,

*Non linear dynamics in an optomechanical beam*, **Combining Light and Sound at the nanoscale, Son et Lumière 2017**, Les Houches, France, 17-28/04/17, M. Colombano

*Mechanical oscillations in lasing microspheres*, **EMRS 2017 Spring Meeting**, Strasbourg, France, 22-26/05/17, D. Navarro

*Self-doping in the triangular lattice of CoO<sub>2</sub> layer of the thermoelectric misfit Bi<sub>2</sub>Sr<sub>2</sub>Co<sub>2</sub>O<sub>y</sub> thin film*, **EMRS 2017 Spring Meeting**, Strasbourg, France, 22-26/05/17, A. Chatterjee

*Towards Phononic circuits*, **Gordon Conference on Topological and Correlated Matter**, Hong Kong, China, 20/06/17, C. M. Sotomayor Torres

*Modulation of coherent phonon emission in optomechanical crystals*, **WOMBAT**, Besançon, France, 2-6/07/17, J. Maire

*Anderson localization to mediate the optomechanical coupling at the nanoscale*, **WOMBAT**, Besançon, France, 2-6/07/17, G. Arregui,

*GHz phonons in Si phononic crystals*, **Wave phenomena and phonon thermal transport scientific school**, Oleron, France, 3-8/09/17, C.M. Sotomayor Torres

*Raman and Brillouin scattering for phononic crystals*, **Wave phenomena and phonon thermal transport scientific school**, Oleron, France, 3-8/09/17, C.M. Sotomayor Torres

*Silicon-based optomechanics: Towards phononic components*, **Photonics Ireland 2017**, Galway, Ireland, 13-15/09/17, C.M. Sotomayor Torres

*Towards a new Nanoelectronics Road Map for Europe: Beyond CMOS*, **SINANO-NEREID workshop**, Leuven, Belgium, 11/09/17, C.M. Sotomayor Torres

*Nanoimprint enabled dynamic surfaces: tailoring the wetting properties of amphiphobic surfaces*, **MNE Conference 2017**, Braga, Portugal, 18-22/09/17, N. Kehagias

*Tuning the temperature dependence of the thermal conductivity in silicon membranes by nanopatterning*, **Nanoscale and Microscale Heat Transfer V. Eurotherm Seminar**, Santorini, Greece, 26/09/17, A. El Sachat

*Modification of thermal conductivity and phonon dispersion relation by means of phononic crystals*, **Therminic**, Amsterdam, The Netherlands, 27-29/9/17, M. Sledzinska

*Fabrication and demonstration of bio-mimicking surfaces using NIL-based*, **7<sup>th</sup> Spanish Workshop in Nanolithography**, Madrid, Spain, 23-25/10/17, A. Francone

*Dependence of the accumulation function on the regularization parameter in the MFP reconstruction technique*, **3<sup>rd</sup> Scientific Meeting BCn-b PhD students in Nanoscience UAB**, Bellaterra, Barcelona, Spain, 7-8/11/17, M.A. Sánchez

*Fabrication of amphiphobic surfaces for biomimetic applications by nanoimprint lithography based processes*, **NNT conference (International Conference on Nanoimprint and Nanoprint Technology)**, Gyeongnam, Korea, 06-11/11/17, N. Kehagias

## Poster

*Thermal Conductivity Measurement of Graphene Nanofluids by Applying 3 $\omega$ -Method*, **Graphene Conference 2017**, Barcelona, Spain, 28-31/03/17, R. Rodríguez

*Non linear dynamics in an optomechanical beam*, **Son et Lumière 2017:Combining Light and Sound at the Nanoscale**, Les Houches, France, 17-28/04/17, M. Colombano

*Study of the impact of the regularization parameter in the phonon mean free path reconstruction*, **EMRS 2017 Spring Meeting 2017**, Strasbourg, France, 22-26/05/17, M. Angel Sánchez

*Novel Graphene nanofluids ideal as coolants for computer cooling sys*, **Wave phenomena and phonon thermal transport scientific school**, Oleron, France, 3-8/09/17, R. Rodríguez

*Dependence of the accumulation function on the regularization parameter in the MFP reconstruction technique*, **Wave phenomena and phonon thermal transport scientific school**, Oleron, France, 3-8/09/17, M.A. Sánchez

*Thermal conductivity of epitaxially grown InP on silicon*, **Wave phenomena and phonon thermal transport scientific school**, Oleron, France, 3-8/09/17, J. Jaramillo

*Thermal Properties of Half-Heusler Superlattices*, **Wave phenomena and phonon thermal transport scientific school**, Oleron, France, 03-08/09/17, E. Chávez

# Physics and Engineering of Nanodevices Group

## 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
- Spin and thermal transport in two-dimensional systems such as topological insulators, graphene and transition metal dichalcogenides
- Control of the magnetic state of ferro- and antiferromagnetic systems by means of the spin-orbit interaction and, particularly, the spin Hall effect
- Coupling in hybrid magnon-phonon-photon systems



## GROUP LEADER



ICREA Research Prof.  
Sergio Valenzuela

Prof. Sergio Valenzuela obtained his PhD in physics in 2001 at the Universidad de Buenos Aires (Argentina) and held research positions at Harvard University and the Massachusetts Institute of Technology (MIT). Since July 2008 Prof. Valenzuela has been an ICREA research professor and leader of the ICN2 Physics and Engineering of Nanoelectronic Devices Group. His research is focused on the unique properties of materials with nanoscale dimensions, motivated by both their intrinsic scientific interest and their potential for advanced electronic applications. His work encompasses spintronics, quantum computation with superconducting circuits and nanoelectromechanical systems (NEMS). Together with his collaborators, he has pioneered the use of non-local devices to study the spin Hall effect of thermopiles to isolate the magnon drag in ferromagnetic materials, and implemented novel qubit control and spectroscopy methods.

Prof. Valenzuela was awarded the 2001 Giambiagi prize and the 2009 IUPAP Young Scientist Prize in Magnetism for his contributions to the field of spintronics, as well as an ERC Starting Grant in 2012. He has authored over 50 articles (*Nature*, *Science*, *Reviews of Modern Physics*, *Nature Materials*, *Nature Physics*, *Physical Review Letters*, among others), three patents, and five books or book chapters.



## GROUP MEMBERS

Arrighi, Aloïs, Severo Ochoa PhD Student

Batlle Porro, Sergi, Visiting Undergraduate Student

Benítez Moreno, Luís Antonio, PhD Student

Bonell, Frédéric, Postdoctoral Researcher

Colombano Sosa, Martín, PhD Student

Costa Cornellà, Aleix, Visiting Undergraduate Student

Costache, Marius Vasile, Senior Researcher

Figueroa García, Adriana Isabel, Postdoctoral Researcher

Forn Diaz, Pol, Visiting Researcher (BSC)

Gebeyehu, Zewdu Messele, PhD Student

González Cuxart, Marc, Severo Ochoa PhD Student

Savero Torres, Williams Fernando, Postdoctoral Researcher

Sierra García, Juan Francisco, Postdoctoral Researcher

Timmermans, Matias, Postdoctoral Researcher

Valenzuela, Sergio Osvaldo, ICREA Research Professor and Group Leader



## NEW PROJECTS & MILESTONES

In 2017 the Physics and Engineering of Nanodevices Group continued its work under the H2020 Graphene Flagship programme to develop spintronic applications with graphene and related 2D materials. The group has experimentally demonstrated anisotropic spin relaxation in graphene caused by spin-orbit proximity effects from a transition metal dichalcogenide, and proposed and observed the generation of thermoelectric spin voltages driven by hot carriers in graphene. The group has continued to make progress in its ERC Starting Grant project to explore the spin properties of materials with large spin-orbit interaction, in particular topological insulators grown in a dual-chamber molecular beam epitaxial (MBE) system to develop spin torque measurements in topological insulator/ferromagnet structures, and study proximity effects by ferromagnetic insulators and molecules. Work has also been carried out within the context of the Spintronics in 2-Dimensional Dirac Systems (S2DDS) project, supported by the Spanish Ministry of Economy, Industry and Competitiveness (MINECO) to investigate the spin Hall effect, and the charge and spin transport properties of graphene, including the growth of CVD graphene, the electrical injection and detection of hot carriers, and spin-to-charge efficiency in graphene/metal hybrids. The group is also participating in the SpinTronicFactory network to coordinate EU spintronics activities, is a member of FWO network (WOG project) on the functional properties of two-dimensional nanostructured materials and represents the Bellaterra node of the recently funded MINECO Spintronics Network. In 2017 a new collaboration was established with researchers at the Barcelona Supercomputing Center on quantum computation. The group also began research on hybrid magnon-phonon-photon systems.

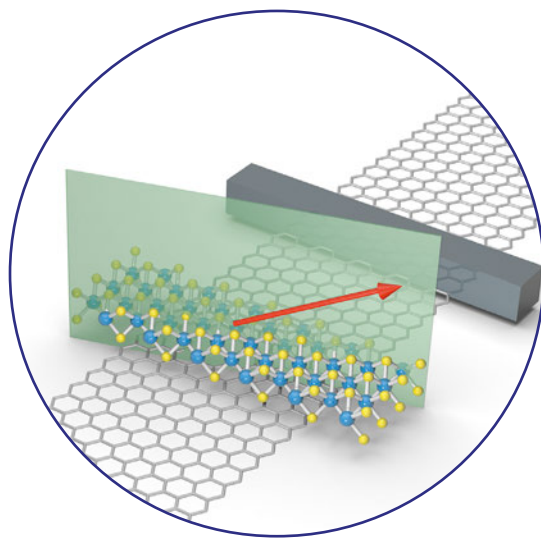
## PUBLICATIONS

**Growth of Twin-Free and Low-Doped Topological Insulators on BaF<sub>2</sub>(111)**, Bonell F., Cuxart M.G., Song K., Robles R., Ordejón P., Roche S., Mugarza A., Valenzuela S.O., *Crystal Growth and Design*; **17 (9)**: 4655-4660. 2017. IF: 4.055

**Spin precession and spin Hall effect in monolayer graphene/Pt nanostructures**, W Saverio Torres, J F Sierra, L A Benítez, F Bonell, M V Costache, S O Valenzuela, *2D Materials*; **4 (4)**: 41008. 2017. IF: 6.937

**Spin precession in anisotropic media**, Raes B., Cummings A.W., Bonell F., Costache M.V., Sierra J.F., Roche S., Valenzuela S.O., *Physical Review B*; **95 (8)**. 2017. IF: 3.836

**The 2017 Magnetism Roadmap**, Sander D., Valenzuela S.O., Makarov D., Marrows C.H., Fullerton E.E., Fischer P., McCord J., Vavassori P., Mangin S., Pirro P., Hillebrands B., Kent A.D., Jungwirth T., Gutfleisch O., Kim C.G., Berger A., *Journal of Physics D: Applied Physics*; **50 (36)**. 2017. IF: 2.588



## BOOKS

**Spin Current**, edited by Sadamichi Maekawa, Sergio O. Valenzuela, Takashi Kimura, Eiji Saitoh, 544p. Ed. *Oxford University Press*, (2017). ISBN: 9780198787075

**Two-dimensional Materials: Properties and Devices**, Chapter 11: *Graphene spintronics*, S. Roche, A.W. Cummings, F. Ortmann and S.O. Valenzuela, Ed. *Cambridge University Press* (2017). ISBN: 9781107163713

## PROJECTS

2014 SGR 56, funded by **AGAUR**, 01/01/14 to 30/04/17, Sergio O. Valenzuela

*SpinBound*, *Exploring the spin physics at the boundaries of materials with strong spin orbit interaction (ERC-2012-STG)*, funded by **EC**, 01/02/13 to 31/01/18, Sergio O. Valenzuela

*2DMD, Heteroestructuras Basadas en Materiales Bidimensionales para Dispositivos de Electrónica Avanzada*, funded by **MINECO**, 30/12/16 to 29/12/19, Sergio O. Valenzuela

*GrapheneCore1, Graphene-based disruptive technologies (H2020-Adhoc-2014-20)*, funded by **EC**, 01/04/16 to 31/03/18, Stephan Roche

## CONTRIBUTIONS

### Invited

**Nanoscale Science Department, Max-Planck Institute of Solid State Research**, Stuttgart, Germany, Jan 17

*Recent progress in experimental graphene spintronics*, **5<sup>th</sup> Joint CNRS-CSIC Workshop. Trends on Spintronics and Nanomagnetism**, Madrid, Spain, 5-6/10/17, S.O. Valenzuela

*Recent progress in experimental graphene spintronics*, **Solvay Workshop "From physics of graphene to graphene for physics"**, Brussels, Belgium, 6-8/09/17, S.O. Valenzuela

*Spin and Hot Carrier Transport in Graphene Based Devices*, **2<sup>nd</sup> EU-Japan Workshop on Graphene and Related 2D Materials**, Barcelona, Spain, 6-8/05/17, S.O. Valenzuela

*Spins, Valleys, and Topological States in 2D and Layered Materials*, **Ohio State University**, USA, 05-08/06/17, S.O. Valenzuela

*Measurement of spin-orbit torques from Rashba and topological surface states*, **2D Materials and Interfaces for Spintronics**, Barcelona, Spain, 23-25/10/17, F. Bonell, M.G. Cuxart, G. Sauthier, M. Goto, S. Miwa, J.F. Sierra, M.V. Costache, K. Song, R. Robles, P. Ordejón, S. Roche, Y. Suzuki, A. Mugarza, S.O. Valenzuela

**Zernike Institute, Groningen University**, Groningen, Netherlands, Nov 17, S.O. Valenzuela

*Recent progress in experimental graphene and topological spintronics*, **Spintec CNRS/CEA**, Grenoble, France, 22/11/2017, F. Bonell

### Oral

*Detection of the spin Hall effect in Pt using graphene-based lateral spin valves*, **Graphene Conference**, Barcelona, Spain, 28-31/03/17, Williams Saverio Torres, J. F. Sierra, L. A. Benitez, F. Bonell, M.V. Costache, S.O. Valenzuela

*Spin-orbit torque-ferromagnetic resonance with topological insulators*, **IEEE Magnetic Frontiers: Topological Insulators**, Nancy, France, 18-21/09/17, F. Bonell, M. Goto, S. Miwa, J. F. Sierra, M. V. Costache, Y. Suzuki, S.O. Valenzuela

*Spin-orbit torque-ferromagnetic resonance with topological insulators*, **4<sup>th</sup> International Symposium on Advanced Magnetic Materials and Applications (ISAMMA)**, Phu Quoc, Vietnam, 10-13/12/17, F. Bonell, M. Goto, S. Miwa, J. F. Sierra, M. V. Costache, Y. Suzuki, S.O. Valenzuela

### Poster

*Hot carrier propagation and detection in monolayer graphene*, **Graphene 2017**, Barcelona, Spain, 28-31/03/17, J.F. Sierra, I. Neumann, M. Costache, S.O. Valenzuela

*Impact of the in-situ rise hydrogen partial pressure on graphene shape evolution during CVD growth*, **Graphene 2017**, Barcelona, Spain, 28-31/03/17, Z. Gebeyehu, A. Arrighi, M. Costache, M.J. Esplandiu, S.O. Valenzuela

