

ANNUAL REPORT 2018



BOARD OF TRUSTEES



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Letter from the Director



2018 was a very successful year for the Catalan Institute of Nanoscience and Nanotechnology (ICN2).

Our scientific activity has resulted in a total of 172 indexed publications and an average impact factor that has increased to a remarkable 8.86 (6.88 in 2017). This figure has been steadily growing in the recent years, with a very relevant increase reported in the present document. Even though the number of articles has been slightly reduced in comparison to previous years, it is worth mentioning that 81% of the publications appeared in journals in the first quartile and 47% in the first decile.

Such high-quality indicators, sustained along the recent years, are among the reasons that facilitated one of the greatest achievements of 2018: being one of the five centres recognised with a Severo Ochoa award and renewing our status as a national centre of excellence. The ICN2 is proud to be awarded this distinction for the second time. The associated grant (€4m over four years, from July 2018 to June 2022) will be devoted to the implementation of a strategic plan that strives for excellence in the research developed at the ICN2 but also in the supporting services and institutional framework that make it possible. A particularly important component of this plan is the recognition of the technology transfer activities as a key objective for the future of ICN2. Our Severo Ochoa workplan includes a series of actions to boost our innovation activities and accelerate the path to the market from the knowledge generated by our researchers.

As you will be able to witness in the following pages, 2018 was an outstanding year in terms of competitive funding attraction (with a historic record of funds gained in competitive calls), the consolidation of new facilities such as the Biolab and the Clean Room and the impact achieved through our outreach and educational programmes. From the technology transfer side, I would like to mention that the Strategy Development Office has gone through a deep redesign that was not yet fulfilled by the end of 2018. Despite of that transformation process, the technology transfer activity of the ICN2 remains notable with 6 new priority patent applications, 1 industrial secret and 3 PCT extensions, out of 17 technologies analysed for patentability in 2018.

During 2018, a new group has been established, under the leadership of Dr Klaas-Jan Tielrooij, who joined us as a Junior Group Leader in September. He enjoys a Ramón y Cajal Fellowship from the Spanish Ministry of Science, Innovation and Universities, and was awarded an ERC Starting Grant shortly after closing the deal to join the ICN2. He leads the ICN2 Ultrafast Dynamics in Nanoscale Systems Group. In turn, the Board of Trustees, following the recommendation of the ICN2's Scientific Advisory Board, decided to close down the Force Probe Microscopy and Surface Nanoengineering, and to assign Dr Fraxedas, its former Group Leader, the task of leading the scientific and strategic activities of collaboration of ICN2 with the neighbouring ALBA Synchrotron. This change will be made effective in early 2019.

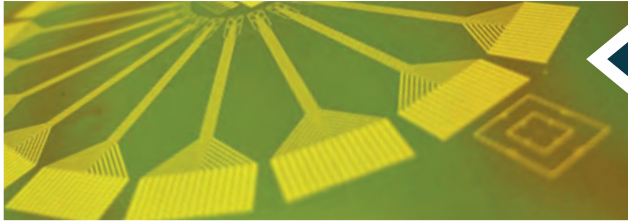
Cooperation within the Barcelona Institute of Science and Technology (BIST) has continued and become stronger. A deeper involvement in the forge and attraction of new talent, as well as initiatives such as the BIST Ignite awards, has allowed an expanding collaboration among the BIST centres. Besides, the two strategic research lines of BIST in which the ICN2 is playing a leading role ("Super-resolution Microscopy" and "Graphene and 2D Materials") are progressing very quickly, and have developed a strategy of investment that will hopefully start producing important results and outcomes during 2019.

Overall, 2018 was an excellent year for the ICN2. 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?



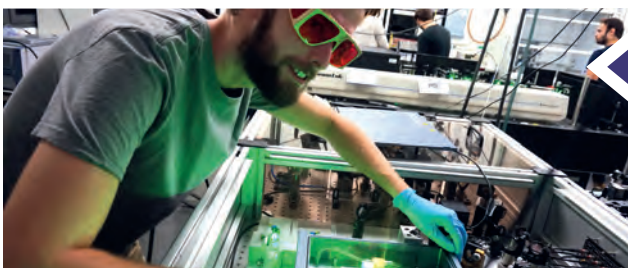
Global leader
in nanoresearch

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

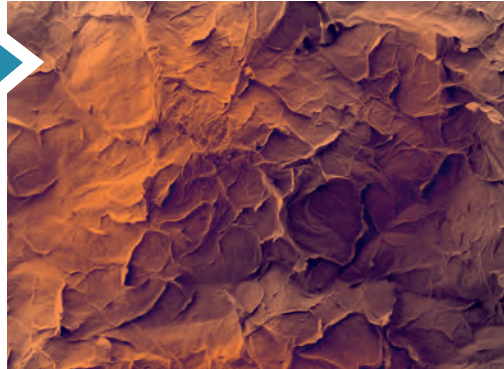
Commitment to equal
opportunities, fair selection
processes and the importance
of the work/life balance



Trainer of the
future generation of
nanoscientists

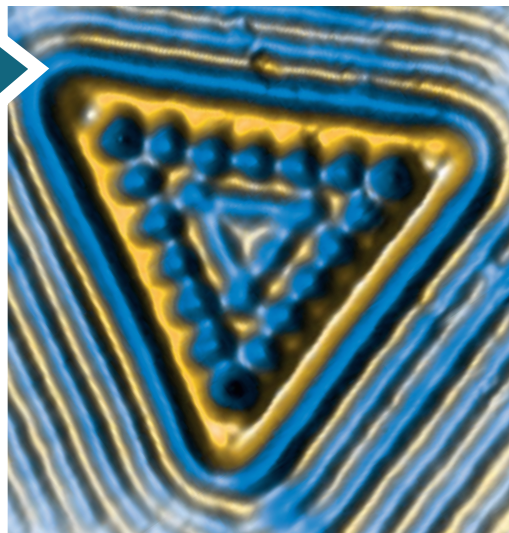
What do we do?

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*

Maria Àngels Chacón, Minister for Business and Knowledge, *Generalitat de Catalunya*

Vice-President*

Rosa Menéndez, President of CSIC (*Consejo Superior de Investigaciones Científicas*)

Secretary

Joan Gómez Pallarès, General Director for Research, Ministry of Business and Knowledge, *Generalitat de Catalunya*

Members

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

Lluís Calvo, Institutional CSIC Coordinator in Catalonia

Francesc Xavier Grau Vidal, Secretary of Universities and Research, Ministry of Business and Knowledge, *Generalitat de Catalunya*

Victor Ramón Velasco Rodríguez, 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. **Steven Louie**, UC Berkeley and Lawrence Berkeley National Laboratory, USA

Dr. **Tapani Ryhänen**, Emberion, Finland

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

Prof. **María Vallet Regí**, Facultad de Farmacia, Universidad Complutense de Madrid, Spain

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 ICREA 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 2018 the ICN2 gathered 18 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**
(No longer existing in 2019)
- Inorganic Nanoparticles
ICREA Prof. **Víctor F. Puntes**
- 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**
- Ultrafast Dynamics in Nanoscale Systems
Dr **Klaas-Jan Tielrooij**

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

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
- Health and Safety
Jose Antonio Pérez Calvo
- Human Resources
Rocío Pérez
- Information Technologies
Jordi Prat Ribas
- Maintenance and Services
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 2018 it had an average workforce of 275 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 2018

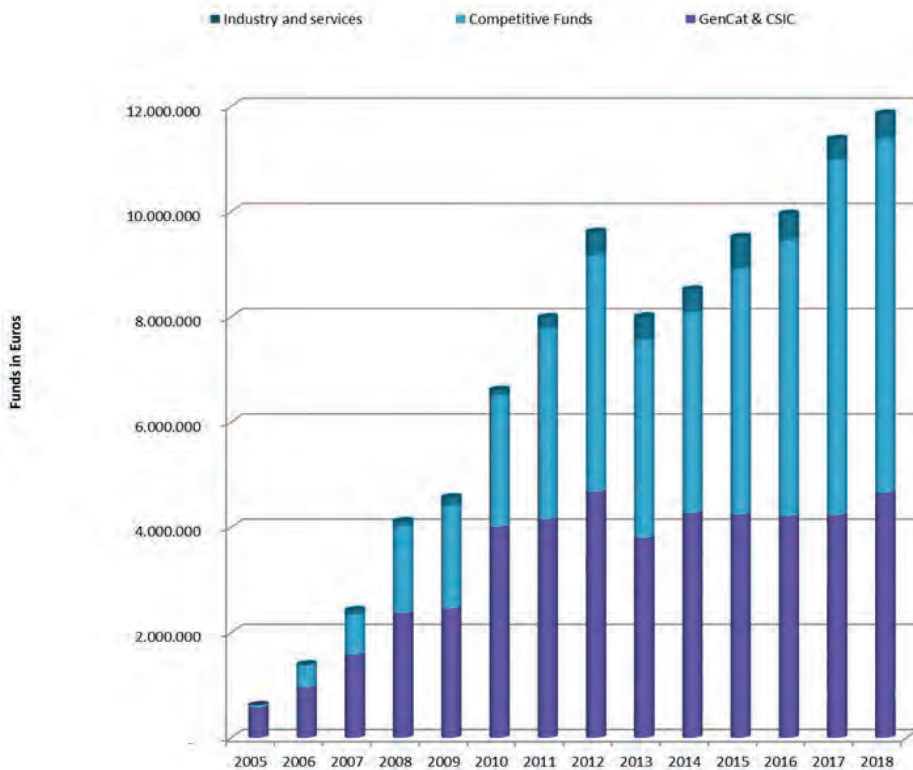
In 2018 the ICN2 Finance Department has continued to roll out the SAP Business One system, developing the web area where budget managers can monitor performance.

This year we have worked towards consolidating 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 2018 stood at €11,855,305, of which 39% were obtained from the Generalitat de Catalunya and the Spanish National Research Council (CSIC), 57% from competitive funding calls, and 4% from industry and services.

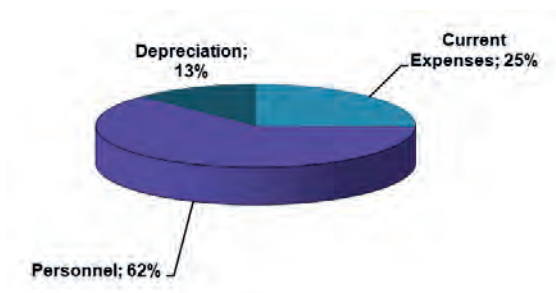
Evolution of ICN2 Operating Funds



EXPENSES

Total expenditure in 2018 came to €11,848,753 including current expenses, personnel costs and depreciation.

Expenditure in 2018



Facilities and Equipment

Total accumulated investment by the ICN2 in scientific equipment, common services and general infrastructure as of year-end 2018 stood at €22,263,518.

During 2018 investment came to a total of €1,666,558, being the most important investments:

- ICN2 access control points
- Nanofabrication facilities furniture
- ATEX hut
- OriginPro Software
- Magnetic vector
- Multi chamber molecular beam epitaxy system
- ASAP 2640 Physisorption Analyser (liquid nitrogen version)
- Magellan Microscope Energy dispersive X-ray (EDX) System
- MBE
- Benchtop centrifuge (Allegra 64R)

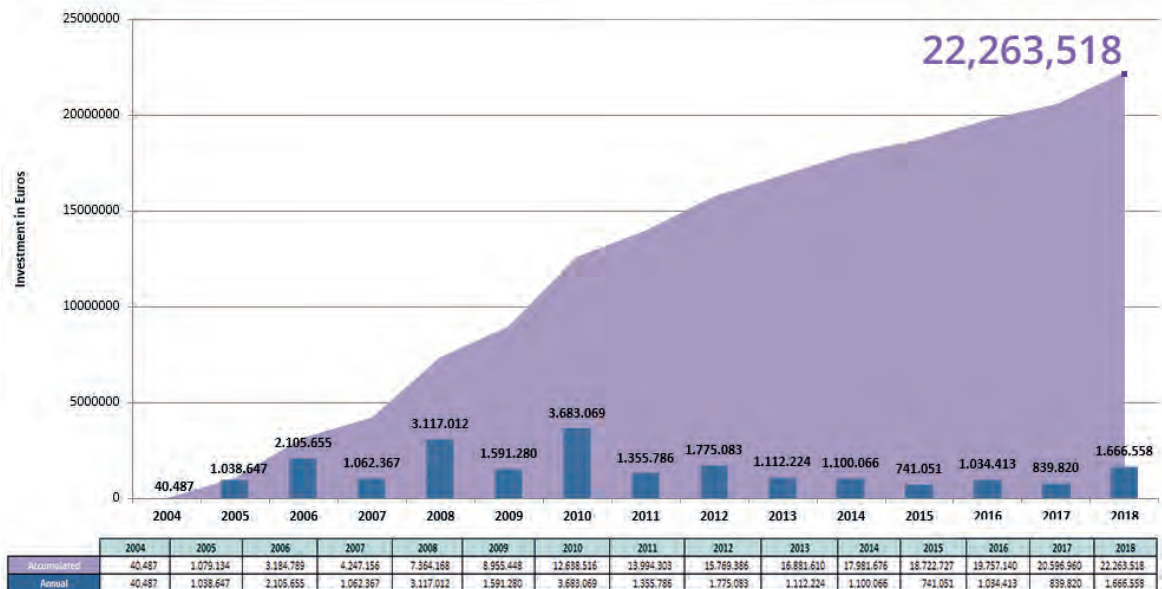


EUROPEAN UNION
European Regional Development Fund

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

- CQ8570 printer
- SPR equipment
- Dell 3050 SFF computer
- 3 400G4SFF laptops
- Halogen lamp
- Bath sonicator
- Precision valve
- Works contract for a BSL-2 type biosafety room
- VIS-NIR PhotoSpectrometer
- PRO 13 Touchbar Quad laptop
- Lateral flow trimming machine
- Dual heater
- Low Energy Electron
- Magnetic vector
- MBE
- Works to equip the nanofabrication premises with a controlled laboratory environment
- Optical lithography equipment for the nanofabrication facilities
- ICP-RIE System for the nanofabrication facilities

Evolution of Investments between 2004 and 2018



Our Research



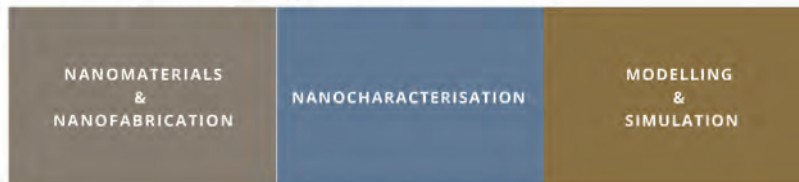
Severo Ochoa Centre of Excellence



4 areas of application



3 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 united 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. It also boosted 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.

On November 2018 the Spanish Research Agency (AEI) published the definitive list of centres and units to be awarded grants under its programme to recognise centres and units of scientific excellence. In total five national research centres were awarded the Severo Ochoa distinction and seven research units named as María de Maeztu units of excellence. The ICN2 was again among the awarded centers renewing its position as reference in national and international research and consolidating its scientific leadership under the previous Severo Ochoa grant.

The ICN2 is proud to be awarded this distinction for the second time, and devotes the associated grant (€4m over four years) to the implementation of a strategic plan that strives for excellence in both the research it develops, and the supporting services and institutional framework that make it possible.

At the heart of this plan, our scientific programme will continue in the pursuit of frontier outcomes in both basic and applied research. Over the coming years, as under the previous Severo Ochoa grant, ICN2 researchers will largely focus on delivering impact in health, ICT, energy and the environment, identified as areas that lend themselves to the application of institutional expertise and to the pursuit of global challenges and growth opportunities. These will be supported by three “enabling platforms” which together constitute a core hub of knowledge, materials, techniques and instrumentation to drive scientific and technological advances in the application areas.

New for the second Severo Ochoa programme is the “technology pipeline”, created to consolidate and further professionalise the support provided by the institute to researchers on the path to market and entrepreneurship. Significant resources will also be devoted to achieving excellence beyond the purely scientific, for instance building on the cultural shift(s) instigated under the first Severo Ochoa in career development, gender awareness and inclusivity, and internal collaboration.

All of the actions proposed in the strategic plan for 2018-2021 have been carefully designed to achieve the goals of robustness and impact. We envision a period of consolidation, on the one hand, of all the achievements of the past four years, and of growth and diversification of the ways in which we interact with the world around us, on the other.

We are honoured by the trust placed in us in the form of this second Severo Ochoa excellence award and will work to uphold the values it represents.

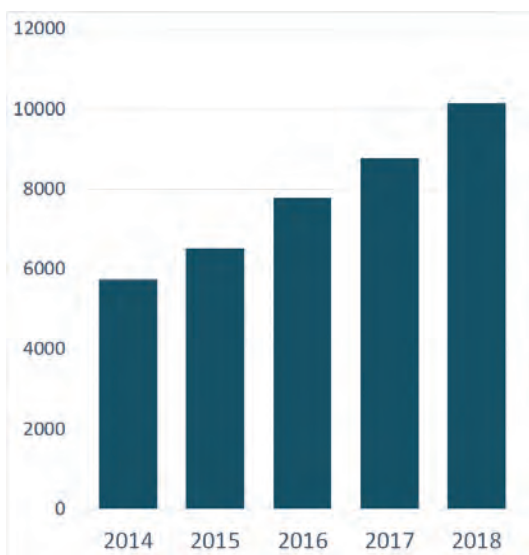
Publications

Once again the ICN2 has performed well in terms of scientific publications. With 172 original papers published in the most influential journals, the average institutional impact factor (IF) has risen from 6.88 in 2017 to 8.86 in 2018.

We are particularly proud of the fact that 136 of these articles (81%) were accepted for publication in first-quartile journals, while 77 (47%) appeared in first-decile journals. Meanwhile, papers authored by ICN2 researchers were cited 10,132 times in 2018.

CITATIONS

Evolution of Citations



Source: Scopus

TOP 10 JOURNALS

Journal	IF	No. articles
<i>Science</i>	41.06	2
<i>Chemical Society Reviews</i>	40.18	3
<i>Nature Nanotechnology</i>	37.49	2
<i>Energy and Environmental Science</i>	30.07	1
<i>Nature Chemistry</i>	26.2	1
<i>Nature Physics</i>	22.73	1
<i>Advanced Materials</i>	21.95	3
<i>Advanced Energy Materials</i>	21.88	1
<i>Accounts of Chemical Research</i>	20.96	1
<i>Journal of the American Chemical Society</i>	14.36	3

Technology Transfer

In 2018 the Technology Transfer Unit of the ICN2 was linked to the structure of the Strategy Development Office, under the overall direction of ICN2 Vice-Director Prof. Jose A. Garrido. A redesign process started leading to the creation of a new Business and Innovation Office that will be fully operative in 2019.

During the year the team 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 and new networking channels.

INTELLECTUAL PROPERTY

17 technologies analysed for patentability

6 new priority patent applications:

- *Electroluminescent sensing devices.*
- *Circuit for the multiplexing and readout of variable resistance sensor arrays.*
- *A nanoporous graphene structure and method of preparation thereof.*
- *Graphene transistor system for measuring electrophysiological signals.*
- *Celda electrolítica y procedimiento para la obtención de grafeno por exfoliación elect.*
- *Methods of forming a porous graphene-based macroscopic structure.*

1 industrial secret

3 PCT extensions

1 KH licensing agreements

- *Earthdas SL, for making graphene batteries.*

2 granted valorisation projects:

- *One Industrial PhD*
- *One RIS3CAT Project (PLASTFUN)*

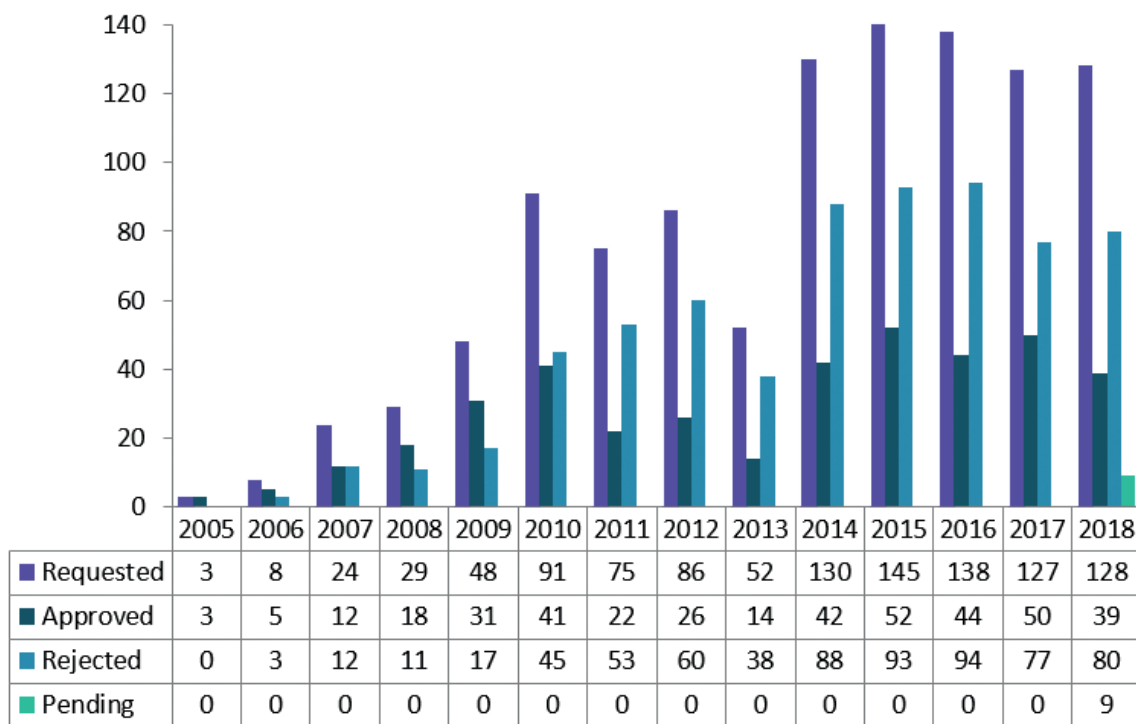
24 Industry Service Actions:

- *Active Contact with 39 Companies*
- *19 NDAs and 4 MTAs Signed*

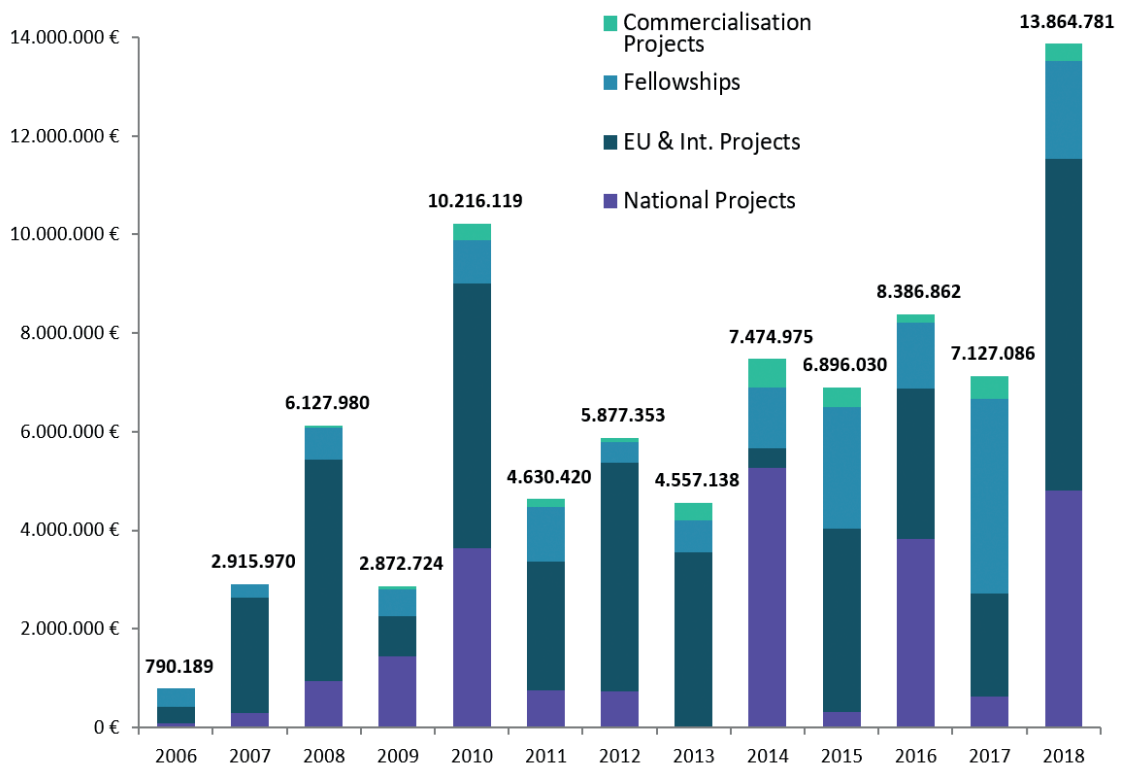
Projects

In 2018 the number of submitted proposals has been very similar to the previous year. Likewise, the success rate is expected to be in line with 2017 once all pending calls are resolved. However, the income from competitive projects has significantly increased. This is because the average amount granted per project has augmented. Outstanding among the awarded projects are the second "Center of Excellence Severo Ochoa" award, an ERC Starting Grant and a H2020 FET Proactive project coordinated by ICN2.

**Outcome of Proposals Submitted by Year
(as of 30/04/2019)**



Evolution of Income from Approved Proposals by Source



Research Groups

The ICN2 currently has 18 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.24**
- > Advanced Electronic Materials and Devices **p.32**
- > Atomic Manipulation and Spectroscopy **p.40**
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- > NanoBioelectronics and Biosensors **p.62**
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- > Nanostructured Functional Materials **p.76**
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- > Physics and Engineering of Nanodevices **p.106**
- > Supramolecular NanoChemistry and Materials **p.112**
- > Theoretical and Computational Nanoscience **p.118**
- > Theory and Simulation **p.124**
- > Ultrafast Dynamics in Nanoscale Systems **p.132**

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

Botifoll Moral, Marc, Fellowship Master Student

David, Jeremy, Postdoctoral Researcher

González Febles, Ana, Visiting TFG Student

Han, Xu, Fellowship Doctoral Student

Infante Carrió, María Francisca, Visiting Degree Student

Koch, Christian, Fellowship Degree Student

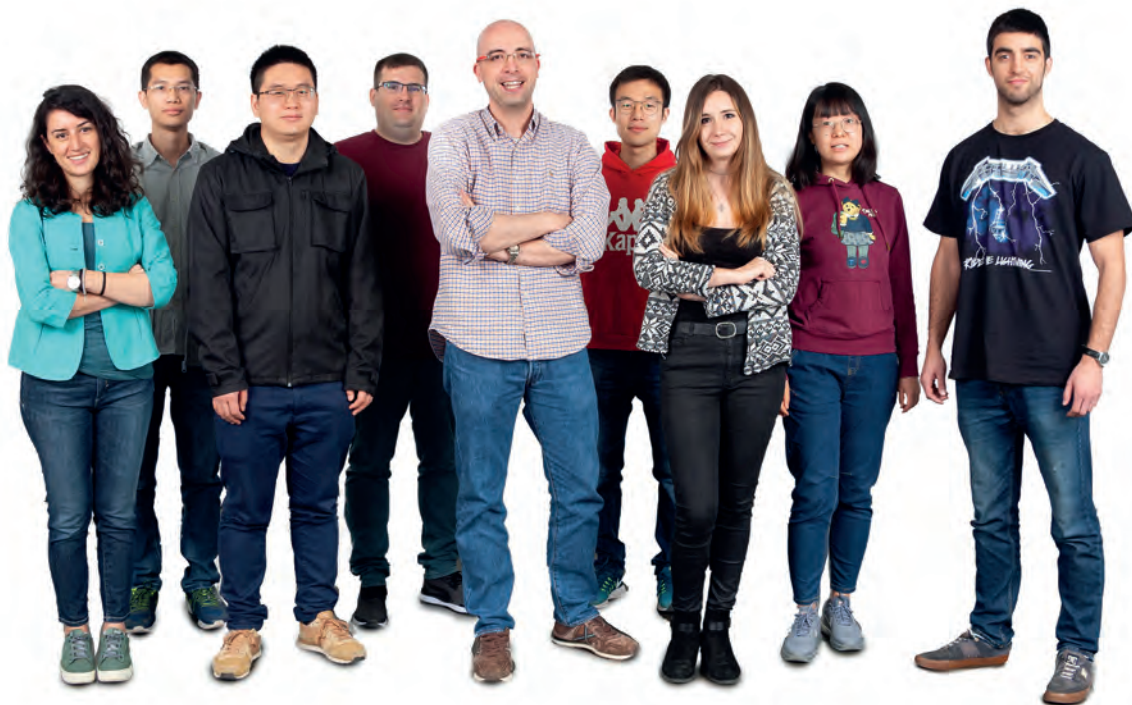


GROUP LEADER



ICREA Research Prof.
Jordi Arbiol

ICREA 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 he began his personal and professional mission to improve Barcelona’s baseline electron microscopy



Martí Sánchez, Sara, Doctoral Student
Spadaro, Maria Chiara, Postdoctoral Researcher
Swoboda, Timm, Visiting Master Student

Tang, Pengyi, Postdoctoral Researcher
Zhang, Ting, Fellowship Doctoral Student
Zhifu, Liang, Doctoral Student

infrastructure, an endeavour 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. In 2019 he became Member of the Executive Board of the International Federation of Societies for Microscopy (IFSM). 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 320 peer-reviewed publications, h-index: 65 WoS (74 GoS), with more than 12750 WoS (16475 GoS) citations.



NEW PROJECTS & MILESTONES

The main weakness of electron microscopy in Catalonia has been the lack of advanced infrastructure. We solved this challenge by establishing strong international collaborations with prestigious microscopy research centers and facilities worldwide. In parallel, in the last 5 years, we've been working at all levels to secure the funding that will allow purchasing modern electron microscopes in the Barcelona area. In this way, we are leading the Scientific part of the METCAM-FIB project (~5 M€), which will allow the acquisition of an advanced electron microscope for materials science and a Focus Ion Beam (FIB). The advanced (S)TEM will be placed at the ALBA-Synchrotron by the end of 2020. The analytic possibilities that the new infrastructure will provide as well as the synergies within the BIST and CSIC institutes, the UAB and the Synchrotron will be at the core of our future plans for the next 5 years.

The new microscopes will allow expanding the group capabilities on the in-situ correlative electron/synchrotron microscopy on energy nanomaterials and will allow a more accurate study on the direct correlation and atomic detection research lines.

The next steps moving forward in the energy nanomaterials research line will be related to the development of in-situ / in-operando experiments in the electron microscope to understand the physical and chemical phenomena promoting the different energy mechanisms (e.g.: photoelectrochemical) with unprecedented resolution. Taking advantage of the synergy with the synchrotron we will work on developing correlative in-situ electron microscopy and Synchrotron experiments (unprecedented in EU), in correlation to the developed theoretical models.

The initial BIST Ignite seeding project (InWOC2) as well as the recently granted ANAPHASE project will help to initially fund the research proposed above. However, the high impact results recently achieved, as well as the preliminary outstanding results just obtained on novel photoelectrochemical earth abundant nanomaterials for water splitting and hydrogen generation (artificial photosynthesis), are encouraging us to prepare an ERC Synergy Grant proposal for the next Call with our ICIQ and ALBA collaborators.

On the other hand, our research line devoted to the direct correlation between atomic scale structure/composition and sub-nanometer scale physical properties will be benefited with the secured funds of the collaborative project with Microsoft for the next years. The new capabilities on the analysis offered by the new infrastructure will allow the study of the novel designed hybrid semiconductor/ superconductor Majorana nanowires for their application in quantum computing and better understand the complex physical phenomena involved in their related devices. The new EU Commission Flagship on Quantum Technology is also a near future objective for funding application (FET and QuantERA calls), together with our collaborators (e.g.: EPFL, Niels Bohr Institute - Univ. Copenhagen, TU Delft, Microsoft), which are some of the main actors on Quantum Technologies in EU.



Ab initio structure determination of Cu_{2-x}Te plasmonic nanocrystals by precession-assisted electron diffraction tomography and haadf-stem imaging, Mugnaioli E., Gemmi M., Tu R., David J., Bertoni G., Gaspari R., De Trizio L., Manna L. *Inorganic Chemistry*; **57 (16)**: 10241-10248. 2018.

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Growth of Au-Pd₂Sn nanorods via galvanic replacement and their catalytic performance on hydrogenation and sonogashira coupling reactions, Nafria R., Luo Z., Ibáñez M., Martí-Sánchez S., Yu X., De La Mata M., Llorca J., Arbiol J., Kovalenko M.V., Grabulosa A., Muller G., Cabot A. *Langmuir*; **34 (36)**: 10634-10643. 2018. 10.1021/acs.langmuir.8b02023. IF: 3.789

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Neuderth P., Hille P., Schörmann J., Frank A., Reitz C., Martí-Sánchez S., De La Mata M., Coll M., Arbiol J., Marschall R., Eickhoff M. *Journal of Materials Chemistry A*; **6 (2)**: 565-573. 2018. 10.1039/c7ta08071a. IF: 9.931

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Mukherjee S., Givan U., Senz S., De La Mata M., Arbiol J., Moutanabbir O. *Nano Letters*; **18 (5)**: 3066-3075. 2018. 10.1021/acs.nanolett.8b00612. IF: 12.080

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Shi Q., Murcia-López S., Tang P., Flox C., Morante J.R., Bian Z., Wang H., Andreu T. *ACS Catalysis*; **8 (4)**: 3331-3342. 2018. 10.1021/acscatal.7b04277. IF: 11.384

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Vaitiekėnas S., Whitticar A.M., Deng M.-T., Krizek F., Sestoft J.E., Palmstrøm C.J., Martí-Sánchez S., Arbiol J., Krogstrup P., Casparis L., Marcus C.M. *Physical Review Letters*; **121 (14)**: 147701, 2018. 10.1103/PhysRevLett.121.147701. IF: 8.839

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Liu J., Wang S., Kravchyk K., Ibáñez M., Krumeich F., Widmer R., Nasiou D., Meyns M., Llorca J., Arbiol J., Kovalenko M.V., Cabot A. *Journal of Materials Chemistry A*; **6 (23)**: 10958-10966. 2018. 10.1039/c8ta01492b. IF: 9.931

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Barreca D., Bigiani L., Monai M., Carraro G., Gasparotto A., Sada C., Martí-Sánchez S., Grau-Carbonell A., Arbiol J., Maccato C., Fornasiero P. *Langmuir*; **34 (15)**: 4568-4574. 2018. 10.1021/acs.langmuir.8b00642. IF: 3.789

Tailoring copper foam with silver dendrite catalysts for highly selective carbon dioxide conversion into carbon monoxide,

Urbain F., Tang P., Carretero N.M., Andreu T., Arbiol J., Morante J.R. *ACS Applied Materials Interfaces, B: Chemical*; **10**: 43650-43660. 2018. 10.1021/acsami.8b15379. IF: 8.097

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Triphenyl phosphite as the phosphorus source for the scalable and cost-effective production of transition metal phosphides, Liu J., Meyns M., Zhang T., Arbiol J., Cabot A., Shavel A. *Chemistry of Materials*; **30 (5)**: 1799-1807. 2018. 10.1021/acs.chemmater.8b00290. IF: 9.890

Ultrasensitive binder-free glucose sensors based on the pyrolysis of in situ grown Cu MOF, Zhang X., Luo J., Tang P., Morante J.R., Arbiol J., Xu C., Li Q., Fransaer J. *Sensors and Actuators, B: Chemical*; **254**: 272-281. 2018. 10.1016/j.snb.2017.07.024. IF: 5.401



PROJECTS

InWoc, In-situ atomic resolution transmission electron microscopy of heterogeneous water oxidation catalysts, funded by **BIST**, 01/01/18 - 31/12/18, Jordi Arbiol

Nanoscopías Electrónicas Avanzadas para el desarrollo y mejora de nuevas rutas fotoelectrocatalíticas para productos de alto valor añadido aprovechando la energía solar (ANAPHASE), funded by **FEDER/Ministerio de Ciencia, Innovación y Universidades** - Agencia Estatal de Investigación/ENE2017-85087-C3-3-R, 01/01/18 - 31/12/18, Jordi Arbiol

Materials characterization of hybrid semi-super Majorana nanowires (CHyMajor), funded by **MICROSOFT**, 01/01/18 - 30/06/18, Jordi Arbiol

CHyMajor2, Materials characterization of hybrid semi-super Majorana nanowires (2), funded by **MICROSOFT**, 30/06/18 - 31/12/18, Jordi Arbiol



CONTRIBUTIONS

Keynote

Free standing nanostructures at atomic scale: from growth mechanisms to properties at the nanoscale, **2018 International Conference on Smart Engineering Materials (ICSEM 2018)**, Romania, 08/03/18, J. Arbiol

Free-standing nanostructures at atomic scale: from growth mechanisms to local properties at the nanoscale, **International Conference on Nanoscience and Nanoengineering (NSNE 2018)**, Las Vegas, USA. 18/04/18, J. Arbiol

Epitaxy at the atomic scale: from core-shell to axial heterojunctions in nanostructures, **EMN Meeting on Epitaxy 2018**, Vienna, Austria. 20/06/18, J. Arbiol

Free-standing nanostructures at atomic scale: from growth mechanisms to local properties at the nanoscale, **The 4th edition of Nanotech France 2018 International Conference and Exhibition (NANOTECH FRANCE 2018)**, France. 29/06/18, J. Arbiol

Free-standing nanostructures at atomic scale: from growth mechanisms to local properties, **International Conference on Materials Science and Engineering (ICMSE 2018)**, Russia. 24/07/18, J. Arbiol

Free-standing nanostructures at atomic scale: from growth mechanisms to local properties, **31st European Crystallographic Meeting (ECM31)**, Oviedo, Spain. 23/08/18, J. Arbiol

Hollow Metal Nanostructures for Enhanced Plasmonics, **2nd International Conference on Nanomaterials and Biomaterials (ICNB 2018)**, Barcelona, Spain. 11/12/18, J. Arbiol