*Magnetic proximity effects in topological insulator/magnetic insulator heterostructures*, **XXIV International Summer School Nicolas Cabrera on Quantum Transport in Topological Materials**, Miraflores de la Sierra, Madrid, Spain, 4-8/09/17, A. Figueroa, F. Bonell, S.O. Valenzuela

*Twin-free Bi<sub>2</sub>Te<sub>3</sub> thin films grown by molecular beam epitaxy*, **IEEE Magnetic Frontiers: Topological Insulators**, Nancy, France, 18-21/09/17, F. Bonell, M. González Cuxart, A. Mugarza, S.O. Valenzuela

*Topological Insulators: Epitaxial growth, Fermi level tuning and Non-equilibrium spin-orbit torques*, **5<sup>th</sup> Joint CNRS-CSIC Workshop. Trends on Spintronics and Nanomagnetism**, Madrid, Spain, 05-06/10/17, F. Bonell, M.G. Cuxart, G. Sauthier, M. Goto, S. Miwa, J.F. Sierra, M.V. Costache, Y. Suzuki, A. Mugarza, S.O. Valenzuela

*Magnetic proximity effects in topological insulator/magnetic insulator heterostructures*, **5<sup>th</sup> Joint CNRS-CSIC Workshop Trends on Spintronics and Nanomagnetism**, Madrid, Spain, 05-06/10/17, A. Figueroa, F. Bonell, S.O. Valenzuela

*Spin precession and spin Hall effect in monolayer graphene/Pt nanostructures*, **2D Materials and Interfaces for Spintronics**, Barcelona, Spain, 23-25/10/17, W. Savero, J. F. Sierra, L. A. Benitez, F. Bonell, M. Costache,, S.O. Valenzuela

*Magnetic proximity effects in topological insulator/magnetic insulator heterostructures*, **2D Materials and Interfaces for Spintronics**, Barcelona, Spain, 23-25/10/17, A. Figueroa, F. Bonell, S.O. Valenzuela



### PARTICIPATED CONGRESSES

**2D Materials & Interfaces for Spintronics**, Barcelona, Spain, 23-27/10/17, *Co-organiser*, S.O. Valenzuela

**Frontiers in Magnetism. Topological Insulators**, Nancy, France, 18-21/9/17, *Scientific Committee*, S.O. Valenzuela

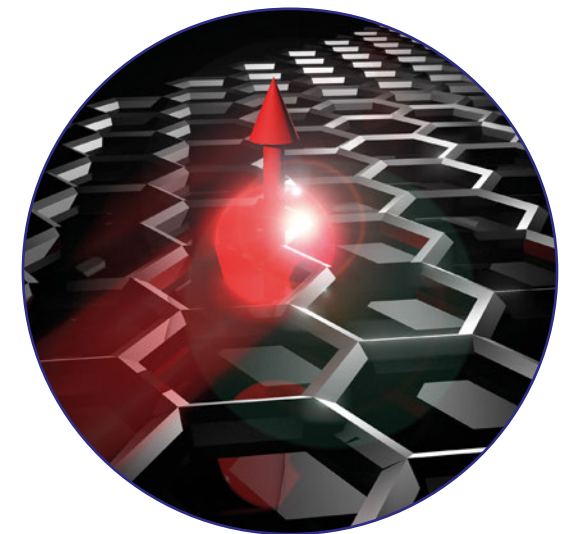
**The European School of Magnetism (ESM)**, Cargese, Corsica, 9-21/10/17, *Scientific Advisory Committee*, S.O. Valenzuela

**GRAPHENE 2017**, Barcelona, Spain, 28-31/3/17, *Scientific Committee*, S.O. Valenzuela



### COURSES

S.O. Valenzuela, **ESONN'17, European School on Nanosciences & Nanotechnologies. Course on Spintronics**, Sept 2017, Grenoble, France



# Supramolecular NanoChemistry and Materials Group

## Main Research Lines

- Nanoporous metal-organic frameworks and related nanoparticles
- Micro- and nanoencapsulation technologies towards the design of new multifunctional nanocarriers

## GROUP MEMBERS

Albalad Alcalá, Jorge, PhD Student  
Arenas Jal, Marta, Visiting PhD Student  
Arnau del Valle, Carla, Master's Fellowship Student  
Avci, Ceren, PhD Student  
Avci, Civan, PhD Student  
Boix i Soler, Gerard, PhD Student  
Cano Sarabia, Antonia, Senior Researcher  
Carné Sánchez, Arnau, Postdoctoral Researcher  
Corvo Alguacil, Laura, Visiting Undergraduate Student

Espín Marti, Jordi, PhD Student  
Fernández De Retana Alda, Sofia, Visiting PhD Student  
García Jimeno, Sonia, Postdoctoral Researcher  
Garzón Tovar, Luís Carlos, PhD Student  
Grancha Marco, Thais María, Postdoctoral Researcher  
Guillerm, Vincent, Postdoctoral Researcher  
Hernández López, Laura, Technician  
Imaz Gabilondo, Inhar, Senior Researcher  
Jarrah, Najmeh, Visiting PhD Student

## GROUP LEADER



ICREA Research Prof. Dr  
Daniel MasPOCH

Dr. Daniel MasPOCH is a chemist who has always maintained a rewarding balance between fundamental and applied research, making pioneering contributions in both in the field of porous metal-organic frameworks (MOFs) and delivery systems. His scientific career began with a degree in chemistry at the Universitat de Girona, followed by a PhD in materials science from the Universitat Autònoma de Barcelona and the Institut de Ciència de Materials de Barcelona. He then spent two years at Northwestern University (USA) as a postdoctoral fellow in the group led by Prof. Chad A. Mirkin. He has been an ICREA research professor and group leader at the ICN2 since September 2011. In 2014



Liu, Yang, PhD Fellowship Student  
MasPOCH Comamala, Daniel, ICREA Research Professor and Group Leader  
Mejías Ruiz, Nereida, Postdoctoral Researcher  
Pérez Carvajal, Javier, Postdoctoral Researcher  
Puga Aranda, Rosa, Scientific Group Administrator  
Rodríguez Hermida, Sabina, Postdoctoral Researcher

Ruiz García, Marta, Visiting PhD Student  
Sanclemente Crespo, Mateo, Visiting Undergraduate Student  
Sanmartí Espinal, Marta, Technician  
Troyano Prieto, Javier, Postdoctoral Researcher  
Vignatti Abellán, Claudia, PhD Student  
Xu, Heng, PhD Student  
Yazdi, Amirali, Severo Ochoa PhD Student

Prof. MasPOCH was awarded a prestigious ERC Consolidator Grant for the InanoMOF project to develop frontier methodologies for the synthesis of nanocomposites made from MOFs. In 2015 he received the Marcial Moreno Mañas Lectureship award. He has authored over 115 papers and five book chapters.

Several technologies and materials developed under his leadership are currently being used by companies with products on the market. In total Prof. MasPOCH has signed more than 15 research contracts with private companies and filed 10 patents, of which four have been licensed. He has also signed four technology transfer contracts that have given rise to different product families such as LuctaCaps® and Fungipol@CP. Most recently he has co-founded the spin-off Ahead Therapeutics S.L.



## NEW PROJECTS & MILESTONES

In 2017 the ICN2 Supramolecular NanoChemistry and Materials Group or “NANOUP” finds itself halfway through the MOFCAS project to develop multifunctional composites based on MOFs as advanced sorbents for biomedical and energy-related applications. Led by Prof. Maspocho this three-year project began in 2016, supported by the Spanish Ministry of Economy, Industry and Competitiveness (MINECO) under its National Programme for Research Aimed at the Challenges of Society. The group has also continued work on the ERC Consolidator Grant project, InanoMOF, achieving the development of several functional nanoMOF@INP composites. Projects that came to an end this year include the NANOFOTOSENS project led by Prof. Laura Lechuga (also of the ICN2) to implement novel photonic nanosensors for the detection of polluting gases in small concentrations. Meanwhile, the European H2020 project ProDIA reached the end of its second year. As part of this project the group is scaling-up the production of nanoporous materials for use in industrial adsorption processes via its spray drying technique.

The group has also continued to collaborate with companies to bring customised micro- and nanoencapsulation technologies to market, working in parallel with different entities. It has also been involved in a new technology transfer action related to the microencapsulation of iron salts, and the creation of new spin-off Ahead Therapeutics, devoted to the validation of a liposome-based platform for the treatment of autoimmune diseases.



## PUBLICATIONS

**Carborane bis-pyridylalcohols as linkers for coordination polymers: Synthesis, crystal structures, and guest-framework dependent mechanical properties**, Tsang M.Y., Rodríguez-Hermida S., Stylianou K.C., Tan F., Negi D., Teixidor F., Viñas C., Choquesillo-Lazarte D., Verdugo-Escamilla C., Guerrero M., Sort J., Juanhuix J., Maspocho D., Planas J.G., *Crystal Growth and Design*; **17 (2)**: 846-857. 2017. IF: 4.055

**Spray drying for making covalent chemistry: Postsynthetic modification of metal-organic frameworks**, Garzón-Tovar L., Rodríguez-Hermida S., Imaz I., Maspocho D., *Journal of the American Chemical Society*; **139 (2)**: 897-903. 2017. IF: 13.858

**Microencapsulation with alginate/CaCO<sub>3</sub>: A strategy for improved phage therapy**, Colom J., Cano-Sarabia M., Otero J., Arriñez-Soriano J., Cortés P., Maspocho D., Llagostera M., *Scientific Reports*; **7**. 2017. IF: 4.259

**Composite Salt in Porous Metal-Organic Frameworks for Adsorption Heat Transformation**, Garzón-Tovar L., Pérez-Carvajal J., Imaz I., Maspocho D., *Advanced Functional Materials*; **27 (21)**. 2017. IF: 12.124

**Continuous One-Step Synthesis of Porous M-XF<sub>6</sub>-Based Metal-Organic and Hydrogen-Bonded Frameworks**, Guillerm V., Garzón-Tovar L., Yazdi A., Imaz I., Juanhuix J., Maspocho D., *Chemistry - A European Journal*; **23 (28)**: 6829-6835. 2017. IF: 5.317

**Liposome-based immunotherapy against autoimmune diseases: Therapeutic effect on multiple sclerosis**, Pujol-Autonell I., Mansilla M.-J., Rodríguez-Fernández S., Cano-Sarabia M., Navarro-Barriuso J., Ampudia R.-M., Rius A., García-Jimeno S., Perna-Barrull D., Cáceres E.M., Maspocho D., Vives-Pi M., *Nanomedicine*; **12 (11)**: 1231-1242. 2017. IF: 4.727

**New synthetic routes towards MOF production at scale**, Rubio-Martínez M., Avci-Camur C., Thornton A.W., Imaz I., Maspocho D., Hill M.R., *Chemical Society Reviews*; **46 (11)**: 3453-3480. 2017. IF: 38.618

**Systematic study of the impact of MOF densification into tablets on textural and mechanical properties**, Dhainaut J., Avci-Camur C., Troyano J., Legrand A., Canivet J., Imaz I., Maspocho D., Reinsch H., Farrusseng D., *CrystEngComm*; **19 (29)**: 4211-218. 2017. IF: 3.474

**Confining Functional Nanoparticles into Colloidal Imine-Based COF Spheres by a Sequential Encapsulation-Crystallization Method**, Rodríguez-San-Miguel D., Yazdi A., Guillerm V., Pérez-Carvajal J., Puentes V., Maspocho D., Zamora F., *Chemistry - A European Journal*; **23 (36)**: 8623-8627. 2017. IF: 5.317

**Core-shell Au/CeO<sub>2</sub> nanoparticles supported in UiO-66 beads exhibiting full CO conversion at 100 °C**, Yazdi A., Abo Markeb A., Garzón-Tovar L., Patarroyo J., Moral-Vico J., Alonso A., Sánchez A., Bastus N., Imaz I., Font X., Puentes V., Maspocho D., *Journal of Materials Chemistry A*; **5 (27)**: 13966-13970. 2017. IF: 8.867

**Leucine zipper motif inspiration: A two-dimensional leucine Velcro-like array in peptide coordination polymers generates hydrophobicity**, Rodríguez-Hermida S., Evangelio E., Rubio-Martínez M., Imaz I., Verdaguer A., Juanhuix J., Maspocho D., *Dalton Transactions*; **46 (34)**: 11166-1170. 2017. IF: 4.029

**Spray drying for making covalent chemistry II: Synthesis of covalent-organic framework superstructures and related composites**, Garzón-Tovar L., Avci-Camur C., Rodríguez-San-Miguel D., Imaz I., Zamora F., Maspocho D., *Chemical Communications*; **53 (82)**: 11372-11375. 2017. IF: 6.319

**Tuning the Endocytosis Mechanism of Zr-Based Metal-Organic Frameworks through Linker Functionalization**, Orellana-Tavra C., Haddad S., Marshall R.J., Abánades Lázaro I., Boix G., Imaz I., Maspocho D., Forgan R.S., Fairen-Jiménez D., *ACS Applied Materials and Interfaces*; **9 (41)**: 35516 - 35525. 2017. IF: 7.504

**Characterization of ApoJ-reconstituted high-density lipoprotein (rHDL) nanodisc for the potential treatment of cerebral  $\beta$ -amyloidosis**, Fernández-De-Retana S., Cano-Sarabia M., Marazuela P., Sánchez-Quesada J.L., García-León A., Montañola A., Montaner J., Maspocho D., Hernández-Guillamón M., *Scientific Reports*; **7 (1)**. 2017.