Invited

Free standing nanostructures at atomic scale: from growth mechanisms to properties at the nanoscale, **Ernst Ruska-Centre for Microscopie and Spectroscopie with Electrons, Forschungszentrum Jülich GmbH**, Germany. 18/01/18, J. Arbiol

Free-standing nanostructures at atomic scale: from growth mechanisms to local properties, **Inauguration Symposium at the National Centre for Electron Microscopy**, Sweden. 12/04/18, J. Arbiol

Energy nanostructures at atomic scale: from growth mechanisms to properties, **Collaborative Conference on Materials Research (CCMR 2018)**, Incheon, South Korea. 26/06/18, J. Arbiol

Energy Nanomaterials: a close look to their atomic scale structure and the influence on their properties at the nanoscale, **Massachusetts Institute of Technology (MIT)**, USA. 28/11/18, J. Arbiol

Oral

Morphology dependent strain relaxation in horizontally grown semiconductor core-shell nanowires and its effect on electronic band alignment, **19th International Microscopy Congress (IMC19)**, Sidney, Australia. 10/09/18, Sara Martí-Sánchez

Free-standing semiconductor nanostructures at atomic scale: from growth mechanisms to local properties at the nanoscale, **19th International Microscopy Congress (IMC19)**, Sidney, Australia. 11/09/18, J. Arbiol

Stars in III-V Nanowires: A 3D reciprocal space study, **Applied Nanotechnology and Nanoscience International Conference - ANNIC**, Germany. 21/10/18, Jeremy David

Morphology dependent strain relaxation in horizontally grown ZnSe@ZnTe core-shell nanowires and its effect on electronic band alignment, **Applied Nanotechnology and Nanoscience International Conference - ANNIC 2018**, Germany, 21/10/18, Sara Martí-Sánchez

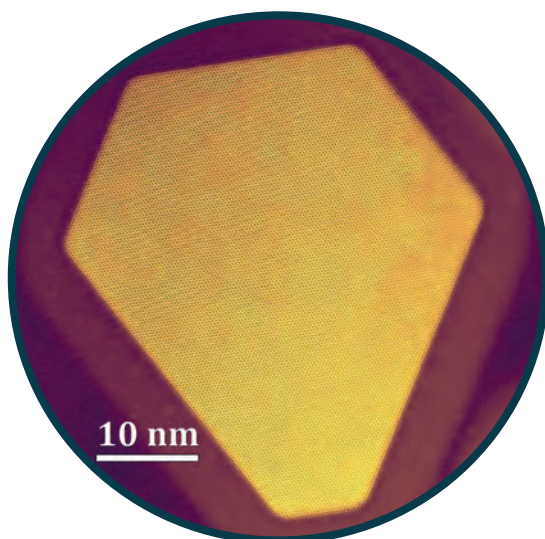
Bottom-up engineering of hematite nanowire heterostructures for water splitting, **nanoGe Fall Meeting 2018**, Spain, 23/10/18, PengYi Tang

Bottom-up engineering of hematite nanowire heterostructures for photoelectrochemical water splitting, **Materials Research Society Fall Meeting 2018 (MRS Fall 2018)**, USA. 28/11/18, PengYi Tang

Morphology dependent strain relaxation in horizontally grown ZnSe@ZnTe core-shell nanowires and its effects on electronic band alignment, **Materials Research Society Fall Meeting 2018 (MRS Fall 2018)**, USA. 28/11/18, Sara Martí-Sánchez

Poster

NiSn bimetallic nanoparticles as stable electrocatalysts for methanol oxidation reaction, **nanoGe Fall Meeting 2018**, Spain. 26/10/18, Ting Zhang





PARTICIPATED CONGRESSES

BIST Winter Workshop on Microscopy, Nanoscopy & Imaging Sciences, Barcelona, Castelldefels, Spain, February 2018. Jordi Arbiol

International Conference on Smart Engineering Materials (ICSEM 2018), Bucharest, Romania, March 2018. Jordi Arbiol

31st European Crystallographic Meeting (ECM31), Oviedo, Symposium Organizer, Spain, August 2018. Jordi Arbiol

Applied Nanotechnology and Nanoscience International Conference 2018 (ANNIC 2018), Berlin, Germany, October 2018. Jordi Arbiol

Materials Research Society Fall Meeting 2018 (MRS Fall 2018) (Symposium NM03: Nanowires and Related 1D Nanostructures - New Opportunities and Grand Challenges), Boston, USA, November 2018. Jordi Arbiol

2nd International Conference on Nanomaterials and Biomaterials (ICNB 2018), Barcelona, Spain, December 2018. Jordi Arbiol



COURSES

Jordi Arbiol, *BIST Winter School on Microscopy, Nanoscopy & Imaging Sciences (Barcelona)*.

BIST-UPF Master of Multidisciplinary Research in Experimental Sciences, Spain, January - February 2018



THESES

Pengyi Tang, *Semiconductor composite materials for energy storage and conversion applications*, 12/7/18, supervised by ICREA Prof. Jordi Arbiol and Prof. Joan Ramón Morante



DISSEMINATION CONTRIBUTIONS

Invited conference

Festival 10alamos9, Veient els àtoms de prop: un viatge al Nanomon, CosmoCaixa, Barcelona, 10/04/18, J. Arbiol

Setmana de la Ciència, Veient els àtoms de prop: un viatge al Nanomon, AGAUR and CRP Vallès Occidental II, Institut Can Planas, Barberà del Vallès, 07/11/18, J. Arbiol



AWARDS

PengYi Tang - **Energy & Environmental Science Poster Prize - International Conference on Renewable Energy - ICREN 2018**, 24-26/04/18, Paris, France

Sara Martí-Sánchez - **Awarded to participate in the IFSM Young Scientists Assembly - 19th International Microscopy Congress - IMC19**, 09-14/09/18, Sydney, Australia

María de la Mata - **2015 PhD Extraordinary Award in Materials Science** by Universitat Autònoma de Barcelona (UAB), Bellaterra

Advanced Electronic Materials and Devices Group

Main Research Lines

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

Garrido, Jose A., ICREA Research Professor and Group Leader and Vice Director

Bonaccini Calia, Andrea, Doctoral Student

Bousquet, Jessica, Postdoctoral Researcher

De la Cruz Sánchez, José Manuel,
Doctoral Student

Del Corro García, Elena, Postdoctoral
Researcher

Del Valle Macià, Jaume, Postdoctoral
Researcher

García Cortadella, Ramón, Doctoral
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Pérez Marín, Antonio Pablo, Technician

Rodríguez Lucas, Elisa, Visiting TFG Student

Ruiz Nicolás, Patricia, Scientific Project
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Salvador Aguilera, Emili, Visiting Master
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Schaefer, Nathan, Doctoral Student

Schäfer, Christian, Doctoral Student

Torralba Gombau, Ricard, Visiting TFG
Student

Viana Casals, Damià, Doctoral Student

Walston, Steven, Postdoctoral Researcher



NEW PROJECTS & MILESTONES

The Advanced Electronic Materials and Devices team focus on the study and application of novel electronic materials, with a strong emphasis on carbon materials such as graphene, though also considering other 2D materials like MoS₂.

The year 2018 has witnessed great advances in the activities of the Advanced Electronic Materials and Devices group.

Within the BrainCom project, the EU FET Proactive coordinated by our team and focused on developing a new generation of neural prostheses able to restore communication in patients with severely impaired language processing abilities, we have reached an important milestone, which is the demonstration of a graphene-based multiplexing technique for high channel count brain implants. A patent has been submitted.

Within the EU Graphene Flagship, our group also participates in the Core 2 phase of the project. During the last year, and together with our partners in the Flagship, we have advanced in a technology for the preparation of high-performing microelectrode arrays based on reduced graphene oxide; the preparation and application of this technology is in the process of being patented. Further, we have demonstrated that sensor arrays based on graphene-based field-effect transistors are capable of mapping infraslow brain activity, which is not possible with standard electrode devices. This work has been published in *Nature Materials* and a patent has been filed.

Also, the GRAFIN project (under the FLAG ERA programme), led by Xavier Navarro from the UAB, has started in 2018. This project focuses on the development of graphene-based flexible neural interfaces for the control of motor neuroprosthetic devices for the peripheral nervous system.

Our team has been awarded with two new EU projects that will start in January 2019. One focused on the development of glucose, pH and humidity sensors (WASP); the other (NANOSMART) on the design, fabrication and validation of a new generation of electronic smart systems based on 2D materials semiconducting electronics

Our efforts to develop graphene-based technologies for retinal prostheses are ongoing with a multidisciplinary BIST Ignite project (THEIA), developed in collaboration with our partners in ICFO, IFAE and the Clinica Barraquer.

A National project founded by the Ministry started in 2018, focused on technologies based in 2D materials for biomedical applications, and with Elena del Corro as co-PI.

At the individual level, Elena del Corro was awarded a Mother in Science grant by BIST - congratulations!

Our group has also received support from the *Generalitat de Catalunya* as a Consolidated Research Group.



PUBLICATIONS

Dexamethasone reduces the foreign body reaction to intraneural electrode implants in the peripheral nerve of the rat, De la Oliva N., Navarro X., del Valle J. *Anatomical Record*; **301(10)**: 1722-1733. 2018. 10.1002/ar.23920. IF:1.373

Flexible graphene solution-gated field-effect transistors: efficient transducers for micro-electrocorticography, Hébert C., Masvidal-Codina E., Suarez-Perez A., Calia A.B., Piret G., Garcia-Cortadella R., Illa X., Del Corro Garcia E., De la Cruz Sanchez J.M., Casals D.V., Prats-Alfonso E., Bousquet J., Godignon P., Yvert B., Villa R., Sanchez-Vives M.V., Guimerà-Brunet A., Garrido J.A. *Advanced Functional Materials*; **28 (12)**: 1703976, 2018. 10.1002/adfm.201703976. IF: 13.325

Lipid monolayer formation and lipid exchange monitored by a graphene field-effect transistor, Blaschke B.M., Böhm P., Drieschner S., Nickel B., Garrido J.A. *Langmuir*; **34 (14)**: 4224-4233. 2018. 10.1021/acs.langmuir.8b00162. IF: 3.789

On the use of Parylene C polymer as substrate for peripheral nerve electrodes, De La Oliva N., Mueller M., Stieglitz T., Navarro X., Del Valle J. *Scientific Reports*; **8 (1)**: 5965, 2018. 10.1038/s41598-018-24502-z. IF: 4.122

Photocurrent generation of biohybrid systems based on bacterial reaction centers and graphene electrodes, Csiki R., Drieschner S., Lyuleeva A., Cattani-Scholz A., Stutzmann M., Garrido J.A. *Diamond and Related Materials*; **89**: 286-292. 2018. 10.1016/j.diamond.2018.09.005. IF: 2.232

Segregation of motor and sensory axons regenerating through bicompartamental tubes by combining extracellular matrix components with neurotrophic factors, del Valle J., Santos D., Delgado-Martínez I., de la Oliva N., Giudetti G., Micera S., Navarro X. *Journal of Tissue Engineering and Regenerative Medicine*; **12 (4)**: e1991-e2000. 2018. 10.1002/term.2629. IF: 4.089

Single-layer graphene modulates neuronal communication and augments membrane ion currents, Pampaloni N.P., Lottner M., Giugliano M., Matruggio A., D'Amico F., Prato M., Garrido J.A., Ballerini L., Scaini D. *Nature Nanotechnology*; **13(8)**: 755-764. 2018. 10.1038/s41565-018-0163-6. IF: 37.490

Time course study of long-term biocompatibility and foreign body reaction to intraneural polyimide-based implants, de la Oliva N., Navarro X., del Valle J. *Journal of Biomedical Materials Research-Part A*; **106 (3)**: 746-757. 2018. 10.1002/jbm.a.36274. IF: 3.231

Understanding the bias dependence of low frequency noise in single layer graphene FETs, Mavredakis N., Garcia Cortadella R., Bonaccini Calia A., Garrido J.A., Jiménez D. *Nanoscale*; **10 (31)**: 14947-14956. 2018. 10.1039/c8nr04939d. IF: 7.233

Uniformly coated highly porous graphene/MnO₂ foams for flexible asymmetric supercapacitors, Drieschner S., Seckendorff M.V., Corro E.D., Wohlketter J., Blaschke B.M., Stutzmann M., Garrido J.A. *Nanotechnology*; **29 (22)**: 225402, 2018. 10.1088/1361-6528/aab4c2. IF: 3.404



PROJECTS

GRAFIN, GRaphene-based Flexible neural Interfaces for the control of Neuroprosthetic devices, funded by **Ministerio de Ciencia, Innovación y Universidades (FLAG ERA 2 2017)**, Ref: PCI2018-092935; 01/04/2018 - 31/03/2021, PI: Jose A. Garrido

BrainCom, High-density cortical implants for cognitive neuroscience and rehabilitation of speech using braincomputer interfases, funded by **European Union's Horizon 2020 research and innovation programme** under grant agreement No 732032, 01/12/2016 - 30/11/2021, Coordinator: Jose A. Garrido

Graphene-based flexible neural interfaces for the peripheral nervous system, funded by **Fundación Ramón Areces**, 02/03/2017 - 01/03/2020, Jose A. Garrido

2DtecBIO, Tecnologías basadas en materiales bidimensionales para aplicación en biomedicina, funded by **FEDER/Ministerio de Ciencia, Innovación y Universidades - Agencia Estatal de Investigación / FIS2017-85787-R**, 01/01/2018 - 31/12/2020, Jose A. Garrido and Elena del Corro

Theia, Towards the implementation of micro-electrode array for retinal prosthesis, funded by **BIST**, 01/01/2018 - 31/12/2019

2017 SGR 1426, funded by **AGAUR**, 01/01/17 - 31/12/2020, Jose A. Garrido

GRAPHENE CORE 2, Graphene Flagship Core Project 2, funded by **European Union's Horizon 2020 research and innovation programme** under grant agreement N° 785219, 01/04/2018 - 31/03/2020

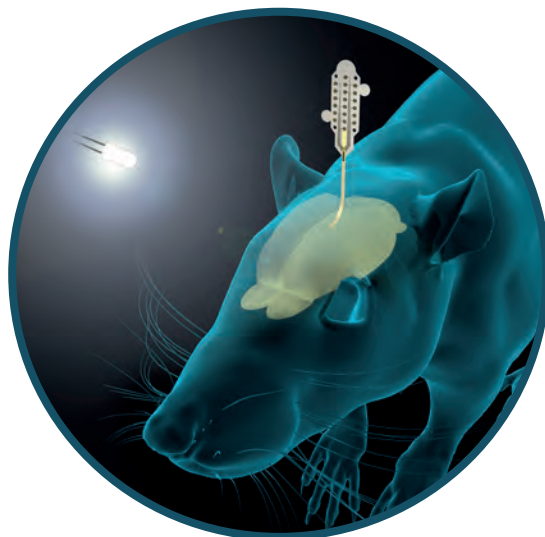
GRAPHENE CORE 1, Graphene-based disruptive technologies, funded by **European Union's Horizon 2020 research and innovation programme** under grant agreement N° 696656, 01/04/2016 - 31/03/2018



TECHNOLOGY TRANSFER

Graphene transistor system for measuring electrophysiological signals, P201831068 (submitted in November 6, 2018)

Circuit for the multiplexing and read-out of variable-resistance sensor arrays, EP18382593 (submitted in August 3, 2018)





CONTRIBUTIONS

Invited

Graphene technologies in neural interfaces, **ICN2 Severo Ochoa International Conference**, Barcelona, Spain, 15/02/18. J. A. Garrido

Biomedical applications of graphene. Functional neural interfases, **Mobile World Congress 2018**, Graphene Innovation Workshop, Barcelona, Spain, 28/02/18. J. A. Garrido

2D electronics for biomedical applications, **BIST Graphene Open Day**, ICFO, Castelldefels, Barcelona, Spain, 17/05/18. J. A. Garrido

Graphene technologies for neural prostheses, **Graphene 2018**, Dresden, Germany. 26/06/18. J. A. Garrido

Oral

Graphene-based flexible electronics for brain neural recordings, **5th International Winterschool on Bioelectronics 2018**, Kirchberg (Tirol), 12-16/03/18. [A. Bonaccini Calia](#), E. Masvidal, R. Garcia, N. Schaefer, E. Del Corro, J. Bousquet, C. Hébert, E. Masvidal, R. Garcia, A. Guimera, E. Prats X. Illa, R. Villa, J. A. Garrido

Graphene Based technology for in vivo neural interface, **MRS 2018 Spring meeting**, Phoenix, Arizona, 02-06/04/18. [C. Hébert](#), A. Bonaccini, E. Masvidal, A. Guimera, R. Garcia, J. De la Cruz, X. Illa, J. Bousquet, E. Del Corro, J. A. Garrido

Graphene based technology for neural interfacing, **International conference on diamond and carbon materials 2018**, Dubrovnik, Croatia, 02-06/09/2108. [C. Hébert](#), A. Bonaccini, E. Masvidal, A. Guimera, R. Garcia, J. De la Cruz, D. Viana, S. Walston, X. Illa, J. Bousquet, E. Del Corro, J. A. Garrido

Low-frequency noise mitigation in graphene field-effect transistors by contact resistance engineering, **Graphene 2018**, Dresden (Germany), 25-26/06/18. [R. Garcia-Cortadella](#), A. Bonaccini Calia, E. Masvidal-Codina, X. Illa, E. del Corro García, J. Bousquet, C. Hebert, R. Villa, A. Guimerà, J. A. Garrido

Graphene solution-gated field-effect transistor arrays for in vivo neural recording, **Journée de la matière condensée 2018**, Grenoble, France, 27-31/08/18. [C. Hébert](#), A. Bonaccini, E. Masvidal, A. Guimera, R. Garcia, J. De la Cruz, X. Illa, J. Bousquet, E. Del Corro, J. A. Garrido

Poster

Characterization and in-vitro assessment of microelectrode technology based on graphene-related materials, **Gordon Conference - Neuroelectronic Interfaces**, Galveston, Texas (USA), 25-30/03/18. S.T. Walston, D. Viana, C. Bullock, X. Illa, R. Caplette, C. Hébert, D. Nguyen, A. Guimerà, S. Picaud, K. Kostarelos, J. A. Garrido

Characterization and in-vitro assessment of graphene-based microelectrode technology for use in neural prostheses, **Graphene Conference 2018**, Dresden (Germany), 26-29/06/18. S.T. Walston, D. Viana, C. Bullock, X. Illa, R. Caplette, C. Hébert, D. Nguyen, A. Guimerà, E. Prats, S. Picaud, K. Kostarelos, J. A. Garrido

NaCl-assisted, low-pressure MOCVD growth of mono- to few layer MoS₂, **Graphene Conference 2018**, Dresden (Germany), 26-29/06/18. C. M. Schäfer, J. M. Caicedo Roque, J. Bousquet, C. Hébert, G. Sauthier, J. Santiso, J. A. Garrido

Growth & characterization of mono- to few layer MoS₂, **BrainCom Summer School**, Barcelona (Spain), 18-20/09/18. C. M. Schaefer, J. Caicedo Roque, E. Del Corro, J. Bousquet, C. Hébert, G. Sauthier, J. Santiso, J. A. Garrido

Flexible graphene-based microelectrodes arrays for in vivo retinal stimulation, **BrainCom**

Summer School, Barcelona (Spain), 18-20/09/18. D.Viana, ST Walston, D Nguyen, X Illa, C Hébert, S Picaud, J. A. Garrido