## PROJECTS

*InanoMOF, Multifunctional micro- and nanostructures assembled from nanoscale metal-organic frameworks and inorganic nanoparticles (ERC-2013-CoG)*, funded by **EC**, 01/04/14 to 31/03/19, Daniel Maspocho

*2014 SGR 80*, funded by **AGAUR**, 01/01/14 to 30/04/17, Daniel Maspocho

*ProDIA, Production, control and demonstration of structured hybrid nanoporous materials for industrial adsorption applications (H2020-NMP-03-2015)*, funded by **EC**, 01/11/15 to 31/10/18, Daniel Maspocho

*MOFNET, Del diseño a las aplicaciones de materiales porosos avanzados basados en redes metalorgánicas*, funded by **MINECO**, 01/12/2015 to 30/11/17, Daniel Maspocho

*MOFCAS, Composites multifuncionales basados en redes metalorgánicas (MOFs) como sorbentes avanzados para aplicaciones biomédicas y energéticas*, funded by **MINECO**, 01/01/16 to 31/12/18, Daniel Maspocho, Inhar Imaz

*GENESIS, High performance MOF and IPOSS enhanced membrane systems as next generation CO<sub>2</sub> capture technologies (H2020-NMBP-2016-2017)*, funded by **EC**, 01/01/18 to 31/12/21, Daniel Maspocho



## TECHNOLOGY TRANSFER

**ICN2PAT\_08\_15** *Synthesis of UiO-66 by Spray Drying combined with continuous flow*, with ref. PCT/EP2017/056404 on 17/03/2017.  
Inventors: Daniel Maspoch (ICREA-ICN2), Ihnar Imaz (ICN2), Luis Carlos Garzón (ICN2)

**ICN2PAT\_09\_16** *A process for the post-synthetic modification of metal organic frameworks*, with ref. PCT/EP2017/082827 on 14/12/2017.  
Inventors: Daniel Maspoch (ICREA-ICN2), Ihnar Imaz (ICN2), Sabina Rodríguez (ICN2), Luis Carlos Garzón (ICN2)

**Industry collaboration** *Development of materials matching specifications (LG)*, with project ref. ICN2PRJ\_05\_16\_LG\_POLARIZER\_FILMS and signature date 01/04/17



## CONTRIBUTIONS

### Invited

*Porous Metal-Organic Frameworks: from bulk to the nanoscale*, **Universidad Jaume I**, Castellón, Spain, 20/01/2017, D. Maspoch

### Oral

*Photothermal activation of metal-organic frameworks using a UV-Vis light source*, **2<sup>nd</sup> European Conference on Metal Organic Frameworks and Porous Polymers (EUROMOF 2017)**, Delft, The Netherlands, 29/10/17 - 01/11/17, J. Espin, L. Garzón-Tovar, A. Carné-Sánchez, I. Imaz, D. Maspoch

*Antigen-Specific Liposomal Nanotherapy Drives Immunoregulation in Human Type 1 Diabetes*, **XI Congrès de la Societat Catalana d'Immunologia**, Barcelona, Spain, 16-17/11/17, S. Rodríguez-Fernandez; I. Pujol-Autonell, F. Briansó, D. Perna-Barrull, M. Cano-Sarabia, S. Garcia-Jimeno, A. Villalba, A. Sanchez, E. Aguilera, F. Vazquez, J. Verdaguer, D. Maspoch, M. Vives-Pi

*Switchable surface hydrophobicity-hydrophilicity of a carborane based MOF*, **XXXVI Biennial Meeting of the Spanish Royal Society of Chemistry**, Sitges, Spain, 25-29/06/17, J. Giner Planas, M.Y. Tsang, S. Rodríguez-Hermida, C. Vignatti, K.C. Stylianou, V. Guillerm, J. Pérez-Carvajal, F. Teixidor, C. Viñas, D. Choquesillo-Lazarte, C. Verdugo-Escamilla, I. Peral, J. Juanhuix, I. Imaz, D. Maspoch

### Poster

*Novel photonic nanosensor integrating MOFs as specific receptors for gas sensing*, **2<sup>nd</sup> European Conference on Metal Organic Frameworks and Porous Polymers (EUROMOF 2017)**, Delft, Netherlands, 29/10/17 - 01/11/17, B. Chocarro-Ruiz, J. Pérez, C. Avci, L. Lechuga, D. Maspoch

*Solid-Gas Phase Post-Modification of Metal-Organic Frameworks through Ozonolysis*, **2<sup>nd</sup> European Conference on Metal Organic Frameworks and Porous Polymers (EUROMOF 2017)**, Delft, Netherlands, 29/10/17 - 01/11/17, H. Xu, J. Albalad, J. Pérez, I. Imaz, D. Maspoch

*Composite salt in porous metal-organic frameworks for adsorption heat transformation*, **2<sup>nd</sup> European Conference on Metal Organic Frameworks and Porous Polymers (EUROMOF 2017)**, Delft, Netherlands, 29/10/17 - 01/11/17, J. Pérez-Carvajal, L. Carlos Garzón-Tovar, I. Imaz, D. Maspoch

*Spray Drying for Making Covalent Chemistry II: Synthesis of Covalent-Organic Framework Superstructures and Related Composites*, **2<sup>nd</sup> European Conference on Metal Organic Frameworks and Porous Polymers (EUROMOF 2017)**, Delft, Netherlands, 29/10/17 - 01/11/17, C. Avci-Camur, L. Garzón-Tovar, D. Rodríguez-San-Miguel, I. Imaz, F. Zamora, D. Maspoch

*Multi-Shelled MOF-INP Composites Synthesized by a Sequential Etching/Re-Growth Approach*, **2<sup>nd</sup> European Conference on Metal Organic Frameworks and Porous Polymers (EUROMOF 2017)**, Delft, Netherlands, 29/10/17 - 01/11/17, I. Imaz, C. Avci, A. Yazdi, X. Ribas, M. Tarres, N. Bastus, V. Puentes, D. Maspoch

*Design and synthesis of new photo-responsive coordination polymers*, **XXXVI Biennial Meeting of the Spanish Royal Society of Chemistry**, Sitges, Spain, 25-29/06/17, J. Espín Martí, J. Albalad Alcalá, I. Imaz Gabilondo, D. Maspoch Comamala

*Composite salt in porous metal-organic frameworks for adsorption heat transformation*, **XXXVI Biennial Meeting of the Spanish Royal Society of Chemistry**, Sitges, Spain, 25-29/06/17, C. Garzón Tovar, J. Perez Carvajal, I. Imaz, D. Maspoch

*Incorporating Inorganic Nanoparticles into Metal-Organic Frameworks for Heterogeneous Catalysis*, **XXXVI Biennial Meeting of the Spanish Royal Society of Chemistry**, Sitges, Spain, 25-29/06/17, A. Yazdi, L.C. Garzón Tovar, J. Patarroyo, F. Merçoçi, N. Bastús, I. Imaz, V. Puentes, D. Maspoch, A. Abo Markeb, A. Alonso, X. Font, T. Gea, A.J. Moral Vico, A. Sanchez Ferrer

*Continuous water-based spray-drying synthesis of MOFs with industrial relevance*, **XXXVI Biennial Meeting of the Spanish Royal Society of Chemistry**, Sitges, Spain, 25-29/06/17, J. Troyano Prieto, C. Avci, L.C. Garzón Tovar, A. Legrand, I. Imaz, D. Maspoch

*Hetero-bimetallic paddlewheel clusters in coordination polymers formed by a water-induced single-crystal to single-crystal transformation*, **XXXVI Biennial Meeting of the Spanish Royal Society of Chemistry**, Sitges, Spain, 25-29/06/17, J. Albalad Alcalá, J. Arriñez Soriano, J. Juanhuix, N. Aliaga Alcalde, I. Imaz, D. Maspoch

*Spray-drying method for the one-step synthesis of ready-to use CO<sub>2</sub> sorbents based on isorecticular M-XF<sub>6</sub>-MOFs*, **XXXVI Biennial Meeting of the Spanish Royal Society of Chemistry**, Sitges, Spain, 25-29/06/17, V. Guillerm, L. Garzón-Tovar, A. Yazdi, I. Imaz, J. Juanhuix, D. Maspoch

*Covalent post-synthetic modification of Metal-Organic Frameworks by Spray Drying technique*, **XXXVI Biennial Meeting of the Spanish Royal Society of Chemistry**, Sitges, Spain, 25-29/06/17, L. Garzón-Tovar, S. Rodríguez-Hermida, I. Imaz, D. Maspoch

*Organocatalytic Tandem and Multicomponent Reactions by Zn-MOF Squaramide Materials under Solvent Free Conditions*, **XXXVI Biennial Meeting of the Spanish Royal Society of Chemistry**, Sitges, Spain, 25-29/06/17, C. Vignatti Abellan, J. Luis, R. Mas, J. Aleman, I. Imaz, D. Maspoch

*Carborane bis-pyridylalcohols as linkers for Coordination Polymers: Synthesis, Crystal Structures and Guest-Framework dependent Mechanical Properties*, **XXXVI Biennial Meeting of the Spanish Royal Society of Chemistry**, Sitges, Spain, 25-29/06/17, M.Y. Tsang, S. Rodríguez-Hermida, K.C. Stylianou, F. Tan, D. Negi, F. Teixidor, C. Vin~as, D. Choquesillo-Lazarte, C. Verdugo-Escamilla, M. Guerrero, J. Sort, J. Juanhuix, D. Maspoch, J. Giner Planas

*INP@MOF Nanocomposites as NIR-Activated Drug Delivery Systems*, **XXXVI Biennial Meeting of the Spanish Royal Society of Chemistry**, Sitges, Spain, 25-29/06/17, G. Boix I Soler, I. Imaz Gabilondo, D. Maspoch Comamala, J. Patarroyo Rengifo, N. Gómez Bastus, V. Franco Puentes

# Theoretical and Computational Nanoscience Group

## Main Research Lines

- Leading-edge theoretical research on quantum transport phenomena in graphene and two-dimensional materials
- Spin dynamics and entanglement properties in Dirac matter (graphene, topological insulators)
- Thermal transport properties and thermoelectricity
- Predictive modelling and multiscale numerical simulation of complex nanomaterials and quantum nanodevices



## GROUP LEADER



ICREA Research Prof.  
Stephan Roche

Prof. Stephan Roche is a theoretician with more than 25 years of experience in the study of transport theory in low-dimensional systems, including graphene, carbon nanotubes, semiconducting nanowires, organic materials and topological insulators.

He has published more than 150 papers in journals such as the *Review of Modern Physics*, *Nature Physics*, *Nano Letters* and *Physical Review Letters* and he is the co-author of the book titled *Introduction to Graphene-Based Nanomaterials: From Electronic Structure to Quantum Transport* (Cambridge University Press, 2014). He received authorisation to supervise PhD students from the Université Joseph Fourier (Grenoble, France) in 2004, since which time he has supervised seven PhD students and some 20 postdoctoral researchers in France, Germany and Spain. In 2009 Prof. Roche was awarded the prestigious Friedrich Wilhelm Bessel Research Award by the Alexander Von-Humboldt Foundation (Germany) and, last but not least, since 2011 he has been actively involved in the European Graphene Flagship project as co-lead of the spintronics work package.



## GROUP MEMBERS

**Barrios Vargas, José Eduard**, Visiting Postdoctoral Researcher

**Cummings, Aron William**, Senior Researcher

**De Moraes Araujo, Bruna Gabrielly**, Research Assistant

**García Aguilar, Jose Hugo**, Postdoctoral Researcher

**Power, Stephen**, Postdoctoral Researcher

**Roche, Stephan**, ICREA Research Professor and Group Leader

**Schou Gregersen, Soren**, Visiting PhD Student

**Song, Kenan**, Severo Ochoa PhD Student

**Vargas Fosada, Rubicelia**, Visiting Senior Researcher

**Vila Tusell, Marc**, PhD Student

## NEW PROJECTS & MILESTONES

In 2017 the group published the following four publications of note:

### *Giant spin lifetime anisotropy in graphene induced by proximity effects*

Models developed by the group this year pointed to a spin lifetime anisotropy several orders of magnitude larger than the 1:1 ratio typically observed in 2D systems. Theoretically inducing a spin filter effect in graphene/TMDC heterostructures via the proximity effect, where transmission is determined by the orientation of the spins that reach it, this represents the first step to achieving direct electric-field tuning of the propagation of spins in graphene.

### *Valley polarised quantum transport generated by gauge fields in graphene*

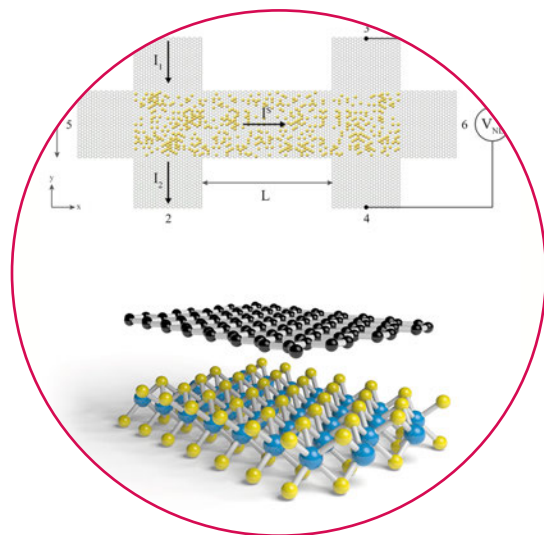
This year the group has also reported on the ability to simultaneously induce a bulk **valley-polarised** dissipative transport and a quantum valley Hall effect in graphene by combining strain-induced gauge fields and real magnetic fields. Their results provide strong experimental basis for a fully valley-polarised device principle.

### *Scale-invariant large non-locality in polycrystalline graphene*

Together with an experimental group at CIC-nanoGUNE, the group reported on scale-invariant non-local transport in large-scale CVD graphene under application of an external magnetic field. The work points to the existence of field-induced spin-filtered edge states whose sensitivity to grain boundaries manifests in the non-local resistance. Found to persist up to the millimetre scale, this suggests that topological Hall effects are highly influenced by the underlying structural morphology, which would limit any practical realisations.

### *Spin Hall effect and weak antilocalisation in graphene/transition metal dichalcogenide heterostructures*

The group has performed a theoretical study of the spin Hall effect and weak antilocalisation in graphene/TMDC heterostructures, calculated using efficient real-space quantum transport methods and realistic tight-binding models parametrised from ab initio calculations. The findings provide guidelines for future experimental study at the upper limits of spin current formation and will enable full exploitation of the potential of 2D materials for spintronic applications.



## PUBLICATIONS

**Large edge magnetism in oxidized few-layer black phosphorus nanomeshes**, Nakanishi Y., Ishi A., Ohata C., Soriano D., Iwaki R., Nomura K., Hasegawa M., Nakamura T., Katsumoto S., Roche S., Haruyama J., *Nano Research*; **10 (2)**: 718-728, 2017. IF: 7.354

**Spin precession in anisotropic media**, Raes B., Cummings A.W., Bonell F., Costache M.V., Sierra J.F., Roche S., Valenzuela S.O., *Physical Review B*; **95 (8)**, 2017. IF: 3.836

**Nanostructured graphene for spintronics**, Gregersen S., Power S.R., Jauho A.-P., *Physical Review B*; **95 (12)**, 2017. IF: 3.836

**Electrical and Thermal Transport in Coplanar Polycrystalline Graphene-hBN Heterostructures**, Barrios-Vargas J.E., Mortazavi B., Cummings A.W., Martinez-Gordillo R., Pruneda M., Colombo L., Rabczuk T., Roche S., *Nano Letters*; **17 (3)**: 1660-1664, 2017. IF: 12.712

**Grain boundary-induced variability of charge transport in hydrogenated polycrystalline graphene**, Vargas J.E.B., Falkenberg J.T., Soriano D., Cummings A.W., Brandbyge M., Roche S., *2D Materials*; **4 (2)**, 2017. IF: 6.937

**Tailoring magnetic insulator proximity effects in graphene: First-principles calculations**, Hallal A., Ibrahim F., Yang H., Roche S., Chshiev M., *2D Materials*; **4 (2)**, 2017. IF: 6.937

**Spin hall effect and weak antilocalization in graphene/transition metal dichalcogenide heterostructures**, Garcia J.H., Cummings A.W., Roche S., *Nano Letters*; **17 (8)**: 5078-5083, 2017. IF: 12.712

**Growth of Twin-Free and Low-Doped Topological Insulators on BaF<sub>2</sub>(111)**, Bonell F., Cuxart M.G., Song K., Robles R., Ordejón P., Roche S., Mugarza A., Valenzuela S.O., *Crystal Growth and Design*; **17 (9)**: 4655-4660, 2017. IF: 4.055

**Valley-polarized quantum transport generated by gauge fields in graphene**, Settnes M., Garcia J.H., Roche S., *2D Materials*; **4 (3)**, 2017. IF: 6.937

**Electron trajectories and magnetotransport in nanopatterned graphene under commensurability conditions**, Power S.R., Thomsen M.R., Jauho A.-P., Pedersen T.G., *Physical Review B*; **96 (7)**, 2017. IF: 3.836

**Scaling properties of polycrystalline graphene: A review**, Isacsson A., Cummings A.W., Colombo L., Colombo L., Kinaret J.M., Roche S., *2D Materials*; **4 (1)**, 2017. IF: 6.937

**Giant Spin Lifetime Anisotropy in Graphene Induced by Proximity Effects**, Cummings A.W., Garcia J.H., Fabian J., Roche S., *Physical Review Letters*; **119 (20)**, 2017.