Towards flexible neural probes based on multiplexed active arrays of graphene transistors, **BrainCom Summer School**, Barcelona (Spain), 18-20/09/18. N. Schaefer, S. Wachter, X. Illa, A. Guimerà, C. Herbert, T. Müller, J. A. Garrido

Graphene flexible electronics for biomedical technologies, **Braincom Summer School**, 18-20/09/18. A. Bonaccini Calia, N. Schaefer, E. Rodriguez-Lucas, E. Del Corro, J. Bousquet, C. Hébert, E. Masvidal, R. Garcia, A. Guimera, E. Prats, X. Illa, R. Villa, J. A. Garrido

Single-Layer Graphene MEAs: a versatile tool for neural recording, **Braincom Summer School**, Barcelona (Spain), 18-20/09/18. J. de la Cruz, A. Guimerà, E del Corro, C. Hebert, J. A. Garrido

Towards flexible neural probes based on multiplexed active arrays of graphene transistors, **Cell-NERF Symposium: Neurotechnologies 2018**, Leuven (Belgium), 30/09-02/10/18. N. Schaefer, S. Wachter, X. Illa, A. Guimerà, C. Herbert, T. Müller, J. A. Garrido

Long-term functionality of transversal intraneural (TIME) electrodes is improved by dexamethasone treatment, **Cell-NERF Symposium: Neurotechnologies 2018**, Leuven (Belgium), 30/09-02/10/18. J. del Valle, N. de la Oliva, I. Delgado, T. Stiedglitz, X. Navarro

Graphene solution-gated field-effect transistors for high density epicortical recordings: sensitivity and yield, **Cell NERF symposium: Neurotechnologies 2018**, Leuven (Belgium), 30/09-02/10/18. R. Garcia-Cortadella, N. Schäfer, A. Guimerà, C. Hebert, J. A. Garrido



PARTICIPATED CONGRESSES

Graphene technology in neural interfaces, **BrainCom summer school, Barcelona**, 18/09/18, J. A. Garrido, *Organiser*



AWARDS

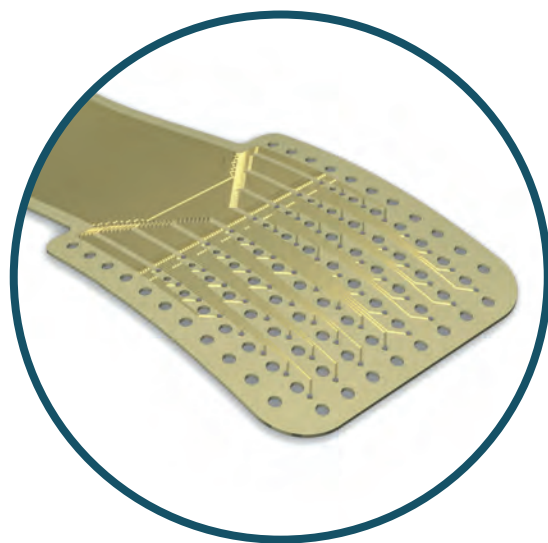
Elena del Corro awarded **Mother of Science by BIST**



DISSEMINATION CONTRIBUTIONS

How to detect an activity in the brain's speech centres using sensors on the brain's surface,

Mobile World CONGRESS 2018, Graphene pavillion, Barcelona, Jose A. Garrido - Group Leader, Andrea P. Bonaccini - ICN2 Doctoral Student , Damia Viana - ICN2 Doctoral Student at Advanced Electronic Materials and Devices Group at ICN2



Atomic Manipulation and Spectroscopy Group

Main Research Lines

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



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 Ramón y Cajal Fellowship. In 2013 he became group leader of the Atomic Manipulation and Spectroscopy Group at the recently constituted 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

Mugarza Ezpeleta, Aitor, ICREA Research Professor and Group Leader

Campos Jara, Sergi, Visiting Degree Student

Diego Lisboa Amaral Lopes, Bárbara, Visiting Master Student

Gastaldo, Michele, Doctoral Student

González Cuxart, Marc, SO Doctoral Student

Kimouche, Amina, Postdoctoral Researcher

López García, Álex, Visiting Master Student

Molina Bom, Nicolau, Visiting PostDoctoral Researcher

Moreno Sierra, César, Senior Researcher

Paradinas Aranjuelo, Marcos, Laboratory Engineer

Saludes Tapia, María Mercedes, Visiting Master Student

Tenorio Tuñas, María, Doctoral Student

Valbuena Martínez, Miguel Angel, Postdoctoral Researcher



NEW PROJECTS & MILESTONES

The work carried out by the Atomic Manipulation and Spectroscopy Group in 2018 has focused mainly on the synthesis and characterisation of carbon-based nanostructures, and on hybrid ferromagnetic/topological insulators heterostructures.

As part of our ongoing research on the synthesis of graphene nanostructures, we have been able to synthesize periodic arrays of 1D graphene nanoribbons (GNR), and more importantly to fuse them into a 2D nanoporous graphene (NPG) sheet, by using on-surface chemistry. This method allows the control on the structure and the possibility to introduce heteroatom dopants or substitutional ligands, both with atomic precision. Our breakthrough achievements in this active field have been to control the distribution of the GNRs into parallel arrays, which also leads to a 2-3 fold increase in reported average length, and their coupling into the first NPG synthesized with bottom-up methods. All these characteristics are crucial for the application of these graphene nanomaterials in devices. As first demonstration, and in collaboration with the ICN2 Physics and Engineering of Nanodevices Group, we have realized NPG-based field effect transistors with state-of-art performance and record fabrication yield. We are currently extending the exploration of the application domains of this novel material to optoelectronics (gate-controlled plasmonics) and membranes for molecular sieving and sensing. This research is carried out within the framework of the FUNMOLDEV project coordinated by the Spanish Ministry of Economy.

In parallel, we are extending our studies on hybrid ferromagnetic/topological insulator heterostructures to the merge of the two functionalities in single-layer metal-organic topological insulators. We do that in a more general project which aims at the synthesis of conducting and magnetic 2D metal-organic frameworks, carried out in collaboration with the ICN2 Nanostructured Functional Materials Group.



PUBLICATIONS

Bottom-up synthesis of multifunctional nanoporous Graphene, Moreno C., Vilas-Varela M., Kretz B., Garcia-Lekue A., Costache M.V., Paradinas M., Panighel M., Ceballos G., Valenzuela S.O., Peña D., Mugarza A., *Science*, **360 (6385)**: 199-203. 2018. IF: 41,058

On-surface synthesis of superlattice arrays of ultra-long graphene nanoribbons, Moreno C., Paradinas M., Vilas-Varela M., Panighel M., Ceballos G., Peña D., Mugarza A., *Chemical Communications*, **54 (9402)**: 9402-9405. 2018. IF: 6,29

Structure and electronic states of vicinal Ag(111) surfaces with densely kinked steps, Ortega J.E., Vasseur G., Piquero-Zulaica I., Matencio S., Valbuena M.A., Rault J.E., Schiller F., Corso M., Mugarza A., Lobo-Checa J., *New Journal of Physics*, **20 (7)**: 073010. 2018. IF: 3,579

Towards microscopic control of the magnetic exchange coupling at the surface of a topological insulator, Philipp Rübmann, Sanjoy K Mahatha, Paolo Sessi, Miguel A Valbuena, Thomas Bathon, Kai Fauth, Sylvie Godey, Aitor Mugarza, Konstantin A Kokh, Oleg E Tereshchenko, Pierluigi Gargiani, Manuel Valvidares, Erika Jiménez, Nicholas B Brookes, Matthias Bode, Gustav Bihlmayer, Stefan Blügel, Phivos Mavropoulos, Carlo Carbone and Alessandro Barla, *Journal of Physics: Materials*, **1 (1)**: 15002. 2018.

Pentacene/TiO₂ anatase hybrid interface study by scanning probe microscopy and first principles calculations, Todorović, M., Stetsovych, O., Moreno, C., Shimizu, T.K., Custance, O., Pérez, R., *ACS Applied Materials and Interfaces*, **10 (40)**: 34718-34726. 2018. IF: 8,097

Real space demonstration of induced crystalline 3D nanostructuring of organic layers, Paradinas M., Pérez-Rodríguez A., Barrena E., Ocal C., *Journal of Physical Chemistry B*, **122 (2)**: 633-639. 2018. IF: 3,146

In-situ scrutiny of the relationship between polymorphic phases and properties of self-assembled monolayers of a biphenyl based thiol, Paradinas M., Munuera C., Buck M., Ocal C., *Journal of Physical Chemistry B*, **122 (2)**: 657-665. 2018. IF: 3,146



PROJECTS

FunMolDev, Nanoestructuras moleculares funcionales para dispositivos optoelectrónicos: Hacia dispositivos de 3 terminales, funded by **MINECO/FEDER, UE**, (MAT2016-78293-C6-2-R), 30/12/2016 - 29/12/2019, IP: Aitor Mugarza

TNSI, Trans-Pyrenean node for scientific instrumentation, funded by **FEDER - INTERREG/POCTEFA** (EFA194/16 TNSI), 01/02/2018 - 31/01/2021, IP: Aitor Mugarza



TECHNOLOGY TRANSFER

EU patent application: **A nanoporous graphene structure and method for preparation thereof**, (Application number: EP18382088.5)



CONTRIBUTIONS

Invited

Electron confinement on surfaces studied by scanning tunneling spectroscopy, **Instituto de Ciencia de Materiales de Aragón (ICMA)**, 05/18, Aitor Mugarza

Bottom-up synthesis of graphene nanostructures: from 0D dots, to 1D ribbons, to 2D porous Graphene, **7th International Conference NANOSEA NANO-structures and nanomaterials Self-Assembly**, France, 04/07/18, Aitor Mugarza

Holey graphene by Lego chemistry, **6th Nano-Carbon Enhanced Materials Consortium**, Cambridge, 11-13/07/18, C. Moreno

Tuning charge and spin interactions at hybrid organic/metal and organic/topological insulator interfaces, **10th International School and Conference on Physics and Applications of Spin Phenomena in Solids**, Austria, 08/08/18, Aitor Mugarza

Engineering nanoporous graphene with atomic precision, **Recent Progress in Graphene & 2D Materials Research (RPGR 2018)**, China, 23/10/18, Aitor Mugarza

From molecules to atomically precise low dimensional materials, **ICMAB-CSIC**, Barcelona, Spain, 12/11/18

Bottom-up synthesis of graphene nanostructures: 0D dots, 1D ribbons and 2D porous graphene, **Institut Néel-CNRS**, Grenoble, France, 06/12/18

Nanoporous graphene, nanoribbons and superlattices with atomic precision, **Smart NanoMaterials 2018: Advances, Innovation and Applications (SNAIA)**, Paris, France, 10-13/12/18, C. Moreno

Synthesizing graphene nanostructures with atomic precision, **University of Barcelona, UB**, 12/18, Aitor Mugarza

Oral

Hierarchical synthesis of nanoporous graphene, **International conference on Novel 2D materials explored via scanning probe microscopy & spectroscopy**, Spain, 25/06/18, Aitor Mugarza

Domains and boundaries in polycrystalline graphene nanostructures, **Fuerzas y Tunel 2018**, Jaca, Spain, 27-29/06/18, S. O. Parreiras, M. Gastaldo, C. Moreno, M. D. Martins, A. Garcia-Lekue, G. Ceballos, R. Paniago, and A. Mugarza

Surface-guided graphene nanoribbon superlattices, **On-Surface Synthesis International Workshop**, Spain, 26/09/18, Aitor Mugarza

Metal-organic topological insulator heterostructure with robust interfacial properties, **Fuerzas y Tunel 2018**, Jaca, Spain, 27-29/06/18, M. G. Cuxart, M. A. Valbuena, F. Bonell, C. Moreno, R. Robles, J. Cruz, I. Imaz, D. Maspoch, C. Nistor, P. Gargiani, P. Ordejón, P. Gambardella, S. O. Valenzuela, and A. Mugarza

Bottom-up synthesis of multifunctional nanoporous graphene, **On-Surface Synthesis International Workshop**, Sant Feliu de Guixols, Girona, Spain, September 24-28/09/18, C. Moreno, M. Vilas-Varela, B. Kretz, A. Garcia-Lekue, M. V Costache, M. Paradinas, M. Panighel, G. Ceballos, S. O. Valenzuela, D. Peña, and A. Mugarza

Bottom up synthesis of multifunctional nanoporous graphene, **Fuerzas y Tunel 2018**, Jaca, 2018, C. Moreno, M. Vilas-Varela, B. Kretz, A. Garcia-Lekue, M. V Costache, M. Paradinas, M. Panighel, G. Ceballos, S. S. Valenzuela, D. Peña, and A. Mugarza

Long and densely aligned graphene nanoribbons by surface-driven interaction, **E-MRS Spring Meeting**, Strasbourg, 2018, C. Moreno, M. Paradinas, M. Vilas-Varela, M. Panighel, G. Ceballos, D. Peña, and A. Mugarza

Poster

Critical role of phenyl substitution and catalytic substrate on the surface-assisted polymerization dibromobianthracene derivatives, **On-Surface Synthesis International Workshop (OSS18)**, Sant Feliu de Guixols (Girona), Spain, 24-28/09/18, C. Moreno, M. Tenorio, M. Panighel, M. Vilas-Varela, G. Sauthier, G. Ceballos, D. Peña, and A. Mugarza

Metal-organic topological insulator heterostructure with robust interfacial properties, **Novel 2D Materials Explored via Scanning Probe Microscopy & Spectroscopy**, Donostia-San Sebastian, Spain, 25-29/06/18, M. G. Cuxart, M. A. Valbuena, C. Moreno, F. Bonell, R. Robles, J. Cruz, I. Imaz, C. Nistor, P. Gargiani, P. Ordejon, P. Gambardella, S. O. Valenzuela, and A. Mugarza

Domains and boundaries in graphene nanostructures, **International Conference on Novel 2D Materials Explored via Scanning Probe Microscopy & Spectroscopy (2D-SPM)**, Donostia-San Sebastian, Spain, 25-29/06/18, S. O. Parreiras, M. Gastaldo, C. Moreno, M. D. Martins, A. Garcia-Lekue, G. Ceballos, R. Paniago, and A. Mugarza



COURSES

Aitor Mugarza, *Master of Multidisciplinary Research in Experimental Sciences*, Barcelona **Institute of Science and Technology (BIST-ICN2)**, 01-02/2018

Aitor Mugarza, *Local Probe Microscopies*, **Master in Advanced Nanoscience and Nanotechnology, UAB**, 10/2018-01/2019



DISSEMINATION CONTRIBUTIONS

Cicle de divulgació científica La Biothèque 2018, 16/11/18, César Moreno

Women in Science, Escola Voramar 14/02/18, César Moreno



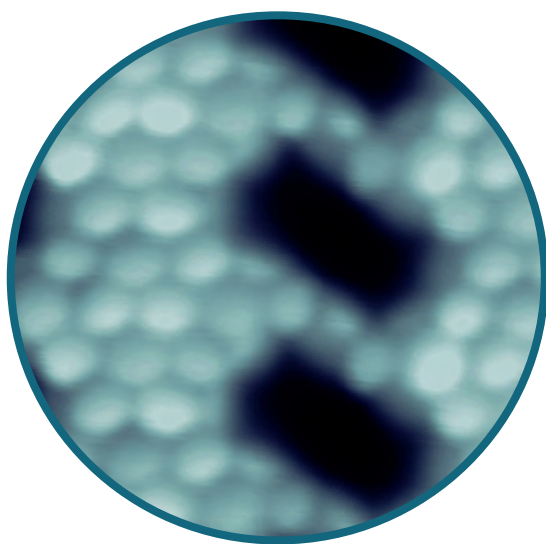
THESES

Michele Gastaldo, *Tailoring the structural and electronic properties of graphene by bottom-up methods*, supervised by ICREA Prof. Aitor Mugarza and Dr. Gustavo Ceballos



AWARDS

Holey graphene membrane voted Molecule of the Year by C&EN journal. The material was presented in *Science* in a joint article by researchers from the ICN2, CiQUS and DIPC. Aitor Mugarza, Group leader and Cesar Moreno, Senior researcher at ICN2



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 140 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

Fraxedas Calduch, Jordi, CSIC Scientific Researcher and Group Leader

Bast, Nour al Hoda, Fellowship Doctoral Student

Esplandiu Egido, María José, CSIC Tenured Scientist

Fetisova, Yuliya, Visiting Master Student

Gramazio, Federico, Doctoral Student

Tiemann, Daniel, Research Engineer

Verdaguer Prats, Albert, Visiting Senior Researcher



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 has been developed and successfully tested for scan frequencies up to ten 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, to study the mass transport of water induced via electro-kinetic and diffusion-osmotic processes.



PUBLICATIONS

Facile synthesis of nanoparticles of the molecule-based superconductor κ -(BEDT-TTF)₂Cu(NCS)₂ [Synthèse aisée de nanoparticules du supraconducteur moléculaire κ -(BEDT-TTF)₂Cu(NCS)₂], Cormary B., Faulmann C., de Caro D., Valade L., de Caro P., Ballesteros B., Fraxedas J. *Comptes Rendus Chimie*; **21 (9)**: 809-813. 2018.

10.1016/j.crci.2018.07.006. IF: 1,877

Impact of the: In situ rise in hydrogen partial pressure on graphene shape evolution during CVD growth of Graphene, Gebeyehu Z.M., Arrighi A., Costache M.V., Sotomayor-Torres C.M., Esplandiu M.J., Valenzuela S.O. *RSC Advances*; **8 (15)**: 8234-8239. 2018.

10.1039/c7ra13169k. IF: 2,936

Interfacial engineering of metal oxides for highly stable halide perovskite solar cells, Mingorance A., Xie H., Kim H.-S., Wang Z., Balsells M., Morales-Melgares A., Domingo N., Kazuteru N., Tress W., Fraxedas J., Vlachopoulos N., Hagfeldt A., Lira-Cantu M. *Advanced Materials Interfaces*; **5 (22)**: 1800367, 2018.

10.1002/admi.201800367.

Quantification of nanomechanical properties of surfaces by higher harmonic monitoring in amplitude modulated AFM imaging, Gramazio F., Lorenzoni M., Pérez-Murano F., Evangelio L., Fraxedas, J. *Ultramicroscopy*; **187**: 20-25. 2018.

10.1016/j.ultramic.2018.01.013. IF: 2,929

Substrate dependence of the freezing dynamics of supercooled water films: a high-speed optical microscope study, Pach E., Rodriguez L., Verdaguer A. *Journal of Physical Chemistry B*; **122 (2)**: 818-826. 2018.

10.1021/acs.jpcc.7b06933. IF: 3,146

Unraveling the operational mechanisms of chemically propelled motors with micropumps, Esplandiu M.J., Zhang K., Fraxedas J., Sepulveda B., Reguera D. *Accounts of Chemical Research*; **51 (9)**: 1921-1930. 2018.