**Record Low Thermal Conductivity of Polycrystalline MoS<sub>2</sub> Films: Tuning the Thermal Conductivity by Grain Orientation**, Sledzinska M., Quey R., Mortazavi B., Graczykowski B., Placidi M., Saleta Reig D., Navarro-Urrios D., Alzina F., Colombo L., Roche S., Sotomayor Torres C.M., *ACS Applied Materials and Interfaces*; **9 (43)**: 37905-37911, 2017. IF: 7.504

**Scale-invariant large nonlocality in polycrystalline graphene**, Ribeiro M., Power S.R., Roche S., Hueso L.E., Casanova F., *Nature Communications*; **8 (1)**, 2017.

## PROJECTS

*MANSPINDIRAC, Spin Manipulation in Dirac Matter*, funded by **MINECO**, 01/01/2016 to 31/12/2018, Stephan Roche / Aron Cummings

*GRAPHENE CORE 2, Graphene Flagship Core Project 2, H2020-SGA-FET-GRAPHENE-2017*, funded by **EC**, 01/04/2018 to 31/03/2020, Stephan Roche

*GRAPHENE CORE1, Graphene-based disruptive technologies (H2020-Adhoc-2014-20)*, funded by **EC**, 01/04/2016 to 31/03/2018, Stephan Roche / Sergio O. Valenzuela / Jose A. Garrido

## CONTRIBUTIONS

### *Invited*

*Tutorial on spintronics and valleytronics in graphene, Annual meeting of the GDR GNT*, Aussois, France, 15/10/17, S. Roche

*Opportunities for spintronic industries with graphene, GRAPHENE CONNECT*, Athens, Greece, 28/09/17, S. Roche

*Theoretical Studies of spin Dynamics in 2D-materials-based heterostructures, GRAPHCHINA 17*, Nanjing, China, 25/09/17, S. Roche

*Advances in 2D Materials-based Spintronics, Recent Progress in Graphene Research 17*, Singapore, 20/09/17, S. Roche

*Spintronics based on 2D Materials: A theoretical perspective, SOLVAY Conference "From physics of graphene to graphene for physics"*, Brussels, Belgium, 06/09/17, S. Roche

*Prospects in 2D Materials-based Spintronics, ECME17*, Dresden, Germany, 31/08/17, S. Roche

*Proximity effects and Spin dynamics in Dirac Matter, Spin Dynamics in the DIRAC Systems- SPICE workshop*, Mainz, Germany, 09/06/17, S. Roche

*Graphene activities and Innovation towards Industries at the ICN2, Innovation Week Barcelona - Graphene Workshop*, Barcelona, Spain, 18/05/17, S. Roche

*Recent progress in 2d Materials-based electronics and spintronics, King Abdullah University of Science and Technology (KAUST)*, Jeddah, Saudi Arabia, 25/04/17, S. Roche

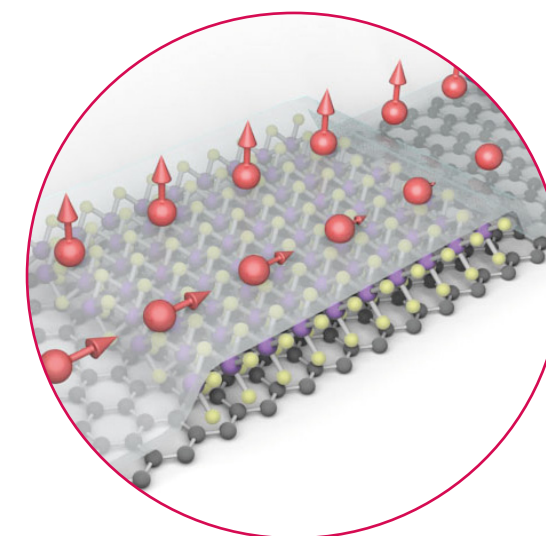
## DISSEMINATION CONTRIBUTIONS

*Revoluciones emergiendo de la planitud, II Festival of Nanoscience and Nanotechnology: 10alamos9*, Barcelona, Spain, 07/03/17, S. Roche

## COURSES

S. Roche, **Seminar on Manipulating valley and spin degrees of freedom in 2D Materials**, Tohoku University, Japan, 02-14/12/17

S. Roche, **Seminar on Proximity effects and Spin dynamics in Dirac Matter**, KAUST, Saudi Arabia, 06-12/03/17





# Theory and Simulation Group

## Main Research Lines

- Development of theoretical methods, numerical algorithms and simulation tools
- Codes: SIESTA and TRANSIESTA
- First-principles simulations at the nanoscale
- Novel physical properties in 2D materials

## GROUP MEMBERS

Akhtar, Arsalan, PhD Student

Alonso Pruneda, José Miguel, CSIC  
Tenured Scientist

Bahmani, Mohammad, Visiting PhD Student

Bernd, Ensing, Visiting Senior Researcher

Costanzo, Francesca, Postdoctoral  
Researcher

Cuadrado Del Burgo, Ramón, Postdoctoral  
Researcher

Dikan, Vladimir, PhD Student

Juan, Dilson, CONICET Predoctoral Student

Guster, Ionel-Bogdan, PhD Student

Huhs, Georg, Visiting Senior Researcher

Iguaz Juan, Joaquim, Visiting Undergraduate  
Student

Illera Robles, Sergio, Severo Ochoa  
Postdoctoral Researcher

Martínez Balagué, Pau, Visiting  
Undergraduate Student

Migani, Annapaola, CSIC Ramón y Cajal  
Researcher

## GROUP LEADER



CSIC Research Prof.  
Pablo Ordejón

Prof. Ordejón earned his degree in physics (1987) and PhD in science (1992) at the Universidad Autónoma de Madrid. He worked as a postdoctoral researcher at the University of Illinois at Urbana-Champaign (USA) from 1992 to 1995, and as assistant professor at the Universidad de Oviedo from 1995 to 1999. In 1999, he obtained a research staff position at the Institut de Ciència de Materials de Barcelona of the Consejo Superior de Investigaciones Científicas (CSIC). In 2007 he moved to the former CIN2 (now ICN2) as the leader of the Theory and Simulation Group, where he is currently a CSIC Research Professor. Since July 2012 he has served as director of the ICN2.

He has published more than 190 scientific articles, which have received over 20,000 citations (h-index of 51). Since 2009 he has served as co-editor of EPL (formerly *Euro Physics Letters*) and since 2004 as

regional editor of *Physica status solidi*. He oversaw the Condensed Matter Physics subject area of the Physics Panel of the Spanish National Evaluation and Foresight Agency (ANEP) from 2003 to 2006, and was the head of the Physics and Engineering Panel of the Access Committee to the Spanish Supercomputing Network from 2005 to 2011. He became a fellow of the American Physical Society in 2005 and in 2017 became a member of the Academia Europaea.

His research is focused on the development of efficient methods for electronic structure calculations in large and complex systems, with contributions to the development of techniques for large-scale atomistic simulations based on first-principles methods such as SIESTA. He has also been involved in the study of the fundamental properties of materials at the atomistic level. His current interests include electronic transport in nanoscale devices and electronic processes at surfaces and 2D materials, among many others. He maintains frequent collaborations with industrial laboratories on the simulation of material processes at the atomic level. He is a co-founder of the spin-off company SIMUNE.



Ordejón Rontomé, Pablo, CSIC Research  
Professor, Group Leader and ICN2 Director

Papior, Nick Rubner, Postdoctoral  
Researcher

Robles Rodríguez, Roberto, Severo Ochoa  
Senior Postdoctoral Researcher

Sentürk, Duygu Gizem, Master's Fellowship  
Student

In 2017 we have continued to focus our efforts on work related to the MaX Centre ([www.max-centre.eu](http://www.max-centre.eu)), one of the eight European Centres of Excellence in HPC Applications supported by the EU under its 2105 H2020 e-infrastructure funding programme.

MaX supports developers and end users of advanced applications for materials simulations, design and discovery, and works at the frontiers of current and future high performance computing (HPC) technologies. It brings together leading developers and users of materials applications, together with top experts in HPC. It is based on the collaboration of 13 teams, including five research groups, like the ICN2 Theory and Simulation Group, which will focus on enhancing the capabilities of the SIESTA package and develop new methodologies for industrial applications of simulation tools in materials science.

We have continued improving the modularity and efficiency of the SIESTA and TRANSIESTA codes. We participated in the organisation of a “SIESTA School” at the Barcelona Supercomputing Center, under the umbrella of MaX activities. Most of the new functionalities developed for SIESTA have been related to the spin-orbit implementation (including a constrained-DFT approach to compute exchange couplings in magnetic materials) and the parallelisation of the Density Functional Perturbation Theory within the code.

The group has continued its participation in NFFAEurope ([www.nffa.eu](http://www.nffa.eu)), a project funded under the H2020-INFRAIA-2014-2015 call “Integrating and opening existing national and regional research infrastructures of European interest”. The NFFA (Nanoscience Foundries and Fine Analysis) is a platform for interdisciplinary research at the nanoscale, in which our group participates as an “installation”

offering computational support for experimental user projects. This year we have received our first approved application, to be executed in 2018.

In 2017 we hosted two international PhD students who came to learn about the techniques developed in the group: Ms. Şentürk, from the Middle East Technical University (Turkey), who spent two months working on novel magnetic 2D materials, and Mr. Bahmani, from the Bremen Center for Computational Materials Science, who spent three months learning about SIESTA and spin-orbit effects in transition metal dichalcogenides.

On the science side of things, in 2017 we made progress in the two research lines we started to develop last year:

#### **Thermal transport at the nanoscale:**

Taking advantage of the expertise of visiting Prof. Colombo on thermal transport at the nanoscale, and coordinated with other theoretical and experimental collaborators, the group has moved forward in this exciting topic, developing new tools and methodologies. In particular, we are exploring the thermal transport properties of 2D materials, which have revealed unusual behaviours (as compared to bulk systems), leading to unexpected intriguing features with significant potential for various front-edge and emerging nanotechnologies (e.g. heat management in nanodevices, thermoelectric energy conversion or the manipulation of lattice heat to engineer phononic devices). The implementation of the Approach to Equilibrium Molecular Dynamics (AEMD) into the SIESTA package will allow other researchers to investigate thermal properties at the nanoscale, from first principles. Within the MaX Centre, and in the context of an industrial collaboration, we have also focused on techniques to study thermal properties in nanofluids, with potential impact on energy storage. Some exciting results have been applied to understand new in-house

experiments (a collaboration between the Novel Energy-Oriented Materials, and the Phononic and Photonic Nanostructures groups and ourselves) on the thermal properties of graphene-dispersed nanofluids.

**Magnetic properties at the nanoscale**, with new developments in SIESTA that make the study of systems with strong spin-orbit effects (including topological insulators) possible, as well as the study of magnetic anisotropies in thin films and other nanostructured materials. We have used the working versions in our study of layered graphene-based magnetic nanostructures (published in *Nature Communications*), frustated magnetic materials, and topological insulators. These materials are very promising in the development of spin-based applications, which are of great interest at the ICN2 as a whole.

In existing research lines, we have made strong progress in:

**Understanding the properties of 2D materials:** In 2017 we have been working on grain boundaries in 2D materials, and 1D polar discontinuities; graphene-based devices for DNA sequencing; insights into the superconducting transition from STM experiments; and novel charge density wave instabilities.

**Understanding nanostructured oxides:** In collaboration with experimental colleagues in Argentina, we studied the mechanisms contributing to oxygen reduction reactions in manganites ( $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$ ), identifying an increased oxygen vacancy concentration close to the surfaces that causes significant ionic conduction and enables the use of these nanostructured materials in solid oxide fuel cells in the “intermediate” temperature range. In addition to this collaboration, and motivated by the MaX Centre, we have established a new research collaboration with industry to advance oxygen diffusion in materials for sensor applications, which will run over the coming years.



**A tunable electronic beam splitter realized with crossed graphene nanoribbons**, Pedro Brandimarte, Mads Engelund, Nick Papior, Aran Garcia-Lekue, Thomas Frederiksen, Daniel Sánchez-Portal, *The Journal of Chemical Physics*; **146 (9)**: 92318. 2017

**Ab initio study of electron-phonon coupling in rubrene**, Ordejón P., Boskovic D., Panhans M., Ortman F., *Physical Review B*; **96 (3)**. 2017. IF: 3.836

**Anisotropic features in the electronic structure of the two-dimensional transition metal trichalcogenide  $\text{TiS}_3$ : Electron doping and plasmons**, Silva-Guillén J.A., Canadell E., Ordejón P., Guinea F., Roldán R., *2D Materials*; **4 (2)**. 2017. IF: 6.937

**Building Complex Kondo Impurities by Manipulating Entangled Spin Chains**, Choi D.-J., Robles R., Yan S., Burgess J.A.J., Rolf-Pissarczyk S., Gauyacq J.-P., Lorente N., Ternes M., Loth S., *Nano Letters*; **17 (10)**: 6203-6209. 2017. IF: 12.712

**Electrical and Thermal Transport in Coplanar Polycrystalline Graphene-hBN Heterostructures**, Barrios-Vargas J.E., Mortazavi B., Cummings A.W., Martinez-Gordillo R., Pruneda M., Colombo L., Rabczuk T., Roche S., *Nano Letters*; **17 (3)**: 1660-1664. 2017. IF: 12.712

**Electrochemical behavior of nanostructured  $\text{La}_{0.8}\text{Sr}_{0.2}\text{MnO}_3$  as cathodes for solid oxide fuel cells**, Sacanell J., Sánchez J.H., Rubio Lopez A.E., Martinelli H., Siepe J., Leyva A.G., Ferrari V.P., Pruneda M., Juan D., Lamas D.G., *ECS Transactions*; **78 (1)**: 667-675. 2017

### Enhanced Cooperativity in Supported

#### Spin-Crossover Metal-Organic Frameworks,

Groizard T., Papior N., Le Guennic B., Robert V., Kepenekian M., *Journal of Physical Chemistry Letters*; **8 (14)**: 3415-3420. 2017. IF: 9.353

#### Field Effect in Graphene-Based van der Waals Heterostructures: Stacking Sequence Matters,

Stradi D., Papior N.R., Hansen O., Brandbyge M., *Nano Letters*; **17 (4)**: 2660-2666. 2017. IF: 12.712

#### Graphene-based synthetic antiferromagnets and ferrimagnets,

Gargiani P., Cuadrado R., Vasili H.B., Pruneda M., Valvidares M., *Nature Communications*; **8 (1)**. 2017. IF: 12.124