10.1021/acs.accounts.8b00241. IF: 20,955



PROJECTS

Simuove, Movimiento de micro/nano-objetos de agua inducido por luz, funded by **MAT2015-68307-P (MINECO/FEDER, UE)**, 01/01/2016 - 31/12/2018, IPs: Jordi Fraxedas / M. J. Esplandiu

PLASTFUN, Planta pilot de peces plàstiques amb superfícies funcionals avançades, funded by **ACCIO**, 01/02/2018 - 31/01/2021, IP: Nikolaos Kehagias

NFFA-Europe, Nanoscience foundries and fine analysis-Europe, funded by **European Union's Horizon 2020 research and innovation programme under grant agreement N° 654360**, 01/09/2015 - 31/08/2019, IP: Pablo Ordejón /Gustavo Ceballos/ José Santiso /Jordi Fraxedas



CONTRIBUTIONS

Keynote

Characterization of directed self-assembled block copolymers prepared on nanopatterned surfaces, **23rd International Conference on Nanomaterials and Nanotechnologies**, London, UK, 15-16/03/18. J. Fraxedas

Invited

Characterization of directed self-assembled block copolymers prepared on nanopatterned surfaces using synchrotron radiation techniques,

International Conference on Condensed Matter and Material Science, Kuala Lumpur, Malaysia, 20-21/06/18. J. Fraxedas

Oral

Micro/Nanomachines self-propelled by chemical gradients: from electrokinetics to diffusion control,

V International Conference on Colloid Chemistry and Physicochemical Mechanics, Saint Petersburg, Russia, 10-14/09/18. K. Zhang, J. Fraxedas, B. Sepúlveda, M. J. Esplandiú

Poster

Interfacial water in silicon-based catalytic motors,
AVS 65 Symposium, Long Beach, CA, USA, 20-26/10/18. J. Fraxedas, K. Zhang, B. Sepúlveda, M. J. Esplandiú, X. Garcia, J. Llorca, V. Perez-Dieste, C. Escudero

Water/methanol solutions characterized by liquid μ -jet XPS and DFT: the methanol hydration case,
5th Annual Ambient Pressure X-ray Photoelectron Spectroscopy Workshop (APXPS 2018), Berlin, Germany, 11-14/12/18. E. Pellegrin, V. Perez-Dieste, C. Escudero, J. Fraxedas, P. Rejmak, N. González, A. Fontseré, J. Prat, S. Ferrer



COURSES

Atomic Force Microscopy & Spectroscopy (AFM&SFS): Fundamentals & Applications, **Master of Multidisciplinary Research in Experimental Sciences (BIST-UPC)**, ICN2, Barcelona, 31/1/2018. M.J. Esplandiú

Master Industrial Chemistry and Introduction to Chemical Research Chemistry for specific materials of interest in research and industry. M.J. Esplandiú

Master Industrial Chemistry and Introduction to Chemical Research Advanced Chemistry: Microscopies, UAB, Barcelona, 25/09/18 - 8/10/18. M.J. Esplandiú

Introduction to Nanoscience and Nanotechnology, **Undergraduate Course in the degree of Nanoscience and Nanotechnology**, UAB, Barcelona, (annual subject 2017/2018 - 2018/2019). M.J. Esplandiú

Discovering the fascinating world of Nanotechnology, **Summer course for secondary school students**, UAB, Barcelona, 02/07/18 - 06/07/18. M.J. Esplandiú



THESES

Federico Gramazio, *Determination of nanomechanical properties of surfaces by atomic force microscopy using higher harmonics*, 16/03/18, supervised by Dr. Jordi Fraxedas and Prof. Francesc Pérez Murano



DISSEMINATION CONTRIBUTIONS

Blog El Món a la Nanoescala,
<http://enciclopedia.cat/divulcat/Jordi-Fraxedas>

Discovering the world of nanotechnology, **Talk in the IV Scientific Day of INS Mercè Rodoreda**, Hospitalet de Llobregat. Barcelona, 16/03/18. M.J. Esplandiú

Què es la Nanotecnologia?, **Talk at the INS Castellar**, Castellar del Vallés, Barcelona, 05/12/18. M.J. Esplandiú

L'aigua sobre les superfícies nanoestructurades, **Crazy for Physics session**, ICN2, 04/05/2018, M.J. Esplandiú, J. Fraxedas

H₂O: què en sabem d'aquesta sorprenent i fascinant molècula?, **Cicle Dilluns de ciència - CSIC**, Residència D'Investigadors, Barcelona, 26/11/18, Jordi Fraxedas

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

F. Puntes, Víctor, ICREA Research Professor and Group Leader

Barbero, Francesco, Doctoral Student

Brandts Busom, Irene, Visiting Doctoral Student

Carulla Urgell, Jordi, Visiting TFG Student

Castellví Corrons, Xavier, Research Assistant

Gómez Bastus, Neus, Senior Researcher

González Naranjo, Daniel, Visiting Master Student

Jiménez Álamo, Carlos, Visiting TFG Student

Martínez Llonch, David, Visiting TFG Student

Martínez Pla, Cristian, Visiting TFG Student

Mondragón Martínez, Laura, Postdoctoral Researcher

Moriones Botero, Oscar Hernando, Doctoral Student

Oliveras Solà, Jana, Research Assistant

Patarroyo Rengifo, Javier, Technician



GROUP LEADER



ICREA Prof.
Víctor F. Puntes

ICREA Research Prof. Víctor F. Puntes' 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 Puntes 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. Amilcar Labarta on giant



Pérez Brizuela, Sara, Visiting TFG Student
Piella Bagaria, Jordi, Technician
Rodríguez Martínez, Gonzalo, Visiting HS Student

Rovira Esteva, Muriel, Postdoctoral Researcher
Wypij, Magdalena, Fellowship Doctoral Student

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 Puntes had 195 peer-reviewed publications and over 12,500 citations.

He 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.



NEW PROJECTS & MILESTONES

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.

In this context, 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.). 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.

In 2018 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. Among them: DANAÉ, a national project funded by the Spanish Ministry of Economy, Industry and Competitiveness 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; and, SOLHYCAT, a BIST project to develop Advanced solar cells to synthesize solar fuels.



PUBLICATIONS

Aging reduces the toxicity of pristine but not sulphidised silver nanoparticles to soil bacteria, Schultz C.L., Gray J., Verweij R.A., Busquets-Fité M., Puentes V., Svendsen C., Lahive E., Matzke M. *Environmental Science: Nano*; **5 (11)**: 2618-2630. 2018.
10.1039/C8EN00054A. I.F.:6.08

Characterization of nanoparticle batch-to-batch variability, Mülhopt S., Diabaté S., Dilger M., Adelhelm C., Anderlohr C., Bergfeldt T., de la Torre J.G., Jiang Y., Valsami-Jones E., Langevin D., Lynch I., Mahon E., Nelissen I., Piella J., Puentes V., Ray S., Schneider R., Wilkins T., Weiss C., Paur H.-R. *Nanomaterials*; **8 (5)**: 311, 2018.
10.3390/nano8050311. IF: 3.504

Effects of systematic variation in size and surface coating of silver nanoparticles on their in vitro toxicity to macrophage RAW 264.7 cells, Sunday Makama, Samantha K Kloet, Jordi Piella, Hans van den Berg Norbert, C A de Ruijter, Victor F Puentes, Ivonne M C M Rietjens, Nico W van den Brink. *Toxicological Sciences*; **162** (1): 79-88, 2018 10.1093/toxsci/kfx228. IF:4.181

Fluorescently labelled nanomaterials in nanosafety research: Practical advice to avoid artefacts and trace unbound dye, Murray R.A., Escobar A., Bastús N.G., Andreozzi P., Puentes V., Moya S.E. *NanoImpact*; **9**: 102-113. 2018. 10.1016/j.impact.2017.11.001. IF :0

Influence of soil porewater properties on the fate and toxicity of silver nanoparticles to *Caenorhabditis elegans*, Schultz, C. L., Lahive, E. , Lawlor, A. , Crossley, A. , Puentes, V. , Unrine, J. M., Svendsen, C. and Spurgeon, D. J. *Environmental Toxicology and Chemistry*; **37**(10): 2609-2618, 2018. 10.1002/etc.4220 IF:3.179

Inter-laboratory comparison of nanoparticle size measurements using dynamic light scattering and differential centrifugal sedimentation, Langevin D., Lozano O., Salvati A., Kestens V., Monopoli M., Raspaud E., Mariot S., Salonen A., Thomas S., Driessen M., Haase A., Nelissen I., Smisdom N., Pompa P.P., Maiorano G., Puentes V., Puchowicz D., Stępnik M., Suárez G., Riediker M., Benetti F., Mičetić I., Venturini M., Kreyling W.G., van der Zande M., Bouwmeester H., Milani S., Rädler J.O., Mülhopt S., Lynch I., Dawson K. *NanoImpact*; **10**: 97-107. 2018. 10.1016/j.impact.2017.12.004. IF: 0.000

Nanotechnology for maternal foetal medicine, Eudald Casals, Muriel F. Gusta, Lena Montana, Manel Mendoza, Nerea Maiz, Elena Carreras, Victor Puentes. *International Journal of Pediatrics and Neonatal Health*; **2**:5, 57-66 , 2018

Plasmonic assemblies of gold nanorods on nanoscale patterns of poly(ethylene glycol): Application in surface-enhanced Raman spectroscopy, Karabel Ocal S., Patarroyo J., Kiremitler N.B., Pekdemir S., Puentes V.F., Onses M.S. *Journal of Colloid and Interface Science*; **532**: 449-455. 2018. 10.1016/j.jcis.2018.07.124. IF: 5.091

Sequential deconstruction-reconstruction of metal-organic frameworks: an alternative strategy for synthesizing (multi)-layered ZIF composites, Avci C., Yazdi A., Tarrés M., Bernoud E., Bastús N.G., Puentes V., Imaz I., Ribas X., MasPOCH D. *ACS Applied Materials and Interfaces*; **10** (28): 23952-23960. 2018. 10.1021/acsami.8b05098. IF: 8.097

Time- and size-resolved plasmonic evolution with nm resolution of galvanic replacement reaction in AuAg nanoshells synthesis, Russo L., Merkoçi F., Patarroyo J., Piella J., Merkoçi A., Bastús N.G., Puentes V. *Chemistry of Materials*; **30** (15): 5098-5107. 2018. 10.1021/acs.chemmater.8b01488. IF: 9.890

Tunable electrochemistry of gold-silver alloy nanoshells, Russo L., Puentes V., Merkoçi A. *Nano Research*; **11** (12): 6336-6345. 2018. 10.1007/s12274-018-2157-y. IF: 7.994

Low-cost strategy for the development of a rapid electrochemical assay for bacteria detection based on AuAg nanoshells,L Russo, J Leva Bueno, JF Bergua, M Costantini, M Giannetto, V Puentes, A Merkoci. *ACS Omega* **3** (12): 18849-18856. 2018.

Nanosafety: Towards safer nanoparticles by design Bastus, N.G., Puentes, V. *Current Medicinal Chemistry*, **25** (35): 4587-4601. 2018. 10.2174/0929867324666170413124915



PROJECTS

PANDORA, Probing safety of nano-objects by defining immune responses of environmental organisms, funded by **European Union's Horizon 2020 research and innovation programme** under grant agreement No 671881, 01/01/2016 - 31/12/2019 IP: Víctor F. Puentes

HISENTS, High level Integrated SEnsor for NanoToxicity Screening, funded by **European Union's Horizon 2020 research and innovation programme** under grant agreement No 685817, 01/04/2016 - 31/03/2019 IP: Víctor F. Puentes

DANAE, Diseño de complejos nanocristales inorgánicos avanzados para la transformación y el almacenamiento óptimo de energía, funded by **MAT2015-70725-R (MINECO/FEDER, UE)**, 01/01/2016 - 31/12/2019, Víctor F. Puentes

SOLHYCAT, Carbon Materials as Charge Transfer Platforms to Convert Sunlight into Fuel with a Nanocrystal-Molecular Catalyst hybrid, funded by **BIST**, 20/04/2018 - 19/12/2018, Víctor F. Puentes

2017 SGR 1431, funded by **AGAUR**, 01/01/2017 - 31/12/2020, Víctor F. Puentes



CONTRIBUTIONS

Invited

Model nanoparticles for nanotechnology risk assessment, **Nanosafety Cluster Meeting**, Athens, Greece, 21/03/18. Víctor F. Puentes

CeO₂ para el tratamiento de la epilepsia refractaria, **Federación Española de Epilepsia**, Madrid, Spain, 23/05/18. Víctor F. Puentes

Intrinsic and extrinsic properties of CeO₂ nanoparticles, **Frontiers in Immunology**, Milano University, Italy, 10/07/18. Víctor F. Puentes

Cytoplasmatic synthesis of Au nanoparticles, **GOLD 2018**, Paris, France, 16/07/18. Víctor F. Puentes

Nanoceria for brain diseases, **1st International Congress on Dravet Syndrome**, Bilbao, Spain, 05/10/18. Víctor F. Puentes

Anti-inflammatory nanoparticles to facilitate tissue engineering, **International Workshop on Self-Assembly and Hierarchical Materials in Biomedicine: Drug Delivery, Tissue Engineering, Sensing and Safety Issues**, San Sebastián, Spain, 09/10/18. Víctor F. Puentes

Targeting the Redoxome in the context of brain hyperactivity, **The use of CeO₂ Nanoparticles in the context of channelopathies, neuroinflammation and epilepsy**, Barcelona, Spain, 27/11/18. Víctor F. Puentes

Cómo trabajar de manera segura con Nanopartículas, Nanotecnología en el sector cosmético: sinergias y nuevas tendencias, Palau Macaya, Barcelona, Spain, 29/11/18. Víctor F. Puentes



PARTICIPATED CONGRESSES

The use of CeO₂ nanoparticles in the context of channelopathies, neuroinflammation and epilepsy, Barcelona, Spain, 27/11/18, *Organiser*, V.F. Puentes



COURSES

Responsible research and innovation in nanotechnology course to 13 PhD fellows under **H2020 ITN PANDORA training program**



THESES

Jordi Piella, *Advanced synthesis and characterization of noble metal nanoparticles*, 08/11/18, supervised by Prof. Víctor F. Puentes

Javier Patarroyo, *Exploring synthetic strategies for the production of complex inorganic nanoparticles*, 16/11/18, supervised by Prof. Víctor F. Puentes

Amirali Yazdi, *Nanoengineering composites made of metal- and covalent-organic frameworks and inorganic nanoparticles using encapsulation techniques*, 30/11/18, supervised by ICREA Prof. Daniel Maspoch, Dr Inhar Imaz and ICREA Prof. Víctor F. Puentes



AWARDS

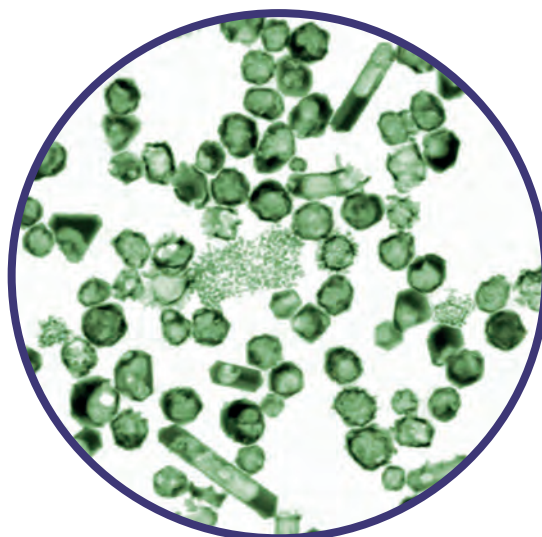
Javier Patarroyo awarded a **poster 2nd price** at *ICPMS 2018, 3rd International Conference on Polyol Mediated Synthesis* (Madrid, 25-27 June 2018). The awarded poster was entitled "*One-pot polypol synthesis of highly monodisperse short green silver nanorods*".



DISSEMINATION CONTRIBUTIONS

Workshop: "Nanoparticles: tools for post world destruction survival", **10alamos9 - Festival de Nanociència i Nanotecnologia**, 10-12/04/18. CosmoCaixa, Barcelona

Ciència i esperit crític, Cicle visions de ciència en homenatge a un dels pares de la ciència. Feynman i l'evolució de la ciència al segle XX, Víctor F. Puentes, 12/02/18. Biblioteca Camp de l'Arpa-Caterina Albert



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 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 240 articles (including eight reviews), with over 16,000 citations and an H-index of 55. He is the author of three patents and his work has given rise to over 225 invited talks at international conferences and workshops.



GROUP MEMBERS

Nogués Sanmiquel, Josep, ICREA Research Professor and Group Leader

Bach Marquès, Èric, Visiting TFG Student

Chaparro Amaro, Oscar Roberto, Fellowship Master Student

Contreras Encinas, María del Carmen, Technician

Estrader Bofarull, Marta, Visiting Postdoctoral Researcher

Gómez Roca, Alejandro, Postdoctoral Researcher

Güell Grau, Pau, Technician

Li, Zhi, Fellowship Doctoral Student

Muro Cruces, Javier, Doctoral Student

Sepúlveda Martínez, Borja, CSIC Tenured Scientist

Shahnazarova, Gubakhanim, Doctoral Student

Zhang, Kuan, SO Doctoral Student

Zhang, Yue, Fellowship Doctoral Student



NEW PROJECTS & MILESTONES

In 2017 the group started work on the MAGOAPP project funded by the Spanish Ministry of Economy, Competitiveness and Industry 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

Atomic-scale determination of cation inversion in spinel-based oxide nanoparticles,

Torruella P., Ruiz-Caridad A., Walls M., Roca A.G., López-Ortega A., Blanco-Portals J., López-Conesa L., Nogués J., Peiró F., Estradé S. *Nano Letters*; **18 (9)**: 5854 - 5861. 2018.

10.1021/acs.nanolett.8b02524. IF: 12.080

Coercivity modulation in Fe-Cu pseudo-ordered porous thin films controlled by an applied voltage: a sustainable, energy-efficient approach to magnetoelectrically driven materials,

Dislaki E., Robbennolt S., Campoy-Quiles M., Nogués J., Pellicer E., Sort J. *Advanced Science*; **5 (8)**: 1800499, 2018.

10.1002/advs.201800499. IF: 12.441

Combining X-Ray whole powder pattern modeling, rietveld and pair distribution function analyses as a novel bulk approach to study interfaces in heteronanostructures: oxidation front in FeO/Fe₃O₄ core/shell nanoparticles as a case study,

Ichikawa R.U., Roca A.G., López-Ortega A., Estrader M., Peral I., Turrillas X., Nogués J. *Small*; **14 (30)**: 1800804, 2018. 10.1002/smll.201800804. IF: 9.598

Enhanced ultrafast nonlinear optical response in ferrite core/shell nanostructures with excellent optical limiting performance,

Perumbilavil S., López-Ortega A., Tiwari G.K., Nogués J., Endo T., Philip R. *Small*; **14 (6)**: 1701001, 2018.

10.1002/smll.201701001. IF: 9.598

Large magnetoelectric effects in electrodeposited nanoporous microdisks driven by effective surface charging and magneto-ionics,

C. Navarro-Senent, J. Fornell, E. Isarain-Chaved, A. Quintana, E. Menendez, M. Foerster, L. Aballe, E. Weschke, J. Nogués. E. Pellicer, J. Sort. *ACS Applied Materials Interfaces*, **10 (51)**: 44897-44905. 2018.

10.1021/acsami.8b17442

Magnetically amplified photothermal therapies and multimodal imaging with magneto-plasmonic nanodomes,

Li Z., Aranda-Ramos A., Güell-Grau P., Tajada J.L., Pou-Macayo L., Lope Piedrafita S., Pi F., G. Roca A., Baró M.D., Sort J., Nogués C., Nogués J., Sepúlveda B. *Applied Materials Today*; **12**: 430 - 440. 2018.

10.1016/j.apmt.2018.07.008

Simultaneous local heating/thermometry based on plasmonic magnetochromic nanoheaters,

Li Z., Lopez-Ortega A., Aranda-Ramos A., Tajada J.L., Sort J., Nogues C., Vavassori P., Nogues J., Sepulveda B. *Small*; **14 (24)**: 1800868, 2018.

10.1002/smll.201800868. IF: 9.598

Tunable magnetism in nanoporous CuNi alloys by reversible voltage-driven element-selective redox processes, Quintana A., Menéndez E., Isarain-Chávez E., Fornell J., Solsona P., Fauth F., Baró M.D., Nogués J., Pellicer E., Sort J. *Small*; **14 (21)**: 1704396, 2018. 10.1002/sml.201704396. IF: 9.598

Unraveling the operational mechanisms of chemically propelled motors with micropumps, Esplandiú M.J., Zhang K., Fraxedas J., Sepúlveda B., Reguera D. *Accounts of Chemical Research*; **51 (9)**: 1921-1930, 2018. 10.1021/acs.accounts.8b00241. IF: 20.955

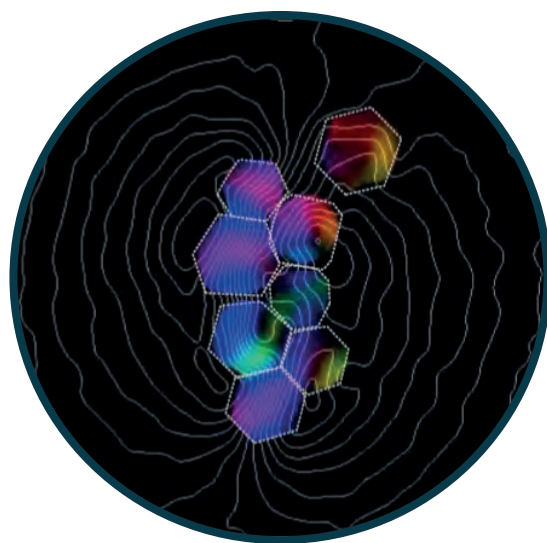
Unravelling the elusive antiferromagnetic order in wurtzite and zinc blende CoO polymorph nanoparticles, Roca A.G., Golosovsky I.V., Winkler E., López-Ortega A., Estrader M., Zysler R.D., Baró M.D., Nogués J. *Small*; **14 (15)**: 1703963, 2018. 10.1002/sml.201703963. IF: 9.598

Voltage-controlled ON-OFF ferromagnetism at room temperature in a single metal oxide film, Quintana A., Menéndez E., Liedke M.O., Butterling M., Wagner A., Sireus V., Torruella P., Estradé S., Peiró F., Dendooven J., Detavernier C., Murray P.D., Gilbert D.A., Liu K., Pellicer E., Nogues J., Sort J. *ACS Nano*; **12(10)**: 10291, 2018. 10.1021/acsnano.8b05407. IF: 13.709

PROJECTS

PAIRED, Magnetically and photochemically actuated bioactive nanowires for remotely controlled drug delivery, funded by **PCIN-2016-093 (MINECO)**, 01/05/16 to 30/04/19, Borja Sepúlveda

MAGOAPP, Nanomateriales magneto-fotónicos multifuncionales para aplicaciones biomédicas: fabricación top-down, bottom-up e híbridas, funded by **MAT2016-77391-R (MINECO/FEDER, UE)**, 30/12/16 to 29/12/19, Josep Nogués, Borja Sepúlveda





CONTRIBUTIONS

Plenary Talk

*Biomedical applications of magnetically controlled magnetoplasmonic nanodomains, **Nanoscience Conference**, Barcelona, Spain, 10/11/18, Borja Sepúlveda*

*Magnetoplasmonic heterostructures for theranostic applications, **23rd International Conference on Nanomaterials and Nanotechnology**, London, United Kingdom, 15/03/18, Alejandro G. Roca*

Keynote

*Magnetoplasmonic nanodomains as a novel structure for biomedical applications, **International Union of Materials Research Societies - International Conference on Electronic Materials (IUMRS-ICEM)**, Daejeon, South Korea, 22/08/18, J. Nogués*

Invited

*Magnetically enhanced and controlled photo-thermal therapies, **HUJI Nano-center Annual Conference**, Death Sea, Israel, 10/02/18, Borja Sepúlveda*

*Heyrosky discussion, **International Workshop on Magneto-Electric Actuation, Magneto-ionics and Related Phenomena in High Surface area Materials**, Trest, Czech Republic, 28/05/18, Alejandro G. Roca*

*Simultaneous local nanoheating/thermometry based on plasmonic magneto-chromic nanodomains, **Collaborative Conference on Materials Research**, Incheon, South Korea, 26/06/18, Josep Nogués*

*Simultaneous local nanoheating/thermometry based on plasmonic magneto-chromic nanodomains, **International Symposium on Metastable, Amorphous and Nanostructured Materials**, Rome, Italy, 03/07/18, Josep Nogués*

*Simultaneous local heating/thermometry based on plasmonic magneto-chromic nanodomains, **International Conference on Small Science**, Rome, Italy, 04/07/18, Josep Nogués*

*Improving the properties of iron oxide in the theranostic applications by the use of elongated nanoparticles, **International Union of Materials Research Societies - International Conference on Electronic Materials (IUMRS-ICEM)**, Daejeon, South Korea, 21/08/18, Alejandro G. Roca*

*Control of photothermal therapies with magnetic fields, **Energy Materials Nanotechnology Barcelona Meeting**, Barcelona, Spain, 10/09/18, Zhi Li*

*Ultrafast optical limiting in ferrite core/shell nanostructures, **European Materials Research Society Fall Meeting (E-MRS)**, Warsaw, Poland, 17/09/18, Josep Nogués*



PARTICIPATED CONGRESSES

Symposium on "Surfaces and Interfaces in Multilayered Thin Films and Nano-composites" at E-MRS (Warsaw, Poland; 2018) - Head Organiser

*Global Congress and Expo on **Materials Science and Engineering** (Rome, Italy, 2018) - Organising Committee*

***International Workshop on Magneto-Electric Actuation, Magneto-ionics and Related Phenomena in High Surface area Materials** (Gavà, Spain, 2018) - Local Organiser*

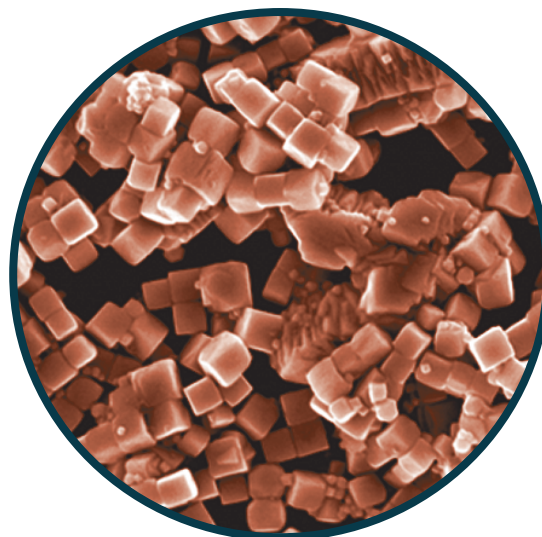
***International Conference on Magnetism & Magnetic Materials** (Paris, France; 2018) - Organising Committee*

*Symposium on "Surfaces and Interfaces of Thin Films, Multilayers and Nanocomposites" at **Materials Research Societies - International Conference on Electronic Materials (IUMRS-ICEM)**, Daejeon, South Korea, 2018. Head organizer, Alejandro G. Roca*



AWARDS

J. Nogués, **Outstanding "Magnetism" Award**, Associazione Italiana di Magnetismo, 2018



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 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 Politècnica 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.



GROUP MEMBERS

Merkoçi Hyka, Arben, ICREA Research
Professor and Group Leader

Alashaini, Somayeh, Visiting Master Student

Álvarez Diduk, Ruslan Raulevich,
Postdoctoral Researcher

Amin, Niloufar, Fellowship Doctoral Student

Balsells Vives, Marc, Technician

Bergua Canudo, José Francisco, Doctoral
Student

Botifoll Moral, Marc, Visiting Degree Student

Calucho Palma, Enric, Fellowship Master
Student

Calucho Palma, Enric, Technician

De La Cruz Morales, Karla, Fellowship
Master Student

Farahmand Nejad, Mohammad Amin,
Fellowship Doctoral Student

Farkhondeh, Golay, Fellowship Doctoral
Student

Fuentes Chust, Celia, Visiting Master Student

Giacomelli, Caterina, Fellowship Master
Student

Golmohammadi, Hamed, Visiting Senior
Researcher

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Hassan, Abdel-Rahim, Fellowship
Postdoctoral Researcher

Hizal Yücesoy, Fehime Jülide, Visiting
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Hu, Liming, Fellowship Doctoral Student

Khater, Mohga, Fellowship Doctoral Student

Kudr, Jiri, Fellowship Postdoctoral Researcher

Martínez Domingo, Carme, Visiting
Doctoral Student

Müller, Mark Alexander, Visiting Master
Student

Nguyen, Emily, Postdoctoral Researcher

Patella, Bernardo, Fellowship Doctoral
Student

Pollap, Aleksandra, Fellowship Doctoral
Student

Puig Font, Anna, Scientific Group
Administrator

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Sena Torralba, Amadeo, Doctoral Student

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Testolin, Anna, Fellowship Doctoral Student

Wong, Xin Yi, Fellowship Doctoral Student

Yang, Qiuyue, Fellowship Doctoral Student

Zhao, Lei, Fellowship Doctoral Student

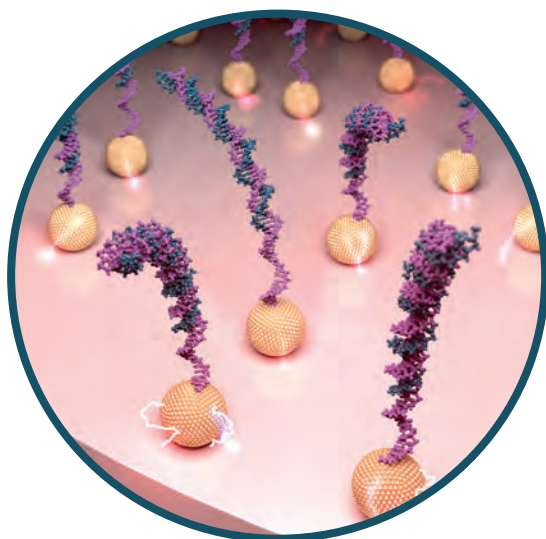


NEW PROJECTS & MILESTONES

In 2018 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 nanodiagnostics platform for monitoring cancer cell-secreted proteins.

In April 2018, the group started his participation in CORE 2 of GRAPHENE FLAGSHIP in relation to graphene-based sensors development. 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 two students defended their PhD theses: Daniel Quesada and Carme Martínez.





PUBLICATIONS

2D materials-based platforms for

electroanalysis applications, Alarcon-Angeles G., Palomar-Pardavé M., Merkoçi A. *Electroanalysis*; **30 (7)**: 1271-1280. 2018. 10.1002/elan.201800245. IF: 2.851

Architecting graphene oxide rolled-up micromotors: a simple paper-based manufacturing technology

Baptista-Pires L., Orozco J., Guardia P., Merkoçi A. *Small*; **14 (3)**: 1702746, 2018. 10.1002/smll.201702746. IF: 9.598

Bioluminescent nanopaper for rapid screening of toxic substances

Liu J., Morales-Narváez E., Orozco J., Vicent T., Zhong G., Merkoçi A. *Nano Research*; **11 (1)**: 114-125. 2018. 10.1007/s12274-017-1610-7. IF: 7.994

Design and fabrication of printed paper-based hybrid micro-supercapacitor by using graphene and redox-active electrolyte

Nagar B., Dubal D.P., Pires L., Merkoçi A., Gómez-Romero P. *ChemSusChem*; **11 (11)**: 1849-1856. 2018. 10.1002/cssc.201800426. IF: 7.411

Electrochromic molecular imprinting sensor for visual and smartphone-based detections

Capoferri D., Álvarez-Diduk R., Del Carlo M., Compagnone D., Merkoçi A. *Analytical Chemistry*; **90 (9)**: 5850-5856. 2018. 10.1021/acs.analchem.8b00389. IF: 6.042

In situ monitoring of PTHLH secretion in neuroblastoma cells cultured onto nanoporous membranes

de la Escosura-Muñiz A., Espinoza-Castañeda M., Chamorro-García A., Rodríguez-Hernández C.J., de Torres C., Merkoçi A. *Biosensors and Bioelectronics*; **107**: 62-68. 2018. 10.1016/j.bios.2018.01.064. IF: 8.173

Microorganism-decorated nanocellulose for efficient diuron removal

Liu J., Morales-Narváez E., Vicent T., Merkoçi A., Zhong G.-H. *Chemical Engineering Journal*; **354**: 1083-1091. 2018. 10.1016/j.cej.2018.08.035. IF: 6.735

Nanomaterial-based devices for point-of-care diagnostic applications

Quesada-González D., Merkoçi A. *Chemical Society Reviews*; **47 (13)**: 4697-4709. 2018. 10.1039/c7cs00837f. IF: 40.182

Photoluminescent lateral flow based on non-radiative energy transfer for protein detection in human serum

Zamora-Gálvez A., Morales-Narváez E., Romero J., Merkoçi A. *Biosensors and Bioelectronics*; **100**: 208-213. 2018. 10.1016/j.bios.2017.09.013. IF: 8.173

Screen-printed electroluminescent lamp modified with graphene oxide as a sensing device

Yakoh A., Álvarez-Diduk R., Chailapakul O., Merkoçi A. *ACS Applied Materials and Interfaces*; **10 (24)**: 20775-20782. 2018. 10.1021/acsami.8b04883. IF: 8.097

Time- and size-resolved plasmonic evolution with nm resolution of galvanic replacement reaction in AuAg nanoshells synthesis

Russo L., Merkoçi F., Patarroyo J., Piella J., Merkoçi A., Bastús N.G., Puentes V. *Chemistry of Materials*; **30 (15)**: 5098-5107. 2018. 10.1021/acs.chemmater.8b01488. IF: 9.890

Tunable electrochemistry of gold-silver alloy nanoshells

Russo L., Puentes V., Merkoçi A. *Nano Research*; **11 (12)**: 6336-6345. 2018. 10.1007/s12274-018-2157-y. IF: 7.994

Uranium (VI) detection in groundwater using a gold nanoparticle/paper-based lateral flow Device

Quesada-González D., Jairo G.A., Blake R.C., II, Blake D.A., Merkoçi A. *Scientific Reports*; **8 (1)**: 16157, 2018. 10.1038/s41598-018-34610-5. IF: 4.122

Low-cost strategy for the development of a rapid electrochemical assay for bacteria detection based on AuAg nanoshells

L Russo, J Leva Bueno, JF Bergua, M Costantini, M Giannetto, V Puentes, A Merkoçi. *ACS Omega*, **3 (12)**, 18849-18856. 2018.



PROJECTS

INTCATCH, Development and application of Novel, Integrated Tools for monitoring and managing Catchments, funded by **European Union's Horizon 2020 research and innovation programme** under grant agreement N° 689341-2, 01/06/2016-31/01/2020, IP: Arben Merkoçi

NACANCELL, Development of a Nanodiagnostic platform for monitoring of Cancer cell secreted proteins, funded by **PCIN-2016-066 (MINECO)**, 01/11/2016-30/10/2019, IP: Arben Merkoçi

INCOSTNANO, Integrated smart cost and effective nanodiagnosics, funded by **FEDER/Ministerio de Ciencia, Innovación y Universidades - Agencia Estatal de Investigación/ MAT2017-87202-P**, 01/01/2018-31/12/2021, Arben Merkoçi

GRAPHENE CORE 2, Graphene Flagship Core Project 2, funded by **European Union's Horizon 2020 research and innovation programme** under grant agreement N° 785219, 01/04/2018-31/03/2020, IP: Stephan Roche, José A. Garrido, Arben Merkoçi, Sergio Valenzuela



CONTRIBUTIONS

Plenary talk

Diagnostics using paper-based platforms, **12 International Symposium on Pharmaceutical Sciences**, Ankara, Turkey, 26-29/06/18, Arben Merkoçi

Keynote

Nanobiosensors for safety and security applications, **NanoSD2018 Security & Defense**, Madrid, Spain, 11-12/12/18, Arben Merkoçi

Graphene-based biosensors for diagnostics, **Graphene Week 2018**, San Sebastian, Spain, 10-14/09/18, Arben Merkoçi

Nanobiosensors design and applications in diagnostics, **Select Biosciences Point-of-Care Diagnostics and Biosensors Europe 2018**, Rotterdam, The Netherlands, 05-06/06/18, Arben Merkoçi

Invited

Graphene-based biosensors. What make graphene and other 2D materials advantageous in comparison to others?, **28th World Congress of Biosensors 2018**, Miami, USA, 15/06/18, Arben Merkoçi

Cost-effective and globally deployable mobile diagnostics using paper-based nanobiosensors, **Point-of-Care Diagnostics & Global Health 2018**, Coronado Island, San Diego, California, USA, 01/10/18, Arben Merkoçi

Graphene-based biosensors for diagnostics, **Tohoku University**, Sendai, Japan, 20/11/18, Arben Merkoçi

Nanomaterials-based biosensors for diagnostics applications, **EPFL**, Lausanne, Switzerland, 10/12/18, Arben Merkoçi

Graphene-Based Biosensors, **EU-Japan Symposium on Application of Graphene and Related 2D Materials**, Tokyo, Japan, 22/11/18, Arben Merkoçi

Nanobiosensors design and applications in diagnostics, **Mendel University in Brno**, Brno, Czech Republic, 06/11/18, Arben Merkoçi

Nanomaterials-based biosensors for diagnostics applications, **Frontiers of Science (FoS) seminar**, Turku, Finland, 11/10/18, Arben Merkoçi

Nanobiosensors in diagnostics, **1st Global Congress of Pharmacy Faculties. Innovation in Pharmacy: Advances and perspectives**, Salamanca, Spain, 25-28/09/18, Arben Merkoçi

Graphene-based biosensors, **International Graphene Innovation Conference (GRAPCHINA)**, Xi'an, China, 19-21/09/18, Arben Merkoçi

Nanobiosensors designs and applications in health diagnostics, environment monitoring, safety and security, **28th Summer PhD School of Information Engineering (SSIE)**, Brixen, Italy, 23-27/07/18, Arben Merkoçi

Nanobiosensors in diagnostics applications, **The 43d Federation of European Biochemical Societies (FEBS) Congress**, Prague, Check Republic, 07-12/07/18, Arben Merkoçi

Nanobiosensors for diagnostics applications, **Istituto Italiano di Tecnologia (IIT)**, Genova, Italy, 31/05/18, Arben Merkoçi

Nanobiosensors for diagnostics, **Catalan Institute for Water Research (ICRA)**, Girona, Spain, 01/03/18, Arben Merkoçi

Nanobiosensors for diagnostics applications, **INL-Lyon Institute of Nanotechnology**, Lion, France, 08/02/18, Arben Merkoçi

Nanobiosensors for diagnostics applications, **Universita degli Studi di Padova**, Padova, Italy, 17/01/18, Arben Merkoçi

Oral

Heavy metals detection using screen printed carbon electrodes, **First Scientific Symposium on Health and Climate Change 2018**, Rome, Italy, 03-05/12/18, Arben Merkoçi

COURSES

A. Merkoçi, **Master's in Nanoscience and Nanotechnology. Subject: Nanodiagnostics**, (6 hours). Universitat Autònoma de Barcelona, Nov/Dec 2018

THESES

Daniel Quesada, *Design and application of nanomaterial-based lateral flow devices*, 26/10/18, supervised by Prof. Arben Merkoçi

AWARDS

ICREA Prof. Arben Merkoçi elected **member of Photonics21 Board of Skateholders**, the main decision-making body of this platform.