#### Growth of Twin-Free and Low-Doped

#### Topological Insulators on BaF<sub>2</sub>(111),

Bonell F., Cuxart M.G., Song K., Robles R., Ordejón P., Roche S., Mugarza A., Valenzuela S.O., *Crystal Growth and Design*; **17 (9)**: 4655-4660. 2017. IF: 4.055

#### Hydrogen Activation by Frustrated Lewis Pairs Revisited by Metadynamics Simulations,

Liu L., Lukose B., Ensing B., *Journal of Physical Chemistry C*; **121 (4)**: 2046-2051. 2017. IF: 4.536

#### Multiscale modeling of spin transport across a diffuse interface,

Chureemart J., Cuadrado R., Chureemart P., Chantrell R.W., *Journal of Magnetism and Magnetic Materials*; **443**: 287-292. IF: 2.63

#### Oxygen Reduction Mechanisms in

#### Nanostructured La<sub>0.8</sub>Sr<sub>0.2</sub>MnO<sub>3</sub> Cathodes for

Solid Oxide Fuel Cells, Sacanell J., Hernández Sánchez J., Rubio López A.E., Martinelli H., Siepe J., Leyva A.G., Ferrari V., Juan D., Pruneda M., Mejía Gómez A., Lamas D.G., *Journal of Physical Chemistry C*; **121 (12)**: 6533-6539. 2017. IF: 4.536

#### Thermal and transport properties of pristine single-layer hexagonal boron nitride: A first

principles investigation, Sergio Illera, Miguel Pruneda, Luciano Colombo, and Pablo Ordejón, *Phys. Rev. Materials*; **1**: 44006. 2017

#### Unconventional Current Scaling and Edge Effects for Charge Transport through

Molecular Clusters, Veronika Obersteiner, Georg Huhs, Nick Papior, Egbert Zojer, *Nano Lett.*; **17 (12)**: 7350-7357. 2017

#### Voltage-Induced Coercivity Reduction in Nanoporous Alloy Films: A Boost toward

Energy-Efficient Magnetic Actuation, Quintana A., Zhang J., Isarain-Chávez E., Menéndez E., Cuadrado R., Robles R., Baró M.D., Guerrero M., Pané S., Nelson B.J., Müller C.M., Ordejón P., Nogués J., Pellicer E., Sort J., *Advanced Functional Materials*; **27 (32)**. 2017. IF: 12.124

#### What Controls Photocatalytic Water Oxidation on Rutile TiO<sub>2</sub>(110) under Ultra-High-Vacuum

Conditions?, Migani A., Blancafort L., *Journal of the American Chemical Society*; **139 (34)**: 11845-11856. 2017. IF: 13.858



## BOOKS

#### On-Surface Atomic Wires and Logic Gates,

Chapter "Band Engineering of Dangling-Bond Wires on the Si (100) H Surface", R Robles, M Kepenekian, C Joachim, R Rurali, N Lorente, *Ed. Springer*, (2017). ISBN: 978-3-319-51846-6



## PROJECTS

NFFA-Europe, Nanoscience foundries and fine analysis-Europe (H2020-INFRAIA-2014-2015), funded by EC, 01/09/2015 to 31/08/2019, Pablo Ordejón

MaX, Materials Design at the eXascale, (H2020-EINFRA-2015-1), funded by EC, 01/09/2015 to 28/02/2018, Pablo Ordejón

SIESTA and the Theory of Instabilities and Transport in Functional and Low-Dimensional Materials, funded by MINECO, 01/01/2016 to 31/12/2018, Miguel Pruneda and Pablo Ordejón



## CONTRIBUTIONS

### Invited

Structural and magnetic properties of atomic magnetic chains supported on Cu<sub>2</sub>N/Cu (100), **2D Materials and Interfaces for Spintronics**, Barcelona, Spain, 23 -25/07/17, R. Robles, D-J. Choi, C. Rubio-Verdú, S. Yan, J.A.J. Burgess, S. Rolf-Pissarczyk, J-P. Gauyacq, M. Ternes, J.I. Pascual, S. Loth, N. Lorente

Electronic instabilities in 2D materials and their interfaces, **1<sup>st</sup> International Workshop Series "Computational and Theoretical Nanoscience"**, IMDEA Nanociencia, Madrid (Spain), 30/11 - 01/12/17, M. Pruneda

Electronic instabilities and metallic grain boundaries in dichalcogenides, **Psi-k Workshop: 2D layered materials for opto-electronics: a theoretical/computational perspective**, CECAM Node Simul, Rome, Italy, 18-19/12/17, M. Pruneda

### Oral

Thermal properties of graphene nanoflakes dispersed in DMF: a classical MD study including QM corrections, **European Materials Research Society (E-MRS). Spring Meeting**, Strasbourg, France, 26-27/05/17, F. Costanzo, B. Ensing, M. Pruneda, P. Ordejón

Thermal properties of graphene nanoflakes dispersed in DMF: a classical MD study including QM corrections, **Nanomaterials & Nanotechnology**, Madrid, Spain, 30-31/03/17, F. Costanzo, B. Ensing, M. Pruneda, P. Ordejón

Thermal conductivity de 2D materials from first principles, **European Materials Research Society (E-MRS). Spring Meeting**, Strasbourg, France, 26-27/05/17, S. Illera, L. Colombo, M. Pruneda, P. Ordejón

Optoelectronic Simulations for Quantum Dot based Devices, **European Materials Research Society (E-MRS). Spring Meeting**, Strasbourg, France, 26-27/05/17, S. Illera, J. D. Prades, A. Cirera.

Thermal conductivity de 2D materials from first principles, **XXXIII Annual Meeting of the Reference Network in Theoretical and Computational Chemistry**, Tarragona, Spain, 5-6/07/17, S. Illera, L. Colombo, M. Pruneda, P. Ordejón.

Ferrocene molecules on metal surfaces: self-assembly and magnetic doping, **XXXIII Annual Meeting of the Reference Network in Theoretical and Computational Chemistry**, Tarragona, Spain, 5-6/07/17, R. Robles, P. Abufager, N. Lorente

### Poster

Thermal energy storage of graphite-like nanoparticles dispersed in solvent, **18<sup>th</sup> International Workshop on Computational Physics and Material Science: Total Energy and Force Methods 2017**, Trieste, Italy, 12/01/2017, F. Costanzo, B. Ensing, P. Ordejón

*Graphene-based synthetic antiferromagnets: an ab-initio study*, **18<sup>th</sup> International Workshop on Computational Physics and Material Science: Total Energy and Force Methods 2017**, Trieste, Italy, 12/01/2017, R. Cuadrado et. al.

*Thermal conductivity of 2D materials from first principles*, **18<sup>th</sup> International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods**, Trieste, Italy, 12/01/2017, S. Illera, L. Colombo, M. Pruneda, P. Ordejon



## DISSEMINATION CONTRIBUTIONS

### *Invited seminar*

*The Role of Relativistic Effects on the Electronic Structure of Materials*, **ALBA Synchrotron Light Source Workshop**, Cerdanyola, Barcelona, Spain, Sep 17, R. Cuadrado

*Thermal transport from first principles simulations*, **ALBA Synchrotron Light Source Workshop**, Cerdanyola, Barcelona, Spain, Sep 17, S. Illera

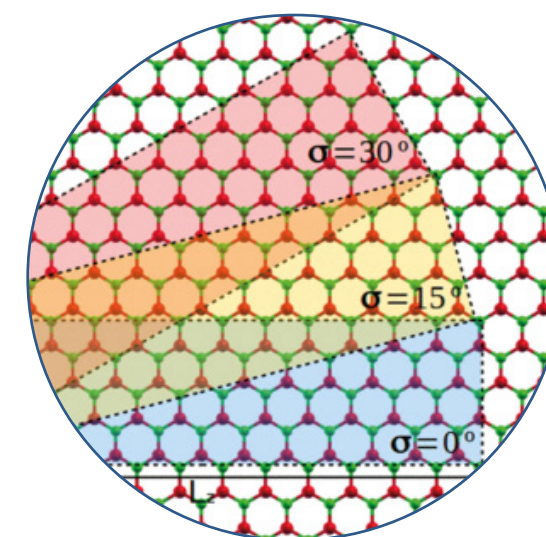
*Magnetic properties of supported molecules*, **ALBA Synchrotron Light Source Workshop**, Cerdanyola, Barcelona, Spain, Sep 17, R. Robles

*Manganite surfaces and 2D materials*, **ALBA Synchrotron Light Source Workshop**, Cerdanyola, Barcelona, Spain, Sep 17, M. Pruneda



## THESES

**Desanka Boskovic**, *Electronic properties of organic semiconductors and low-dimensional materials*, 10/07/17, supervised by Prof. Pablo Ordejón



# Research Support Division



Research at the ICN2 is supported by the Research Support Division, a centralised support infrastructure that provides shared access to specialised equipment, services and expertise. It offers ICN2 research groups and neighbouring centres a repository of advanced services for the development of new methods, materials and instruments, and in doing so fosters multidisciplinary collaborations within the institute and beyond. Led by Dr Gustavo Ceballos, the division is made up of three Research Support Units and a series of Core Research Facilities. It is staffed with highly-qualified scientists and technicians with diverse skillsets that bring added value to the ICN2 and all of its research groups.

## Research Support Units

Led by scientists with extensive research experience, the units develop novel experimental equipment, setups and techniques. Their combined expertise enables ICN2 research groups to conduct experiments at the frontier of science in a way that would not be possible without specialised support.

- Instrumentation Unit **p.138**
- Electron Microscopy Unit **p.140**
- Nanomaterials Growth Unit **p.144**

## Core Research Facilities

The Core Research Facilities constitute a body of specialised equipment, technologies and services. Very much service-oriented, these facilities are run by highly-qualified personnel and allow ICN2 scientists to efficiently and cost-effectively meet their ambitious research goals.

- Nanofabrication Facility **p.148**
- Photoemission Spectroscopy (XPS&UPS) Facility **p.150**
- Molecular Spectroscopy and Optical Microscopy Facility **p.151**
- X-Ray Diffraction Facility **p.152**
- Mechanical Workshop Facility **p.154**

# Instrumentation Unit

## Main Activities

- Design, development and improvement of advanced precision instrumentation
- Modification of commercial instrumentation to match particular experimental requirements
- Scientific computing
- Data acquisition
- 3D-CAD design of precision devices
- Vacuum technology (HV, UHV)
- Cryogenics

## UNIT MEMBERS



**Ceballos, Gustavo**, Head of Research Support Division and Unit Leader



**Maymó, Marc**, Research Engineer

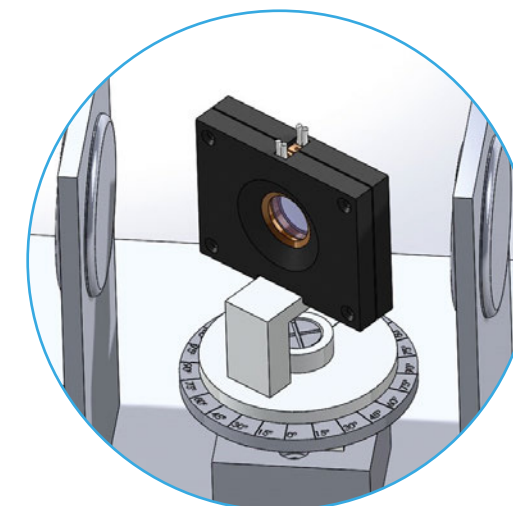
## UNIT LEADER

Dr Gustavo Ceballos earned his degree in chemistry at the Universidad Central de Venezuela in 1989. He obtained his PhD in 1996 at the Institut für Physikalische und Theoretische Chemie der Universität Bonn (Germany). In 1997 he moved to the Institut für Experimentalphysik der Freie Universität Berlin to complete his postdoctoral studies, and from 2001 to 2002 he worked at the Low-Temperature Scanning Tunnelling Microscopy Group at the Fritz Haber Institute of the Max Planck Society, also in Berlin. From 2002 to 2006 he was a research scientist at the XSTM and Low-Temperature STM of Nanostructures Division at the Laboratorio Nazionale TASC-INFM (Trieste, Italy). In 2006 he joined the then ICN as a senior scientist and eventually created the ICN2 Instrumentation Unit. He actively participates in the research led by the ICN2 Atomic Manipulation and Spectroscopy Group.

Throughout his career Dr Ceballos has made modifications to existing instruments or experimental setups, as well as developing new ones to meet the needs of the new experiments he has devised.

## NEW PROJECTS & MILESTONES

The unit provides scientific and technical assistance in applied physics, precision instrumentation, microengineering, nanotechnology, scientific computing and the 3D-design of precision devices. Its central goal is to help address challenging instrumentation requirements in both basic and applied research. In 2017 the unit developed several novel setups to enable new experiments in the fields of magnetometry, spectroscopy and synthesis of nanomaterials. The unit has also brought its expertise to dissemination activities, specifically where the design and construction of prototypes and technology demonstrators have been required.



## PUBLICATIONS

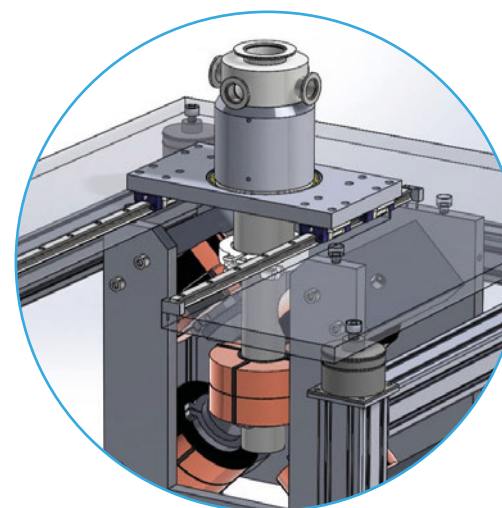
**Symmetry forbidden morphologies and domain boundaries in nanoscale graphene islands**, Parreiras S.O., Gastaldo M., Moreno C., Martins M.D., Garcia-Lekue A., Ceballos G., Paniago R., Mugarza A. *2D Materials*; **4 (2, 025104)** 2017. IF: 6.937

## PROJECTS

*Functional Molecular Nanostructures for Optoelectronic Devices: towards 3-terminal devices (MAT2016-78293-C6-2-R)*, funded by **MINECO**, 30/12/16 to 29/12/19, Aitor Mugarza

*2DMD, Heteroestructuras Basadas en Materiales Bidimensionales para Dispositivos de Electrónica Avanzada*, funded by **MINECO**, 30/12/16 to 29/12/19, Sergio O. Valenzuela

*Nanoscience Foundries and Fine Analysis in Europe (NFFA-Europe) (H2020-INFRAIA-2014-2015)*, funded by **EC**, 01/2016 - 12/2019, Prof. Giorgio Rossi (CNR, Italy)



# Electron Microscopy Unit

## Main Activities

- Use of 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 on the interaction of nanomaterials and biological entities

## UNIT MEMBERS



Ballesteros Pérez, Belén,  
Unit Leader



Belarre Triviño, Francisco  
Javier, CSIC Technician



Rosado Iglesias, Marcos,  
Specialist Technician

## UNIT LEADER

Dr Belén Ballesteros earned her degree in chemistry with honours at the Universitat Autònoma de Barcelona (UAB) in 2001, going on to obtain her PhD in 2006 at the Institut de Ciència de Materials de Barcelona (ICMAB-CSIC).