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). From 2013 to 2017 she was 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 250 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 the spin-off company *SENSIA, SL* in 2004 and the co-founder of the company *BIOD, SL* in 2010.



Prof. Lechuga is associate editor of the *Optics and Laser Technology and Analyst (RSC)* journals. 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 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

Lechuga Gómez, Laura, Full Professor and Group Leader

Andreu Guarro, Meritxell, Visiting Master Student

Calvo Lozano, Olalla, Doctoral Student

Cancelli, Giulia, Fellowship Master Student

Cerf, Camille, Fellowship Master Student

Chocarro Ruiz, Blanca, SO Doctoral Student

Dey, Priyanka, Research Engineer

Díaz Luis-Ravelo, Heriberto J., Technician

Estévez Alberola, Maria Carmen, Senior Researcher

Fabri Faja, Núria, Doctoral Student

Guiu Tort, Roger, Technician

Leuermann, Jonas, Visiting Doctoral Student

Llop Castelbou, Jessica, Scientific Group Administrator

López Muñoz, Gerardo Arturo, Fellowship Doctoral Student

Minguillón Rosa, Xavier, Visiting Degree Student

Muradas Belinchón, David, Visiting Degree Student

Peláez Gutiérrez, Enelia Cristina, Technician

Pepió Tàrrega, Belén, Visiting Degree Student

Portela Otaño, Alejandro Ernesto, Postdoctoral Researcher

Prada Vargas, Yuly Andrea, Visiting Doctoral Student

Ramírez Priego, Patricia, Technician

Robles, Denise, Fellowship Doctoral Student

Sierra Montoya, Miquel, Visiting Degree Student

Soler Aznar, Maria, Senior Researcher



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 2018 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 for further integration in portable platforms. New solutions based on vertical adiabatic tapers for light incoupling in the nanometric structures of

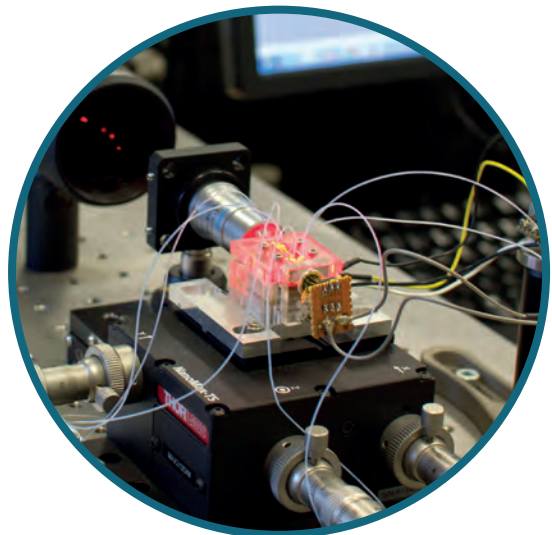
the bimodal waveguide biosensor have been successfully implemented, allowing incoupling with the tolerances required for a multiplexed point-of-care. New designs of the multiplexed version of the nanointerferometric sensors have further expanded the capabilities of this ultrasensitive technology.

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 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 demonstrated a new and unique methodology for the direct detection of epigenetic marks (as methylation) in double strands of DNA. We have also successfully demonstrated miRNA detection in biological media at exceptionally low detection limits, which has allowed us to stratify between healthy patients and those with bladder cancer with a simple urine analysis.

In addition, we have started a new research line in collaboration with the oil company CEPSA within the framework of the project DIONISOS (RETOS-Colaboración, RTC-2017-6222-5)

We have also 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.





PUBLICATIONS

A CO₂ optical sensor based on self-assembled metal-organic framework nanoparticles,

Chocarro-Ruiz B., Pérez-Carvajal J., Avci C., Calvo-Lozano O., Alonso M.I., MasPOCH D., Lechuga L.M. *Journal of Materials Chemistry A*; **6 (27)**: 13171-13177. 2018. 10.1039/c8ta02767f. IF: 9.931

A low-cost integrated biosensing platform based on SiN nanophotonics for biomarker detection in urine,

Martens D., Ramirez-Priego P., Murib M.S., Elamin A.A., Gonzalez-Guerrero A.B., Stehr M., Jonas F., Anton B., Hlawatsch N., Soetaert P., Vos R., Stassen A., Severi S., Van Roy W., Bockstaele R., Becker H., Singh M., Lechuga L.M., Bienstman P. *Analytical Methods*; **10 (25)**: 3066-3073. 2018. 10.1039/c8ay00666k. IF: 2.073

Gold/silver/gold trilayer films on nanostructured polycarbonate substrates for direct and label-free nanoplasmonic biosensing,

López-Muñoz G.A., Estévez M.-C., Vázquez-García M., Berenguel-Alonso M., Alonso-Chamarro J., Homs-Corbera A., Lechuga L.M. *Journal of Biophotonics*; **11 (8)**: e201800043, 2018. 10.1002/jbio.201800043. IF: 3.768

Interferometric nanoimmunosensor for label-free and real-time monitoring of Irgarol 1051 in seawater,

Chocarro-Ruiz B., Herranz S., Fernández Gavela A., Sanchís J., Farré M., Marco M.P., Lechuga L.M. *Biosensors and Bioelectronics*; **117**: 47-52. 2018. 10.1016/j.bios.2018.05.044. IF: 8.173

Label-free and real-time detection of tuberculosis in human urine samples using a nanophotonic point-of-care platform,

Ramirez-Priego P., Martens D., Elamin A.A., Soetaert P., Van Roy W., Vos R., Anton B., Bockstaele R., Becker H., Singh M., Bienstman P., Lechuga L.M. *ACS Sensors*; **3 (10)**: 2079-2086. 2018. 10.1021/acssensors.8b00393. IF: 5.711

Label-free DNA-methylation detection by direct ds-DNA fragment screening using poly-purine hairpins,

Huertas C.S., Aviñó A., Kurachi C., Piqué A., Sandoval J., Eritja R., Esteller M., Lechuga L.M. *Biosensors and Bioelectronics*; **120**: 47-54. 2018. 10.1016/j.bios.2018.08.027. IF: 8.173

Nanoplasmonic biosensor device for the monitoring of acenocoumarol therapeutic drug in plasma,

Peláez E.C., Estevez M.-C., Portela A., Salvador J.-P., Marco M.-P., Lechuga L.M. *Biosensors and Bioelectronics*; **119**: 149-155. 2018. 10.1016/j.bios.2018.08.011. IF: 8.173



PROJECTS

URINETEST, Métodos Rápidos de análisis de péptidos inmunogénicos alimenticios en orina, funded by RTC-2016-5452-1 (**MINECO/FEDER, UE**), 01/04/2016 - 31/12/2018, IP: Laura Lechuga

PreDICT, Point-of-care Nanoplasmonic Platforms for Novel High-Value Diagnostics and Therapy Follow-Up, funded by TEC2016-78515-R (**MINECO/FEDER, UE**), 30/12/2016 - 29/12/2019, Laura Lechuga

RAIS, Scalable, point-of-care and label free microarray platform for rapid detection of Sepsis, funded by **European Union's Horizon 2020 research and innovation programme** under grant agreement No 644956, 01/03/2017 - 31/03/2018, IP: Laura Lechuga

DIONISOS, Desarrollo de Inmunorreactivos y biosensores para el análisis de trazadores en yacimientos, funded **FEDER/Ministerio de Ciencia, Innovación y Universidades - Agencia Estatal de Investigación/** RTC-2017-6222-5, 01/07/2018 - 30/06/2021, IP: Laura Lechuga



CONTRIBUTIONS

Keynote

Nanophotonic point-of-care biosensor platforms for advanced and portable diagnostics, **IEEE NEMS 2018**, 13th IEEE International Conference on Nano/Micro Engineered and Molecular Systems, Singapore, 22/04/18, Laura M. Lechuga

Photonic label-free biosensors for real-time analysis of untreated clinical and environmental samples, **GRC (Gordon Research Conference) on Bioanalytical sensors**, Boston, USA, 24/06/18, Laura M. Lechuga

Next generation of nanosensing devices for universal health care, **Encuentro de Científicos Peruanos en Europa (SINAPSIS)**, Spain, 24/10/18, Laura M. Lechuga

Invited

Nanophotonic biosensor platforms for ultrasensitive bioanalysis, **Institute of Chemical Research of Catalonia (ICIQ)**, Tarragona, Spain, 02/02/18, Laura M. Lechuga

Point-of-care devices in the Diagnostics area: state-of-the-art and future developments, **Laboratori de Referència de Catalunya, S.A**, Barcelona, Spain, 07/03/18, Laura M. Lechuga

Nanobiosensor devices as advanced tools for precision medicine and healthcare, **ICN2 Severo Ochoa International Conference 2018**, Barcelona, Spain, 15/02/18, Laura M. Lechuga

Nanomedicina: hacia el diagnóstico de precisión y la medicina personalizada, **Seminarios Facultad de Medicina y Enfermería, Univ. del País Vasco**, Bilbao, Spain, 12/04/18, Laura M. Lechuga

Nanophotonic biosensor platforms for ultrasensitive bioanalysis, **Physics Department, Chalmers University of Technology**, Gotenburg, Sweden, 24/05/18, Laura M. Lechuga

Nanodispositivos biosensores para el diagnóstico clínico avanzado, **Foro CIBER (CIBER-BBN-CIBERES-CIBERER)**, Instituto de Salud Carlos III, Madrid, Spain, 08/05/18, Laura M. Lechuga

Ultrasensitive nanophotonics biosensors for the label-free and real-time detection of analytes, **Workshop Biosensors for Security**, Bologna, Italy, 09/05/18, Laura M. Lechuga

Nanophotonic point-of-care biosensor platforms for ultrasensitive and label-free bioanalysis of untreated samples, **Nanotechnology Institute, University of Miami**, Miami, USA, 03/08/18, Laura M. Lechuga

Nanophotonic biosensor platforms for ultrasensitive and multiplex analysis at the point-of-care, **IEEE RAPID Conference**, IEEE Research and Applications of Photonics in Defense Conference, USA, 22/08/18, Laura M. Lechuga

Silicon photonics biosensors, **Summer school Micro and Optical Technologies in Biomedical Science**, Wallis, Switzerland, 10/09/18, Laura M. Lechuga

Nanophotonic point-of-care biosensors for early Sepsis diagnosis and treatment followup, **Hospital Vall d'Hebrón and VHIR**, Barcelona, SPAIN, 13/09/18, Laura M. Lechuga

Moving nanophotonics biosensors to point-of-care diagnostics applications, **Master on Multidisciplinary Research in Experimental Sciences (BIST)**, Barcelona, Spain, 17/09/18, Laura M. Lechuga

Photonic point-of-care nanobiosensors platforms for universal health diagnostics, **The Latin America Optics and Photonics (LAOP) Conference (OSA Conferences)**, Perú, 12/11/18, Laura M. Lechuga

Oportunidades y desafíos de la nanobiotecnología para la salud, **Unidad de Posgrado, Facultad de Farmacia y Bioquímica, Universidad Nacional Mayor de San Marcos**, Lima, Perú, 16/11/18, Laura M. Lechuga

Nanophotonic point-of-care biosensor platforms for ultrasensitive and label-free bioanalysis of untreated samples, **RMIT University**, Melbourne, Australia, 20/11/18, Laura M. Lechuga

Nanophotonic biosensor platforms for ultrasensitive and multiplex analysis at the point-of-care, **Smart Nanomaterials: Advances, Innovation and Application Conference**, France, 10/12/18, Laura M. Lechuga

Nanophotonic point-of-care biosensors for ultrasensitive and label-free bioanalysis of untreated samples, **Exeter University**, Exeter, UK, 18/12/18, Laura M. Lechuga

Oral

Au/Ag Nanostructures based on Blu-ray optical discs with integrated microfluidics for multiplexed, **Europtrode 2018**, Italy, 25/3/18, G.A. López-Muñoz; M.-C. Estevez; M. Vázquez-García; M. Berenguel-Alonso; J. Alonso-Chamarro; A. Homs-Corbera; L.M. Lechuga

Use of a microarray reader for the fast, label-free and multiplexed measurement of biomarkers for Sepsis detection, **Europtrode 2018**, Italy, 25/3/18, N. Fabri-Faja; R.A. Terborg; F. Yesilköy; O. Calvo; P. Dey; M.-C. Estévez; J. Pello; A. Belushkin; P. Soetaert; M. Rabaey; H. Altug; V. Pruneri; L.M. Lechuga

Photonic label-free biosensors for real-time analysis of untreated clinical and environmental samples, Laura M. Lechuga, **GRC (Gordon Research Conference) on Bioanalytical sensors**, Valencia, Spain, 24/06/18

Towards photonic biosensing using a three-port mach-zehnder interferometer in a silicon nitride platform, **ECIO 2018**, Spain, 30/05/18, J. Leuermann; A. Sánchez-Postigo; A. Fernandez-Gavela; I. Molina-Fernandez; L.M. Lechuga; R. Halir

Fast, multiplex and label-free quantification of sepsis biomarkers with an innovative optical point-of-care platform, **IBERSENSOR 2018**, Spain, 17/09/18, N. Fabri-Faja; O. Calvo; P. Dey; R. A. Terborg; M.-C. Estévez; F. Yesilköy; J. Pello; A. Fàbrega; J.C. Ruiz Rodriguez; A. Belushkin; J. González-López; H. Altug; V. Pruneri; L.M. Lechuga

Bimodal waveguide interferometric biosensors for highly sensitive point-of-care diagnosis, **IBERSENSOR 2018**, Spain, 17/09/18, L.M. Lechuga, C. S. Huertas, J. Maldonado, D. Grajales and C. Domínguez

Label-free SPR monitoring of gluten immunogenic peptide in urine for celiac disease follow-up, **IBERSENSOR 2018**, Spain, 17/09/18, E.C. Peláez; M.-C. Estévez; C. Sousa; L. Moreno; A. Cebolla; L.M. Lechuga

Nanodispositivos biosensores para el diagnóstico clínico avanzado, **Foro CIBER (CIBER-BBN-CIBERES-CIBERER)**, Madrid, Spain, 17/09/18, Laura M. Lechuga

Poster

Label-free SPR monitoring of gluten immunogenic peptide in urine for celiac disease follow-up, **EUROPTRODE 2018**, Italy, 25/3/18, E.C. Peláez; M.-C. Estévez; C. Sousa; L. Moreno; A. Cebolla; L.M. Lechuga

Integrating Metal-Organic Frameworks in a nanophotonic sensor for specific environmental monitoring, **EUROPTRODE 2018**, Italy, 25/3/18, B. Chocarro-Ruiz; J. Pérez; D. MasPOCH; L.M. Lechuga

Multiplexed photonic nanointerferometric biosensors in silicon nitride platform for ultrasensitive analysis, **ECIO 2018**, Spain, 30/05/18, R. Guiu, D. Grajales, A. Fernández-Gavela, C. Domínguez and L.M. Lechuga

HSPX Protein tuberculosis biomarker evaluated in sputum samples by plasmonic biosensing, **IBERSENSOR 2018**, Spain, 17/09/18, E.C Peláez; M.-C. Estévez; A. Mongui; M.C. Menéndez; M.J. García; C. Toro; O. L. Herrera; P. Del Portillo; L.M. Lechuga



DISSEMINATION CONTRIBUTIONS

La revolución de la Nanomedicina, **Festival de Nanociencia y Nanotecnología 10alamos9**, Barcelona, 10/04/18, Laura Lechuga

Nanomedicina: Hacia el diagnóstico precoz, el tratamiento personalizado y la medicina de precisión, **Conferencia en la Unidad de posgrado, Facultad de Medicina y Bioquímica**, Lima, Perú, 16/11/18, Laura M. Lechuga

Nanomedicina: Hacia el diagnóstico precoz, el tratamiento personalizado y la medicina de precisión, **Ciclo de conferencias CSIC, Residencia de Investigadores**, Barcelona, España, 17/01/18, Laura M. Lechuga

Participation at Round table - Women Scientists, Celebrating Women in Science, **International Day of Women and Girls in Science, ICN2**, Barcelona (Spain), 13/02/18, L.M. Lechuga.

Nanotecnología: la fuerza de lo muy pequeño, **International Day of Women and Girls in Science, Puerto de Santa María**, Cádiz (Spain), 20/02/18, L.M. Lechuga

Nanomedicina: hacia el diagnóstico de precisión y la medicina personalizada, **Semana de la Ciencia de la Nueva España**, Oviedo (Spain), 22/03/18, L.M. Lechuga

El increíble mundo nanotecnológico, **I Certamen gaditano de robótica libre (ROByCAD)**, Cádiz (Spain), 25/05/18, L.M. Lechuga

Work-life balance: An informal discussion, **SRUK-CERU meeting**, London (UK), 17/12/18, Invited: L.M. Lechuga



PARTICIPATED CONGRESSES

ECIO 2018. European Conference on Integrated Optics 2018, 30/05 - 01/06, Valencia (Spain). *Local Organising Committee*. L.M. Lechuga



THESES

Daniel Grajales, *Lab-on-a-chip Integration of the Bimodal Waveguide Nanointerferometric Biosensor*, 14/09/18, supervised by Prof. Laura M. Lechuga and Dr. José Ramón Sendra

Gerardo López, *Simple and low cost nanostructured plasmonic biosensor for sensitive and multiplexed biodetection*, 19/10/18, supervised by Prof. Laura M. Lechuga and Dr. M. Carmen Estévez



AWARDS

Prof. Laura M. Lechuga **joined the Analyst Editorial Board as an Associate Editor.**

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

Ruiz Molina, Daniel, CSIC Tenured Scientist and Group Leader

Ayala García, Álex, Visiting Doctoral Student

Bellacanzone, Christian, SO Doctoral Student

Carrasco Campuzano, Marc, Visiting Degree Student

Carrascal Marín, Aleix, Visiting Master Student

Casagualda Clapés, Carolina, Visiting Doctoral Student



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.