During her doctoral studies, she undertook research stays at various European universities, including the Universiteit Twente (Netherlands), Universitetet i Oslo (Norway), University of St Andrews (UK) and Universidad de la Laguna. In July 2006 she took a postdoctoral research position at the University of Oxford, where she worked in electron microscopy imaging and the analysis of carbon nanotubes, inorganic nanotubes and related materials. She has been the head of the Electron Microscopy Unit at the ICN2 since April 2009.

Dr Ballesteros has authored 64 peer-reviewed articles with over 1100 citations.



## NEW PROJECTS & MILESTONES

During 2017 the Electron Microscopy Unit consolidated its range of research support activities, providing scientific and technical support not only to internal users, but to an increasing number of external users. This year also saw the unit's first PhD student, Elzbieta Pach, defend her PhD thesis. The unit also hosted a visiting student from King's College London (Kuo-Ching Mei).

As in previous years, the team actively participated in the outreach activities organised at the ICN2, such as the *Escolab*, *Professors i Ciència* and *Bojos per la Física* programmes. Dr Belén Ballesteros also gave a series of lectures on nanotechnology at the Fundació Universitària Bages-UManresa.

Research-wise, the Electron Microscopy Unit has continued to devote efforts to the study of functional carbon nanomaterials for biomedical applications and the characterisation of single-layered inorganic nanotubes. For instance, we have proved the versatility of the templating strategy through the encapsulation of a range of metal halide inorganic nanotubes inside carbon nanotubes.

## PUBLICATIONS

**Encapsulation of two-dimensional materials inside carbon nanotubes: Towards an enhanced synthesis of single-layered metal halides**, Sandoval S., Pach E., Ballesteros B., Tobias G., *Carbon*; **123**: 129-134. 2017. IF: 6.337

**Evaluation of the immunological profile of antibody-functionalized metal-filled single-walled carbon nanocapsules for targeted radiotherapy**, Perez Ruiz De Garibay A., Spinato C., Klippstein R., Bourgoignon M., Martincic M., Pach E., Ballesteros B., Ménard-Moyon C., Al-Jamal K.T., Tobias G., Bianco A., *Scientific Reports*; **7**: 42605, 2017. IF: 4.259

**Filling Single-Walled Carbon Nanotubes with Lutetium Chloride: A Sustainable Production of Nanocapsules Free of Nonencapsulated Material**, Kierkowicz M., González-Domínguez J.M., Pach E., Sandoval S., Ballesteros B., Da Ros T., Tobias G., *ACS Sustainable Chemistry and Engineering*; **5 (3)**: 2501-2508. 2017. IF: 5.951

**Functionalization of Polypyrrole Nanopipes with Redox-Active Polyoxometalates for High Energy Density Supercapacitors**, Dubal D.P., Ballesteros B., Mohite A.A., Gómez-Romero P. *ChemSusChem*; **10 (4)**: 731-737. 2017. IF: 7.226

**Multi-scale analysis of the diffusion barrier layer of gadolinia-doped ceria in a solid oxide fuel cell operated in a stack for 3000 h**, Morales M., Miguel-Pérez V., Tarancón A., Slodczyk A., Torrell M., Ballesteros B., Ouweltjes J.P., Bassat J.M., Montinaro D., Morata A., *Journal of Power Sources*; **344**: 141-151. 2017. IF: 6.395

**Nanosecond Laser-Assisted Nitrogen Doping of Graphene Oxide Dispersions**, Kepic D., Sandoval S., Pino Á.P.D., György E., Cabana L., Ballesteros B., Tobias G., *ChemPhysChem*; **18 (8)**: 935-941. 2017. IF: 3.075

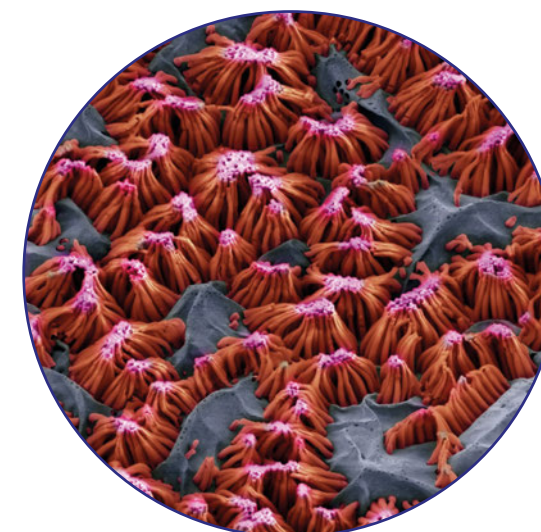
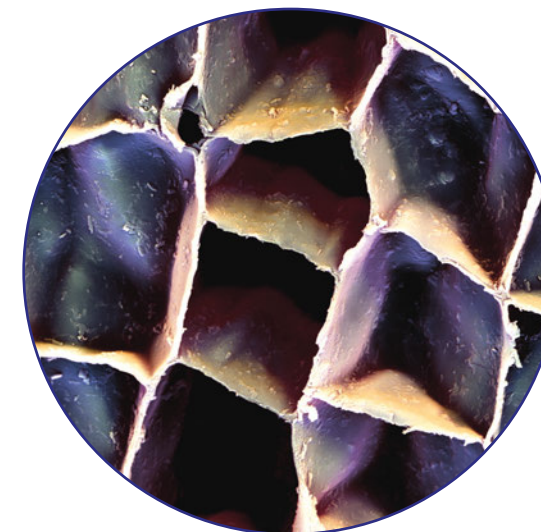
**Raman antenna effect from exciton-phonon coupling in organic semiconducting nanobelts**, Wang M., Gong Y., Alzina F., Svoboda O., Ballesteros B., Sotomayor Torres C.M., Xiao S., Zhang Z., He J., *Nanoscale*; **9 (48)**: 19328-19336. 2017

## THESES

**Elzbieta Pach**, *Electron Microscopy Studies on Functional Carbon Nanotubes*, 19/07/17, supervised by Dr Belén Ballesteros

## COURSES

Belén Ballesteros. *Nanotechnology and societal challenges: how to do more with less*, **Fundació Universitària del Bages**, Mar 2017, 8 hours, Manresa, Spain.





# Nanomaterials Growth Unit

## Main Activities

- Pulsed laser deposition of epitaxial thin films and characterisation of different materials (mainly oxides), looking at strain and relaxation mechanisms, and the microstructural and functional properties of ultrathin films (oxide ionic conducting, thermoelectric, ferroelectric, ferromagnetic, metal-insulating transitions, transparent conducting, etc.).
- MOCVD growth of 2D layers of transition metal dichalcogenides
- Structural characterisation by RHEED and advanced XRD, and high temperature electronic transport properties. Surface composition segregation and its effect on oxygen surface exchange kinetics and ageing phenomena.
- 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)



## UNIT LEADER

Dr José Santiso earned his degree in physics at the Universitat Autònoma de Barcelona (UAB) in 1988, later obtaining his PhD from the Universitat de Barcelona (UB) in 1993.

After his doctoral studies, he worked as a visiting scientist at Cambridge University (UK) from 1994 to 1996. He then joined the Institut de Ciència de Materials de Barcelona (ICMAB) as a research associate and became a CSIC tenured scientist in 2002. In 2007 he moved to the former CIN2 as the leader of the Pulsed Laser Deposition and Nanoionics Group, which later became the ICN2 Nanomaterials Growth Unit. In 2012 he received the Sōmiya Award from the International Union of Materials Research Society (IUMRS) for his contributions to solid state ionics. More recently in 2014 he obtained a grant from the Japan Society for the Promotion of Science to join the International Institute for Carbon-Neutral Research (I<sup>2</sup>CNER, Kyushu University) for a three-month research visit.

In 2015 Dr José Santiso spent three months at the Massachusetts Institute of Technology (USA). The aim of this visit was to consolidate the collaboration between groups working in the field of oxide thin films for energy applications.

Dr Santiso has authored more than 120 articles, and has around 1200 citations and an h-index of 21.



## UNIT MEMBERS



Santiso López, José, CSIC  
Tenured Scientist and Unit Leader



Caicedo Roque, José  
Manuel, Research Engineer



Magrasó Solà, Anna,  
Postdoctoral Researcher



Rodríguez Domínguez,  
Laura, PhD Student



Chatterjee, Arindom,  
Severo Ochoa PhD Student



Bagués, Nuria,  
Visiting PhD Student



## NEW PROJECTS & MILESTONES

Our unit produces films by means of a pulsed laser deposition technique, and works in close and frequent collaboration with many ICN2 research groups, as well as with external collaborators. Our unit carries out preliminary structural characterisation, primarily by X-ray diffraction.

We are also involved in the development of advanced methods for the characterisation by X-ray diffraction of epitaxial thin films. These include in-plane diffraction, GISAXS analysis, as well as 3D reciprocal space mapping. This microstructure research is complemented with HRTEM characterisation.

We are particularly interested in surface and interfacial 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 in-operando characterisation by XRD in different solid state electrochemical devices.

In 2017 we have also continued to develop a thin film MOCVD process for the growth of high-quality ultrathin transition metal dichalcogenides, starting with MoS<sub>2</sub>, in collaboration with the ICN2 group led by Prof. José A. Garrido. We have plans to scale this process up for 2" wafers.

## PUBLICATIONS

**Domain wall magnetoresistance in BiFeO<sub>3</sub> thin films measured by scanning probe microscopy**, N. Domingo, S. Farokhipoor, J. Santiso, B. Noheda & G. Catalán, *Journal of Physics: Condensed Matter*; **29 (33)**: 334003, 2017

**On the persistence of polar domains in ultrathin ferroelectric capacitors**, Pavlo Zubko, Haidong Lu, Chung-Wung Bark, Xavi Martí, José Santiso, Chang-Beom Eom, Gustau Catalán and Alexei Gruverman, *Journal of Physics: Condensed Matter*; **29**: 284001, 2017

## PROJECTS

*Designing advanced functionalities through controlled Nanoelement integration in oxide thin films (DAFNEOX)*; Marie Skłodowska-Curie Actions, Research and Innovation Staff Exchange (RISE). Call: **H2020-MSCA-RISE-2014**, Sep 2015 to Aug 2018, Dr Alberto Pomar (ICMAB-CSIC)

*Designing rules for enhancing surface kinetics in functional oxides for clean energy technologies (SURKINOX)*, funded by **M-ERA.NET**, José Santiso

*Fundamental aspects of thin film growth of oxide heterostructures controlling their resistive switching behaviour (FUN-TO-BE)*, funded by **CNRS-CSIC**, 01/2016 - 12/2018, José Santiso and Mónica Burriel (LMGP Grenoble-CNRS)

*BrainCom, High-density cortical implants for cognitive neuroscience and rehabilitation of speech using braincomputer interface*, (H2020-FETPROACT-2016-2017), funded by **EC**, 01/12/16 to 30/11/21, Jose A. Garrido

*Nanoscience Foundries and Fine Analysis in Europe (NFFA-Europe) (H2020-INFRAIA-2014-2015)*, funded by **EC**, 01/2016 - 12/2019, Prof. Giorgio Rossi (CNR, Italy)

*Oxide Nanoelectronics Group. Emerging Research Group (SGR 1216\_2014)*, funded by **Generalitat de Catalunya**, 01/2015 - 12/2018, Gustau Catalán (ICN2)

*Paredes de dominio, interfaces y dominios de antifase en antiferroeléctricos*, funded by **MINECO**, 30/12/16 to 29/12/19, Gustau Catalán and José Santiso

RED Consolider: *Funcionalización superficial de materiales para aplicaciones avanzadas (FUNCOAT+)* (MAT2015-69035-REDC), funded by **MICINN**, 2015-2018, Agustín Rodríguez González-Elipse (ICMSE-CSIC)

## CONTRIBUTIONS

### Invited

*Electro-chemo-mechanical coupling in energy storage and conversion materials: In-situ X-ray diffraction exploration of chemical expansion in thin films of mixed ionic-electronic conducting oxides*, **Solid State Ionics Conference 21**, Padova, Italy, 18-23/06/17, José Santiso, A. Chatterjee, J.M. Caicedo, A. Magrasó

### Oral

*Characterization of the surface exchange kinetics of Fe-doped CaTiO<sub>3</sub> thin films by time resolved X-ray Diffraction*, **Solid State Ionics Conference 21**, Padova, Italy, 18-23/06/17, Anna Magrasó, J.M. Caicedo, J. Padilla, J. Santiso

*In Situ Investigation of Strain Effects on the Redox Behaviour of Thin Film La<sub>0.5</sub>Sr<sub>0.5</sub>Mn<sub>0.5</sub>Co<sub>0.5</sub>O<sub>3-δ</sub>*, **Solid State Ionics Conference 21**, Padova, Italy, 18-23/06/17, C. van den Bosch, A. Cavallaro, J. Santiso, G. Cibir, S. Skinner, A. Aguadero

*Role of the electrodes on the electrical characteristics of La<sub>2</sub>NiO<sub>4</sub>-based memristive devices*, **Solid State Ionics Conference 21**, Padova, Italy, 18-23/06/17, K. Maas, M. Boudard, Q. Raffay, J.M. Caicedo, C. Jimenez, S. Bagdzevicius, J. Santiso, M. Burriel

### Oral

*Solid oxide fuel cells and electrolyzers: Study of oxygen surface exchange in epitaxial double perovskite GdBaCo<sub>2</sub>O<sub>5+δ</sub> thin film heterostructure by in-situ X-ray diffraction applying external bias*, **Solid State Ionics Conference 21**, Padova, Italy, 18-23/06/17, A. Chatterjee, J.M. Caicedo Roque, J. Zapata, J. Santiso

## DISSEMINATION CONTRIBUTIONS

### Invited lecture

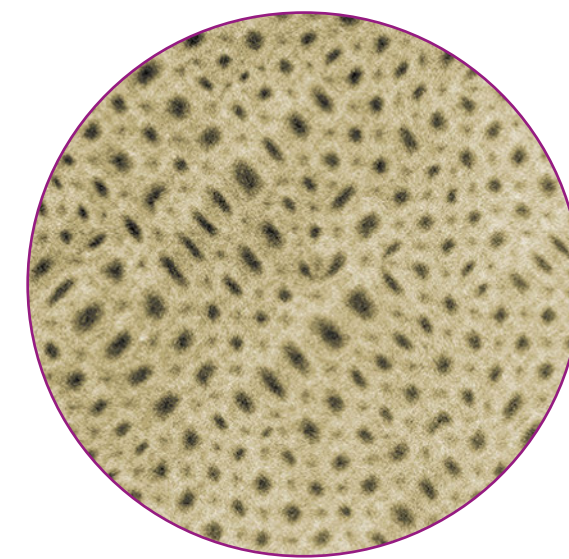
*X-Ray diffraction advanced techniques for Thin Film Materials Characterisation*, **Imperial College Centre for Doctoral Training, Advanced Characterisation of Materials, Summer Retreat – CDT**, Sant Feliu de Guixols, Girona, Spain, 19-22/07/17, J. Santiso

## THESES

**Nuria Bagués**, *Atomic and electronic structure of self-organized defects in epitaxial films of functional perovskite-type oxides*, 06/06/17, supervised by Dr José Santiso López and Dr Felip Sandiumenge Ortíz

## AWARDS

Arindom Chatterjee, Jose Manuel Caicedo Roque, James Zapata and Jose Santiso, **Best Poster Award for Solid Oxide Fuel Cells and Electrolyzers** at the Solid State Ionics Conference 21, *Study of oxygen surface exchange in epitaxial double perovskite GdBaCo<sub>2</sub>O<sub>5+δ</sub> thin film heterostructure by in-situ X-ray diffraction applying external bias*



# Nanofabrication Facility

The Nanofabrication Facility focuses on the design and development of fabrication methods and techniques at the nanoscale for basic and applied research. Providing high quality services to both internal and external users, it aims to support the fabrication and characterisation of nano materials and structures, and the integration of devices at all length scales. It also offers support, assistance and training to ensure researchers and other users are able to operate the available equipment safely and efficiently.

## FACILITY MEMBERS



Pérez, Raúl, Severo Ochoa  
Research Engineer



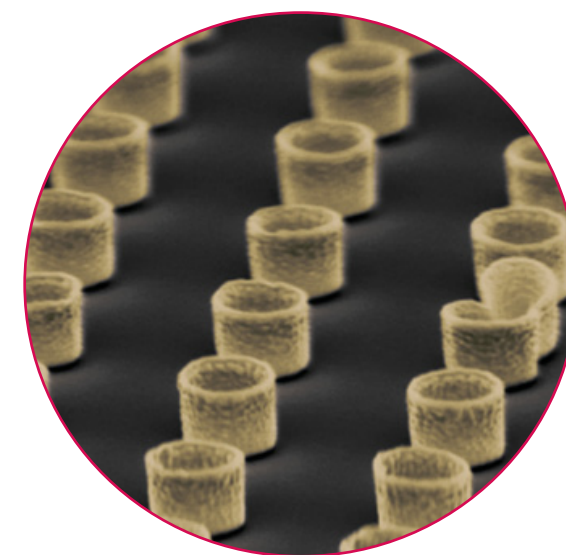
Borrisé, Xavier, Research  
Engineer

## AVAILABLE TECHNIQUES

- Electron-beam lithography (EBL)
- Focused ion beam (FIB)
- Thermal and UV-nanoimprint lithography (NIL)
- Atomic force microscopy (AFM)
- E-beam evaporation
- Sputter coating
- Plasma cleaning
- Wedge bonding
- Spin coating
- Optical microscopy
- 3D optical profiler
- Stylus profilometer

## NEW PROJECTS & MILESTONES

In 2017 work in relation to the Nanofabrication Facility has been focused on the design and construction of a new environmentally-controlled area within the main ICN2 building. This included the specification and purchase of specialised equipment that will boost existing nanofabrication services at the ICN2. With a focus on dry etching and photolithography processes (and combined with the existing evaporation systems), this new equipment will allow the development and fabrication of fully functional micro and nanodevices. In addition to providing essential micro and nanofabrication capabilities for research on electronic, optoelectronic and 2D materials and devices, this facility is intended to facilitate 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 photonics and phononic devices.



# Photoemission Spectroscopy (XPS&UPS) Facility

The Photoemission Spectroscopy Facility is equipped with a state-of-the-art XPS and UPS system (SPECS PHOIBOS 150 hemispherical energy analyser) that enables chemical and electronic characterisation of the surface of a wide range of materials. It provides services to both internal and external users for routine XPS analysis, as well as for long-term experiments to characterise the electronic structure of samples requiring in-situ preparation and modification.

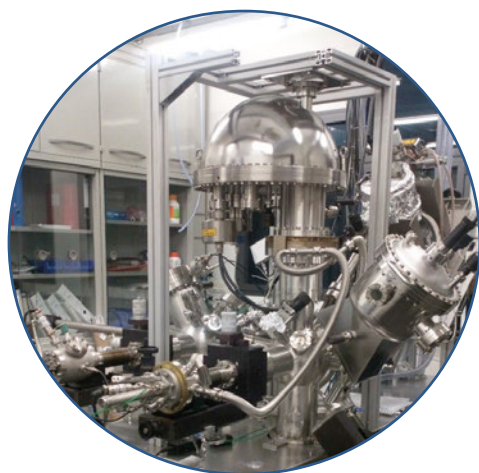
## FACILITY MEMBERS



**Sauthier, Guillaume**,  
Research Technician of the  
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



# Molecular Spectroscopy and Optical Microscopy Facility

The Molecular Spectroscopy and Microscopy Facility is a set of laboratories that allow researchers access to state-of-the-art equipment for the comprehensive physicochemical and structural characterisation of materials at the macro and nano scales. It has been equipped to deliver not only routine analysis, but also highly demanding techniques and applications, meeting the need for basic and specific scientific analysis. Besides offering technical support and training for the equipment that can be self-operated, the facility also performs case studies to be able to offer advice to researchers or develop devices that enhance the performance of existing equipment.

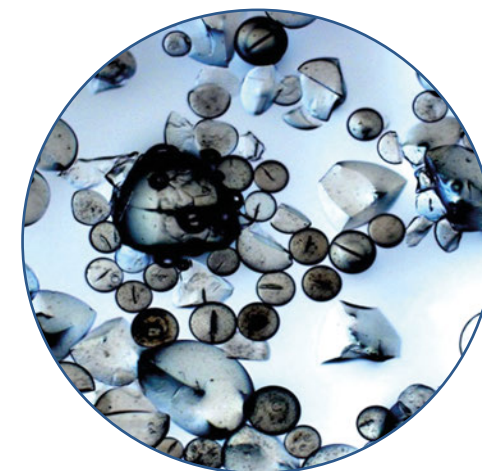
## FACILITY MEMBERS



**Saiz, Javier**, Research  
Technician of the Molecular  
Spectroscopy and Optical  
Microscopy Facility

## AVAILABLE TECHNIQUES

- FT-IR spectroscopy and microscopy
- UV-vis spectroscopy
- Dynamic light scattering and zeta potential
- Optical microscopy
- Fluorescence microscopy
- Static contact angle



# X-Ray Diffraction Facility

This facility is equipped with two advanced X-ray diffractometers (X'Pert MPD and MRD from PANalytical). These pieces of equipment are used to perform X-ray diffraction (XRD) analysis of nanopowders and thin films, and by doing so support the research activities of ICN2 groups and the surrounding research community. The instruments are quite versatile, allowing performance of routine powder analysis and phase identification, to more sophisticated measurements, including glancing angle diffraction, X-ray reflectometry, diffuse scattering studies in nanopowders (SAXS), high-resolution analysis and reciprocal space mapping in epitaxial films, in-plane diffraction, as well as diffraction under non-ambient conditions (high temperature and controlled atmosphere).

## FACILITY MEMBERS



**Padilla, Jessica**, Research Technician of the 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
- 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)

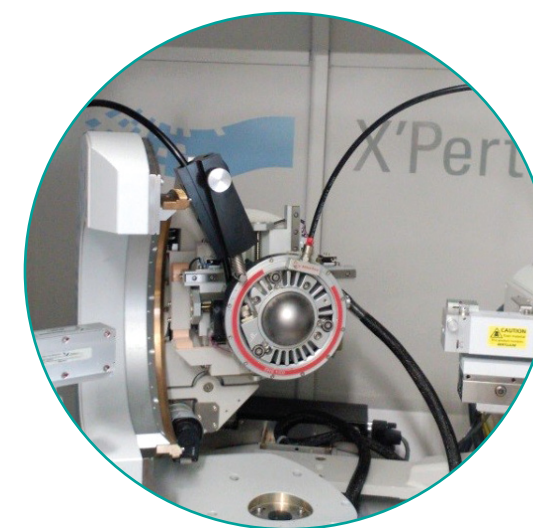
## PUBLICATIONS

**Electric-Field-Adjustable Time-Dependent Magnetoelectric Response in Martensitic FeRh Alloy**, Fina I., Quintana A., Padilla-Pantoja J., Martí X., Macià F., Sánchez F., Foerster M., Aballe L., Fontcuberta J., Sort J., *ACS Applied Materials and Interfaces*, **9 (18)**: 15577-15582. 2017

## CONTRIBUTIONS

### *Invited*

*Magnetic, magnetostructural and magnetoelectric properties of cobalt-based oxides*, **24<sup>th</sup> Congress General Assembly of the International Union of Crystallography 2017**, 21-28/08/2017, Hyderabad, India. *Acta Crystallographica Section A: Foundations and Advances* 73(a2):C1310, 2017, J. L. García-Muñoz, J. Herrero-Martín, J. Padilla-Pantoja, B. Bozzo, I. Urcelay, and, J. Blasco



# Mechanical Workshop

## NEW PROJECTS & MILESTONES

The Mechanical Workshop was created with the aim of supporting researchers by offering high-quality design, fabrication and repair of equipment and instrumentation for research projects. Our workshop specialises in both CNC and traditional machining for variety of materials.

This year the facility ran at full capacity, offering a broad range of custom machining services for the design, fabrication and assembly of devices and parts for ICN2 researchers. Also in 2017 a manual folding and cutting machine was incorporated in the facility, offering new capabilities for metal parts processing. A small 3D printer was also acquired in order to test and evaluate the possibility of offering 3D printing services in a near future. So far it has been used for some prototyping and its potential is still being explored.

## FACILITY MEMBERS

## AVAILABLE TECHNIQUES



León, Rafael, Severo Ochoa  
Mechanical Workshop Technician

- 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
- Folding and cutting machine



# Strategy Development Office



# Strategy Development Office

In 2017 the ICN2 formally inaugurated its new Strategy Development Office with the primary goal of anticipating and providing a response to the challenges faced by the institute on the long and short term. This involves addressing issues at the national and international levels to improve the institute's responsiveness to an ever-changing global context.

Led by Vice-Director Prof. Jose A. Garrido, it marks a pivotal change in the institute's management structure, pursuing the double objective of improving its resourcefulness when securing funds for future research and driving forward the business development and transfer of in-house technologies.

All of the actions of this office are aligned with the ICN2's mission to become a world-leading research institution.



## MAIN ACTIVITIES

- Design and implementation of the ICN2 Strategic Plan
- Preparation and coordination of strategically-important institutional projects
- Advanced research funding support to individual researchers and groups
- Support in forging closer and productive relationships with industry, and the business and innovation communities



## OFFICE MEMBERS

**Del Rey, Alfonso**, Knowledge and Technology Transfer Officer

**Benítez, Núria**, Research Development Officer

**Garrido Ariza, Jose**, ICREA Research Professor, Group Leader and Vice-Director

**Pons, Nadia**, Business Development Officer

**Reverter Cendros, Jordi**, Knowledge and Technology Transfer Officer

**Tienda, Dulce**, Strategy Development Officer



# Management and Services



# Management and Services

Research at the ICN2 is underpinned, protected and promoted by a comprehensive set of management and support services. Overall responsibility for these services, distributed across seven departments, lies with the ICN2 General Manager Mr Lluís Bellafont.



## **COMPETITIVE FUNDING**

The ICN2 Competitive Funding Department is devoted to supporting the researchers in managing competitive funding bids and projects, in compliance with the terms and requirements of the various funding agencies throughout the life of each funded project. This includes providing comprehensive support for the preparation and submission of proposals and, upon grant acceptance, fulfilling all administrative and reporting requirements for active grants, as well as budget management.

The philosophy of the department is based on establishing a fluid dialogue with the researcher in which the assigned project manager becomes the go-to contact for all steps related to project management. In this way, researchers can devote their time almost exclusively to the technical development of their project, minimising their involvement in financial control and deadlines.

## **FINANCE**

The ICN2 Finance Department is split into two areas: administration and accounting.

The administration team oversees all of the institute's administrative functions. Each research group, unit, facility and department has a contact person responsible for all administrative tasks in order to ensure fluid communication and adaptation of the service to the specific needs of unit in question. Sales and billing management is also carried out by this team.

Meanwhile, the accounting team is responsible for the overall financial reporting and control. Reporting is carried out both internally and externally, in fulfilment of the institute's legal obligations as set out by the Spanish tax office and other public bodies, trustees, dashboards and internal economic reports. Its responsibilities include financial analysis, budget monitoring, treasury and public tenders.

## **HUMAN RESOURCES**

The ICN2 Human Resources Department focuses on the people of the ICN2, providing effective talent attraction, selection, development and assessment processes, as well as a set of user-friendly guidelines and tools. Its mission is to support growth and career development through the cultivation of an attractive institutional environment.

The department's policies contribute to making the ICN2 a workplace where people can thrive, share their experience and exchange new ideas. The institute was awarded the European Commission's HR Excellence in Research logo in recognition of its commitment to career development, equal opportunities, transparency and favourable working conditions.

## **INFORMATION TECHNOLOGY**

The ICN2 IT Department provides technical support to the whole of the ICN2 community. In 2017 it continued the implementation of the ICN2 network, IP communication, firewalls etc. It also led work on the new ICN2 Intranet.

## **LEGAL ADVISORY**

Under the supervision of the general manager, the position of Legal Advisor serves the entire institute as its in-house attorney. It offers counsel on all rules and regulations that affect the ICN2, informing of the duties and obligations that must be observed in different situations and drafting and negotiating the legal instruments required to carry out different activities.

Of recent creation and still in the process of adapting to the complexities of the institute, the ultimate objective of the position of Legal Advisor is to provide added value in the analysis and implementation of the different norms that apply to the ICN2, such that it fulfils its objectives more efficiently.

### **MAINTENANCE AND SAFETY**

The ICN2 Maintenance and Safety Department manages all building facilities and plays a key role in the configuration of new spaces. Its members work to keep over 40 laboratories in optimal condition.

The department also oversees management of external service providers in such as cleaning, gardening, reception, security, courier, post, etc.

Another of the department's main roles is to coordinate the Risk Prevention Plan, supervising and editing all safety procedures. Additionally it organises the annual routine medical examinations offered to all ICN2 members and liaises with health and safety-related companies and organisations.

### **MARKETING AND COMMUNICATION**

The ICN2 Marketing and Communication Department offers a range of services to enable and optimise dissemination of the knowledge generated at the ICN2. Its goal is to maximise impact across all key stakeholder groups, while respecting the principles of responsible research and innovation (RRI).

Among its responsibilities is the management of the ICN2 website, social networks and institutional image. It provides graphic design services to ensure that the quality of visual support material is on a par with the science being developed, as well as writing support for important public-facing and internal texts. Its actions are aimed at finding the most effective way to engage a range of audiences, from the internal community to industry to the interested layman. The department also supports and leads the organisation of high-impact events that raise the profile of the ICN2 in different contexts, and delivers a strong line in education outreach.



# Events and Dissemination



- > Science and Industry **p.168**
- > Public Outreach and Education Sector **p.172**
- > Community-Building **p.178**
- > Media Impact **p.180**

# Science and Industry

ICN2 researchers are active contributors to the nanoscience and nanotechnology communities, including through the organisation of scientific events of international scope. Together with their counterparts in management and support, they also enjoy a strong presence at trade fairs.

## CONFERENCES AND WORKSHOPS

### Graphene 2017

Barcelona International Convention Centre (CCIB),  
March 2017



- This prestigious event brought academia and industry together to find new ways to integrate graphene technologies into practical applications.
- Over 250 speakers presented their latest graphene-based achievements, including Nobel Prize laureates Andre Geim and Albert Fert.
- Together with ICFO, the ICN2 was the local organiser of this conference that gathered over 1000 graphene experts from around the world.

### BIST Founding Conference

Centre de Cultura Contemporània de Barcelona (CCCB), March 2017

- The Barcelona Institute of Science and Technology (BIST) Founding Conference brought together 300 participants, including leading scientific experts from Barcelona and beyond.
- Jean-Pierre Sauvage, winner of the 2016 Nobel Prize in Chemistry, opened the conference as keynote speaker.
- The conference included many thought-provoking sessions, including dialogues run by experts in the four research areas that BIST has identified as strategic: chemical biology, graphene, big data and microscopy.



### EU Flagship-Japan Second Workshop

Casa Convalescència, UAB Campus, May 2017

- Organised by the ICN2, this workshop focused on the recent advances in 2D materials and heterostructures achieved by researchers from the Graphene Flagship and Japan.
- Over 40 participants looked at material production, device fabrication and the exploration of electronics, photonics and spintronics in novel structures.



### VIII International Congress on Analytical Nanoscience and Nanotechnology (NyNA 2017)

Casa Convalescència, UAB Campus, July 2017

- With over 100 attendees, the event was a unique opportunity to create enduring links and discuss progress in areas such as diagnostics, safety and security, environmental monitoring and other industrial applications.
- ICN2 group leaders ICREA Prof. Arben Merkoçi, Prof. Laura Lechuga and ICREA Prof. Jordi Arbiol formed the organising committee.



### Taiwan-Spain Workshop on 2D Materials and Interfaces for Spintronics

UAB Campus, October 2017

- The event brought together some 50 researchers from Taiwan and Spain working in the rapidly evolving field of 2D materials and interfaces for spintronics.
- It was co-organised by the ICN2 and the National Center for Theoretical Sciences (NCTS), with ICN2 group leaders ICREA Prof. Aitor Mugarza, ICREA Prof. Stephan Roche and ICREA Prof. Sergio Valenzuela as main coordinators.



## 100xCiencia 2

Alicante, October 2017

- 100xCiencia.2 brought together the vanguard of Spanish research: representatives of the Severo Ochoa and María de Maeztu centres of excellence.
- “Co-creating Value in Scientific Research” was the theme of this meeting devoted to the transfer of scientific knowledge.
- The ICN2 was part of the organising committee, also giving a talk on its vision and actions in relation to creating social and socioeconomic impact.



## 3<sup>rd</sup> Scientific Meeting of BNC-b Students

ICMAB, November 2017

- The aim of this event was to present the work performed by PhD students at the institutions making up the Barcelona Nanotechnology Cluster–Bellaterra: namely, ICMAB, ICN2, IMB-CNM, UAB and ALBA Synchrotron.
- The event included presentations and poster sessions, as well as various invited speakers who shared their experiences of working in companies and as science communicators.
- The participants reflected on the skills acquired during their PhD that are transferrable outside of academia.



## ICN2 BOOTH AT TRADE SHOWS AND FAIRS

### Mobile World Congress (MWC)

Fira de Barcelona, February 2017

- For the second consecutive year, the MWC offered a selection of the most promising applications based on 2D materials like graphene in the Graphene Flagship's Graphene Experience Zone.



- The ICN2 presented two technologies: innovative electronic retina prostheses for patients who have lost their sight but still have a functional optic nerve, and a patented sensor that can be fitted to a mobile phone, with oenology and pollution detection applications.

### Expoquimia

Fira de Barcelona, October 2017

- ICN2 representatives shared their knowledge and experiences at Expoquimia, both as speakers and from an institutional booth shared with members of the Advanced Materials Cluster (Cluster MAV).
- This is a key event and meeting point for the national and international chemical sectors.



## CAREERS FAIRS

### University of Barcelona Careers Fair (Fira d'Empreses)

UB Faculty of Physics, May 2017

- The ICN2 was among the nearly 100 companies and research institutes to interact with students taking the first steps towards a career in science.
- We promoted a research career at the ICN2, pointing to our Jobs Portal as the main way of finding out about open positions.



## EVENT ATTENDANCE

ICN2 researchers also attended many other events during the course of 2017. Details can be found in the group sections. In total our researchers participated in 162 international conferences in 2017, giving a total of 188 talks (118 as invited speakers) and 72 poster presentations.

# Public Outreach and Education Sector

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. Actions in this area are a joint effort between the institute's professional support services and scientists.

## EDUCATION PROGRAMMES

The ICN2 is a regular and active participant in the following regional and national science education programmes:

### NanoEduca

Scientists, teachers and communicators work together on this initiative to bring nanoscience into the classroom, co-founded by the ICN2 together with the Universitat de Barcelona (UB), Universitat Autònoma de Barcelona (UAB) and CESIRE.

This programme includes the design and production of an experiment kit related to the world of nano, the **NanoKit**. These are intended to offer teachers a set of interactive experiences in nanoscience that can be linked to more established subjects like Chemistry, Physics, Mathematics and even Philosophy.

In 2017 some 100 kits were distributed to schools throughout Catalonia via the Catalan Ministry of Education. This was made possible thanks to the efforts of the ICN2 and collaborators, and funding from the ICN2 Severo Ochoa research programme, the Fundación Española para la Ciencia y la Tecnología - Ministerio de Economía, Industria y Competitividad (FECYT-MINECO) and the Fundació Catalana per a la Recerca i la Innovació (FCRi).



### Mad for Physics (*Bojos per la Física*)

The Fundació Catalunya / La Pedrera has developed a programme to open the doors of the region's top research institutes to outstanding secondary school students in different subjects. The ICN2, IFAE and the UAB are the coordinators of the series of events devoted to Physics.

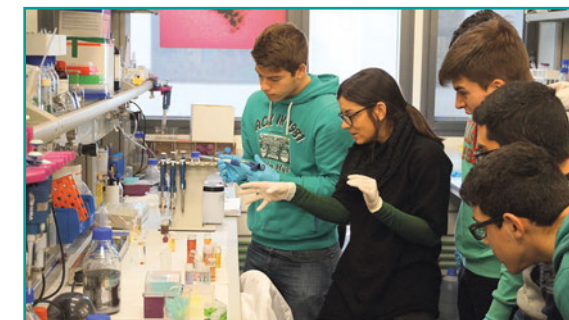
Over the course of the year, 25 outstanding students are invited to interact with researchers from the ICN2, IFAE, UAB, ICMAB and ICFO. The idea is to provide these students experiment-based experiences over 16 sessions, while conveying a sense of what it's like to be a physics researcher.



### ESCOLAB

These lab tours offer young students the opportunity to enter a research facility and interact with real scientists. They are short-term actions which, when combined with follow-up activities, allow to real bonds to be formed with budding young scientists and lead to greater overall engagement with science in general and nanoscience in particular.

ESCOLAB is an initiative led by Barcelona City Council in which the ICN2 has played a role from the outset.



## EVENTS AIMED AT A YOUNG PUBLIC

### Youth Mobile Festival (YoMo)

March 2017, Fira de Barcelona

- This year we presented the NanoKit educational project to the STEAM community, alongside the UB, UAB and CESIRE.



### Festival 10alamenos9

April 2017, Barcelona, UAB Campus and other venues

- In its second edition, the 10alamenos9 Festival of Nanoscience and Nanotechnology was back with over 100 activities to choose from across five locations in Spain.
- The festival kicked off at UAB Campus in Bellaterra with a tour of the different research facilities and a talk from ICREA Prof. Stephan Roche.
- The ICN2 coordinated the activities on the UAB Campus with the participation of the UAB, ICMA B and CNM-CSIC, in an educational activity funded by the Spanish Foundation for Science and Technology (FECYT).



### NanoEduca Schools Contest

May 2017, Universitat de Barcelona

- Part of the **NanoEduca** programme, this annual event brings students together in a scientific conference-like setting for the final stage of a video and poster contest. Young students can get a taste of what it's like to "do science", presenting their 'findings' before an audience of peers.



### Barcelona Science Fair

May 2017, Parc de la Ciutadella de Barcelona

- The ICN2 was at the 2017 Barcelona Science Fair together with collaborating institutions such as the UAB, ICMA B and CRESIB.
- With a central booth devoted to discovering the nanoworld, ICN2 researchers and communicators interacted with a large audience made up of families and science lovers.



### Sabadell Science Fair

September 2017, Sabadell

- The ICN2 participated in this family-friendly science event in the nearby town of Sabadell.
- With activities and experiments aimed at a young public, the ICN2 gave an overview of what it means to work at the nanoscale, also highlighting some of the products derived from the research carried out by the ICN2 community.



### "Welcome to the nanoscale!" exhibition

Sep–Nov 2017, Gas Museum, Sabadell

- The temporary exhibition was co-organised by the ICN2 at the Gas Natural Fenosa Gas Museum in Sabadell (Barcelona) in collaboration with the Institute of Nanoscience of Aragon and the Spanish Foundation for Science and Technology (FECYT).
- The idea behind this exhibition was to shine a spotlight on nanoscience and nanotechnology, and show how it can and already is being applied to the benefit of society.



### OTHER OUTREACH

#### TEDxValencia

April 2017, Valencia

- Prof. Laura M. Lechuga, leader of the Nanobiosensors and Bioanalytical Applications Group, shared her ideas on the present and future of biosensors in a TEDx talk.
- The talk reflected on glucose monitors, the Spanish cucumber scandal and Gattaca, all in the context of the research carried out at the ICN2.





### Nano2All Citizen Debate

June 2017, Centre de Cultura Contemporània de Barcelona (CCCB)

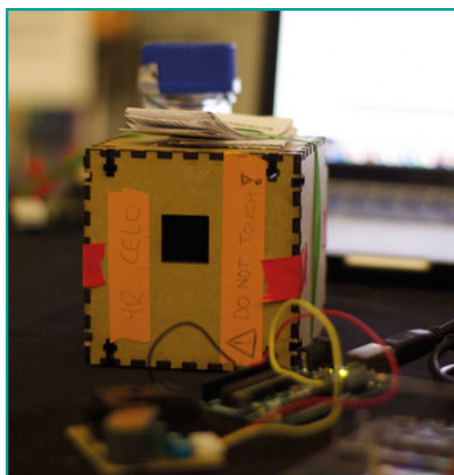
- Nano2All is a European project that brings together 12 project partners across Europe and beyond to put into practice the principles of responsible Research and Innovation.
- Its aim is to support responsible research and policy-making in nanotechnologies through consultation and engagement with all stakeholders from civil society to industry.
- One of its main lines of actions are its citizen dialogues, one of which was organised by the ICN2 in Barcelona to gauge the impressions and understanding of the general public in areas of nano research and technology development.



### Maker Faire Barcelona

June 2017, Fira de Barcelona

- The Maker Faire originated in the San Francisco Bay Area in 2006 as a meeting point for the tech-influenced DIY community. It has gone on to bring together the creative and the curious around the world ever since.
- The ICN2 was there demonstrating a DIY Arduino-based sensor for measuring air quality. It monitors the presence of particulate matter, a substance identified as affecting more people than any other pollutant.



### CSIC Science Mondays (*Lunes de Ciencia*)

November 2017, Barcelona

- Numerous ICN2 researchers participated in this series of talks aimed at the popularisation of science.
- Science Mondays is a well-established initiative led by the Spanish National Research Council (CSIC) and is open to the entire CSIC research community in Catalonia.



# Community-Building

The ICN2 also organises a series of events designed to build and consolidate community within both the ICN2 and the immediate scientific context.

## MANUEL CARDONA LECTURES

The Manuel Cardona lecture series offers the ICN2 community and beyond the opportunity to interact with some of the most prominent researchers in nano-related fields. They stand as a tribute to Prof. Manuel Cardona, a key figure in our institutional history.

In 2017 we hosted Dr Prof. **Young Hee Lee**, director of the Center for Integrated Nanostructure Physics in Seoul (Korea). Invited by ICREA Prof. Stephan Roche, he gave a talk with the title "Recent progresses in 2D materials in CINAP". While here he also gave a short interview discussing changes to the 2D materials landscape and how Korea is rising to the challenge.

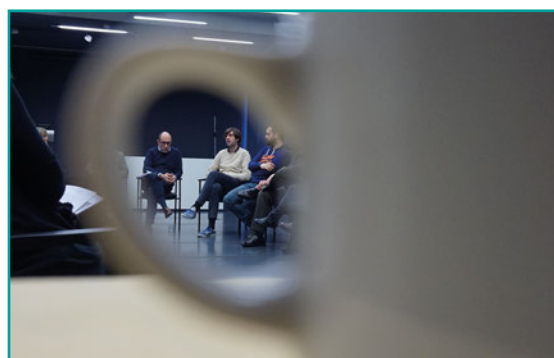
Both his lecture and interview can be found on the ICN2 YouTube channel.



## COFFEE WITH PABLO

In 2017 Human Resources launched the "Coffee with Pablo" initiative. It is designed as an informal channel for internal communication to allow all ICN2 employees the opportunity to hear and be heard directly by the ICN2 Director. Led by Director Prof. Pablo Ordejón the sessions cover a range of topics chosen in advance by those planning to attend.

In 2017 one such coffee session was held.



## ICN2 SEVERO OCHOA SCIENTIFIC WORKSHOPS

Since the kick-off of the ICN2 Severo Ochoa research programme, the institute has organised an annual scientific workshop that brings together ICN2 researchers from all career stages and all of the institute's research groups to share progress in their respective fields.

This year we were also joined by top influencers in innovation and technology transfer in Spain and beyond.



## ICN2 INVITED SEMINARS

The ICN2 hosts regular scientific lectures by international researchers outlining their latest results in topics adjacent to those pursued at the ICN2.

In 2017 a total of 35 seminars were held, delivered by researchers from centres in the United States (5), Europe (20), Spain (4) and the rest of the world (7).



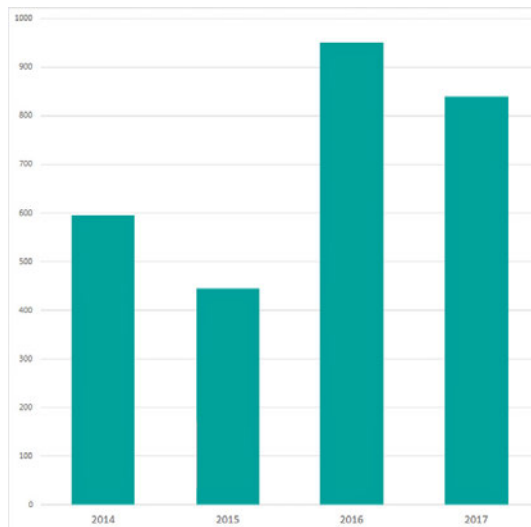
# Media Impact

In 2017 the ICN2 continued its efforts to reach out to the general and scientific public through the media. Close working relationships with journalists, ten scientific press releases and other research-related news articles scored a high total number of journalistic impacts for the ICN2.

The following chart shows the number of online impacts identified on journalistic websites over the past four years.



Number of online journalistic impacts per year  
Source: Meltwater



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Marketing and Communication Department  
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