Chen, Jing, Visiting TFG Student

Contreras Pereda, Noemí, Doctoral Student

García Martínez, Beatriz, Doctoral Student

García Pardo, Javier, Postdoctoral
Researcher

González Monje, Pablo, Technician

Julià López, Alejandro Ricar, Doctoral
Student

Kropova, Mariia, Visiting Master Student

Martínez Agudo, Xantal, Visiting TFG
Student

Moghzi, Faezeh, Visiting Doctoral Student

Montpeyó Garcia-Moreno, David,
Doctoral Student

Moreno Villaecija, Miguel Ángel, Doctoral
Student

Novio Vazquez, Fernando, Postdoctoral
Researcher

Otaegui Rabanal, Jaume Ramón, Visiting
Master Student

Pepió Tárrega, Belén, Visiting TFG Student

Pradas García, Eddim, Visiting Master
Student

Rivas Dapena, Antón, Fellowship Master
Student

Roscini, Claudio, Senior Postdoctoral
Researcher

Rubirola Vila, Pau, Visiting TFG Student

Sabater Algarra, Yolanda, Visiting Master
Student

Sedó Vergara, Josep, Senior Postdoctoral
Researcher

Simó Costa, Cristina, Visiting Master Student

Solorzano Rodríguez, Rubén, Visiting
Doctoral Student

Stepanova, Ekaterina, Visiting Master
Student

Suárez García, Salvio, Doctoral Student

Teuber, Jeremy, Visiting Master Student

Torres Pierna, Héctor, Visiting Doctoral
Student

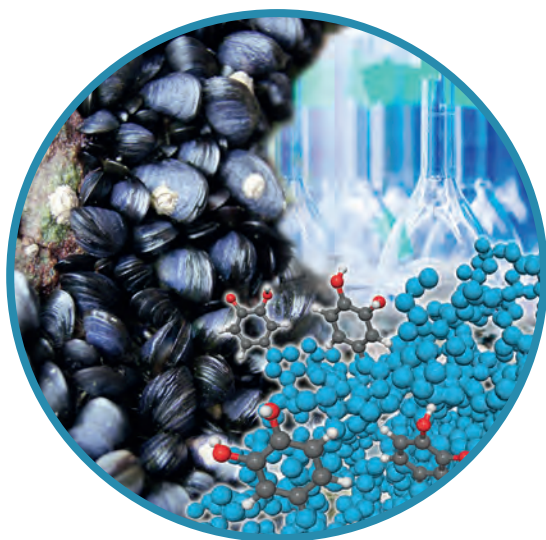
Xiaoman, Mao, Doctoral Student

Zhang, Junda, Doctoral 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

A hexa-quinoline based: C 3-symmetric chemosensor for dual sensing of zinc(ii) and PPI in an aqueous medium via chelation induced “OFF-ON-OFF” emission, Sinha S., Chowdhury B., Adarsh N.N., Ghosh P. *Dalton Transactions*; **47 (19)**: 6819-6830. 2018. 10.1039/c8dt00611c. IF: 4.099

Biochemical and MALDI-TOF mass spectrometric characterization of a novel native and recombinant cystine knot miniprotein from *Solanum tuberosum* subsp. *andigenum* cv. Churqueña, Cotabarren J., Tellechea M.E., Tanco S.M., Lorenzo J., Garcia-Pardo J., Avilés F.X., Obregón W.D. *International Journal of Molecular Sciences*; **19 (3)**: 678, 2018. 10.3390/ijms19030678. IF: 3.687

Carbon nanotube-based nanocomposite sensor tuned with a catechol as novel electrochemical recognition platform of uranyl ion in aqueous samples, Muñoz J., Montes R., Bastos-Arrieta J., Guardingo M., Busqué F., Ruíz-Molina D., Palet C., García-Orellana J., Baeza M. *Sensors and Actuators, B: Chemical*; **273**: 1807-1815. 2018. 10.1016/j.snb.2018.07.093

Crystal structure and mechanism of human carboxypeptidase O: Insights into its specific activity for acidic residues, García-Guerrero M.C., Garcia-Pardo J., Berenguer E., Fernandez-Alvarez R., Barfi G.B., Lyons P.J., Aviles F.X., Huber R., Lorenzo J., Reverter D. *Proceedings of the National Academy of Sciences of the United States of America*; **115 (17)**: E3932-E3939. 2018. 10.1073/pnas.1803685115. IF: 9.504

Dual T1/ T2 nanoscale coordination polymers as novel contrast agents for MRI: a preclinical study for brain tumor, Suárez-García S., Arias-Ramos N., Frias C., Candiota A.P., Arús C., Lorenzo J., Ruiz-Molina D., Novio F. *ACS Applied Materials and Interfaces*; **10 (45)**: 38819-38832. 2018. 10.1021/acsami.8b15594. IF: 8.097

Dual-fluorescent nanoscale coordination polymers via a mixed-ligand synthetic strategy and their use for multichannel imaging, Nador F., Wnuk K., García-Pardo J., Lorenzo J., Solorzano R., Ruiz-Molina D., Novio F. *ChemNanoMat*; **4 (2)**: 183-193. 2018. 10.1002/cnma.201700311. IF: 3.173

Molecular-based upconversion in homo/heterogeneous liquids and in micro/nanostructured solid materials, Latterini L., Massaro G., Penconi M., Gentili P.L., Roscini C., Ortica F. *Dalton Transactions*; **47 (26)**: 8557-8565. 2018. 10.1039/c8dt00020d. IF: 4.099

Off/On fluorescent nanoparticles for tunable high-temperature threshold sensing, Julià López A., Ruiz-Molina D., Landfester K., Bannwarth M.B., Roscini C. *Advanced Functional Materials*; **28 (28)**: 1801492, 2018. 10.1002/adfm.201801492. IF: 13.325

Polydopamine-like coatings as payload gatekeepers for mesoporous silica nanoparticles, Moreno-Villaécija M.-A., Sedó-Vegara J., Guisasaola E., Baeza A., Regí M.V., Nador F., Ruiz-Molina D. *ACS Applied Materials and Interfaces*; **10(9)**: 7661-7669. 2018. 10.1021/acsmi.7b08584. IF: 8.097

Pt(IV)-based nanoscale coordination polymers: Antitumor activity, cellular uptake and interactions with nuclear DNA, Adarsh N.N., Frias C., Ponnoth Lohidakshan T.M., Lorenzo J., Novio F., García-Pardo J., Ruiz-Molina D. *Chemical Engineering Journal*; **340**: 94-102. 2018. 10.1016/j.cej.2018.01.058. IF: 6.735

Solvent-tuned supramolecular assembly of fluorescent catechol/pyrene amphiphilic molecules, Nador F., Wnuk K., Roscini C., Solorzano R., Farauto J., Ruiz-Molina D., Novio F. *Chemistry-A European Journal*; **24 (55)**: 14724-14732. 2018. 10.1002/chem.201802249. IF: 5.160

Sonochemical synthesis of a novel nanoscale 1D lead(II) [Pb₂(L)₂(I)₄]_n coordination polymer, survey of temperature, reaction time parameters, Hayati P., Suárez-García S., Gutiérrez A., Molina D.R., Morsali A., Rezvani A.R. *Ultrasonics Sonochemistry*; **42**: 320-326. 2018. 10.1016/j.ultsonch.2017.11.033. IF: 6.012

Sonochemical synthesis of optically tuneable conjugated polymer nanoparticles, Bellacanzone C., Roscini C., del Carmen Ruiz Delgado M., Ponce Ortiz R., Ruiz-Molina D. *Particle and Particle Systems Characterization*; **35 (2)**: 1700322, 2018. 10.1002/ppsc.201700322. IF: 4.384

Sonochemical synthesis of two novel Pb(II) 2D metal coordination polymer complexes: New precursor for facile fabrication of lead(II) oxide/bromide micro-nanostructures, Hayati P., Suárez-García S., Gutierrez A., Şahin E., Molina D.R., Morsali A., Rezvani A.R. *Ultrasonics Sonochemistry*; **42**: 310-319. 2018. 10.1016/j.ultsonch.2017.11.037. IF: 6.012

Spin-crossover in an exfoliated 2D coordination polymer and its implementation in thermochromic films, Salvio Suárez-García, Nayarassery N. Adarsh, Gábor Molnár, Azzedine Bousseksou, Yann Garcia, Marinela M. Dîrtu, Javier Saiz-Poseu, Roberto Robles, Pablo Ordejón, and Daniel Ruiz-Molina *ACS Applied Nano Materials*; **1 (6)**: 2662-2668. 2018. 10.1021/acsnm.8b00341

Surface functionalization of metal-organic frameworks for improved moisture resistance, Castells-Gil J., Novio F., Padiál N.M., Tatay S., Ruíz-Molina D., Martí-Gastaldo C. *Journal of Visualized Experiments*; 2018 **139**: e58052, 2018. 10.3791/58052. IF: 1.184



BOOKS

Bioinspired Catechol-Based Systems: Chemistry and Applications, Marco d'Ischia, Daniel Ruiz-Molina, *Biomimetics*, ISBN: 978-3-03842-813-8



PARTICIPATED CONGRESSES

International workshop on Bioinspired adhesives and functional coatings based on catechol, ICN2, Campus UAB, Barcelona, Spain, 10-11/10/18, *Co-organiser*, Daniel Ruiz-Molina



PROJECTS

MICROREP, Microcápsulas inteligentes con repelentes de mosquitos y fragancias de aplicación en textiles que eviten la propagación de enfermedades tropicales, funded by RTC-2016-5670-1 (**MINECO/FEDER, UE**), 01/09/2016 - 31/12/2019, IP: Daniel Ruiz-Molina

NanoSVim, Materiales nanoestructurados de índice variable de aplicación en la industria óptica oftálmica, funded by RTC-2016-4822-6 (**MINECO/FEDER, UE**), 01/09/2016 - 31/03/2019, IP: Daniel Ruiz-Molina

TeraCat, Materiales Basados en Catecoles para Teranóstica de la Enfermedad de Parkinson, funded by MAT2015-70615-R (**MINECO/FEDER, UE**), 01/01/2016 - 31/12/2018, Daniel Ruiz-Molina

2017 SGR 694, funded by **AGAUR**, 01/01/2017 - 31/12/2020, Daniel Ruiz-Molina



THESES

David Montpeyó, *Nanotechnological strategies for coating and encapsulation of therapeutic proteins*, supervised by CSIC Tenured Scientist Daniel Ruiz-Molina, Dr. Fernando Novio and Prof. Julia Lorenzo



AWARDS

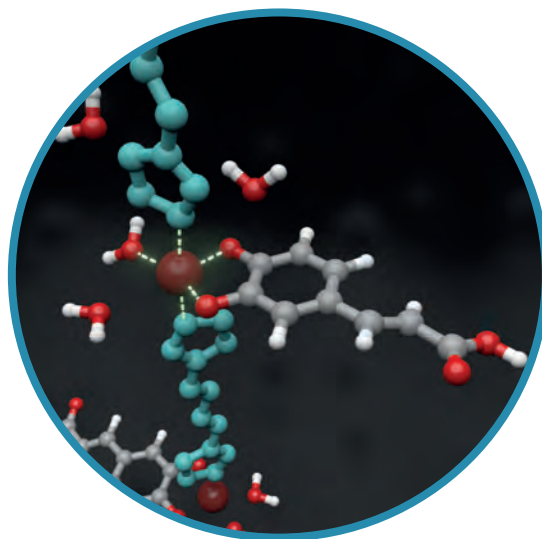
Noemí Contreras receives a **“la Caixa” fellowship** for her doctoral degree in 2D MOF materials for electronic applications.



DISSEMINATION CONTRIBUTIONS

Nanocentres al carrer, Festival 10alamenos9, 10/2/18 - Guided visit to ICN2, Miguel Moreno and Yolanda Sabater, PhD Students at Nanostructured Functional Materials Group

El poder de la Nanotecnologia com a eina de la 4^a Revolució Industrial, Invited Conference, Setmana de la Ciència, Ajuntament de Viladecans, 14/11/18, Miguel Moreno, PhD Student at Nanostructured Functional Materials Group



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

Lira Cantu, Mónica, CSIC Research Scientist and Group Leader

Capdevila Ibáñez, Laia, Visiting TFG Student
Echeverria Troya, Fernando, Fellowship Doctoral Student

Gallardo Ponce, Norma Janette, Visiting Degree Student

Martínez Rojas, Vanessa Celia, Visiting Doctoral Student

Mingorance Ferrer, Alba, SO Doctoral Student

Narymany Shandy, Amir, Fellowship Degree Student

Pereyra Marina, Jose Carlos, Fellowship Doctoral Student



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.



Reyna Velázquez, Yegraf, Fellowship
Doctoral Student

Santigosa Murillo, Elia, Fellowship Doctoral
Student

Xie, Haibing, SO Postdoctoral Researcher

Perez-Tomas, Amador, JIA postdoctoral
Researcher

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) and established the ICN2 Photovoltaic Energy Group in 2007.

Since then she has directly managed more than 60 researchers, including visiting professors, postdoctoral students, eight PhD students (four in progress), over 32 Masters and undergraduate students, project managers and 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 15 scientific conferences and is currently a scientific referee for more than 15 international and European research agencies, and 52 scientific journals. She is member of the editorial board of *SN Applied Science (Nature)*, *Journal of Materials Chemistry C (RSC)*, *Journal of Physics Energy (IOP)*, *Journal of Photonics for Energy (SPIE)* and *Frontiers in Energy Research: Solar Energy (Frontiers)*. She is a member of the advisory board for the Nanotechnology and Chemical Science degree (INCQ) of the *Instituto Tecnológico y de Estudios Superiores de Monterrey (Mexico)*.

Her research interests lie in the synthesis and application of nanostructured materials for high efficient and high stable next-generation thin-film solar cells: halide-perovskite, dye-sensitised, all-oxide and organic solar cells. Currently, the group has developed halide perovskite solar cells with > 21 % efficiency and 1000 h stability under continuous illumination. The group also focuses on the application of solar cells in printed battery-less, self-powered electronics for the IoT (on flexible, transparent and/or smart materials).

Dr Lira-Cantú has more than 120 publications, among them 96 published papers, 9 patents and 10 book chapters, 1 edited book and several technical reports (h index 41, *Google Scholar*)



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

A solar transistor and photoferroelectric memory, Pérez-Tomás A., Lima A., Billon Q., Shirley I., Catalan G., Lira-Cantú M. *Advanced Functional Materials*; **28 (17)**: 1707099, 2018. 10.1002/adfm.201707099. IF: 13.325

Nanofibers as promising materials for new generations of solar cells, AE Shalan, A Barhoum, AM Elseman, MM Rashad, M Lira-Cantú, *Handbook of Nanofibers*, A. Barhoum, et al Eds. Springer Int Pub. 2018, Pages 1-33

Interfacial engineering of metal oxides for highly stable halide perovskite solar cells, Mingorance A., Xie H., Kim H.-S., Wang Z., Balsells M., Morales-Melgares A., Domingo N., Kazuteru N., Tress W., Fraxedas J., Vlachopoulos N., Hagfeldt A., Lira-Cantu M. *Advanced Materials Interfaces*; **5 (22)**: 1800367, 2018. 10.1002/admi.201800367.

Reconsidering figures of merit for performance and stability of perovskite photovoltaics, Khenkin M.V., Anoop K.M., Visoly-Fisher I., Galagan Y., Di Giacomo F., Patil B.R., Sherafatipour G., Turkovic V., Rubahn H.-G., Madsen M., Merckx T., Uytterhoeven G., Bastos J.P.A., Aernouts T., Brunetti F., Lira-Cantu M., Katz E.A. *Energy and Environmental Science*; **11 (4)**: 739 - 743. 2018. 10.1039/c7ee02956j. IF: 30.067

Wide and ultra-wide bandgap oxides: Where paradigm-shift photovoltaics meets transparent power electronics, Pérez-Tomás A., Chikoidze E., Jennings M.R., Russell S.A.O., Teherani F.H., Bove P., Sandana E.V., Rogers D.J. *Proceedings of SPIE - The International Society for Optical Engineering*; **10533 (105331Q)** 2018. 10.1117/12.2302576



BOOKS

M. Lira-Cantu Editor. **The future of Semiconductor Oxides in Next-Generation Solar Cells**. Elsevier Ghenadii Korotcenkov, Metal Oxide Series Editor. 2018. ISBN: 9780128111659. <https://www.elsevier.com/books/the-future-of-semiconductor-oxides-in-next-generation-solar-cells/lira-cantu/978-0-12-810419-4>

Book Chapter: *Stability of molecular devices: halide perovskite solar cells*, Y Reyna, A Pérez-Tomás, A Mingorance, M Lira-Cantú. In **Molecular Devices for Solar Energy Conversion and Storage**, Haining Tian, Gerrit Boschloo and Anders Hagfeldt (Eds.). Pages 477-531. 2018 *Springer Nature Switzerland AG*. DOI 10.1007/978-981-10-5924-7
Print ISBN 978-981-10-5923-0
Online ISBN 978-981-10-5924-7



PROJECTS

European Network to connect research and innovation efforts on advanced Smart Textiles (CONTEXT), funded by **European Union's Horizon 2020 research and innovation programme** under grant agreement N° CA17107. 05/2018 - 04/2022, coordinated by: Dra. Ariadna Detrell (ES), Monica Lira-Cantu as member.

Ultrafast opto-magneto-electronics for non-dissipative information technology (MAGNETOFON), funded by **European Union's Horizon 2020 research and innovation programme** under grant agreement N° CA17123. 05/2018 - 04/2022, coordinated by: Prof. dr. Andrei I. Kirilyuk (NL), Monica Lira-Cantu as MC member.

StableNextSol, Stable Next-Generation Photovoltaics: Unravelling Degradation Mechanisms of Organic Solar Cells by Complementary Characterization Techniques, funded by **European Union's Horizon 2020 research and innovation programme** under grant agreement N° MP1307, 20/03/2014 - 19/03/2018, coordinated by: Mónica Lira-Cantú

EFFECT, Expanding ferroelectric photovoltaics conventional playground, funded by ENE2015-74275-JIN (**MINECO/FEDER, UE**), 19/01/2017- 18/01/2020, Amador Pérez

GraPerOS_PSC, Nanomateriales para celdas solares tipo perovskita de alta eficiencia y estabilidad, funded by ENE2016-79282-C5-2-R (**MINECO/FEDER, UE**), 30/12/2016 - 29/12/2019, Mónica Lira-Cantú

ORGENERGY, Materiales orgánicos optoelectrónicos para la energía, funded by CTQ2016-81911-REDT (**MINECO**), 01/07/2017 - 30/06/2019, Mónica Lira-Cantú

2017 SGR 329, funded by **AGAUR**, 01/01/2017 - 31/12/2020, Mónica Lira-Cantú



CONTRIBUTIONS

Invited

Halide Perovskite Solar Cells: The stability challenge, ICN2 Severo Ochoa international Conference, Barcelona (Spain) 15-16/02/2018. Mónica Lira-Cantú

Last-generation of photovoltaic devices fabricated at ICN2, Reunión Ciencia y tecnología de Superficies (CyTeS), Barcelona (Spain) 08/03/2018. Mónica Lira-Cantú

Recent concepts and future opportunities for oxides in solar cells, 2018 TO-BE Spring Meeting, Sant Feliu de Guixols (ES), 12-14/03/2018. Mónica Lira-Cantú

Oxides for Stable perovskite Solar Cells, Meeting of the Spanish Photovoltaic Excellence network. Madrid, March 9, 2018.

Novel Metal Oxides as Transport Layers in Halide Perovskite Solar Cells, HOPV18, Benidorm (Spain), 28-31/05/2018. Mónica Lira-Cantú

Solution processing oxides for emerging photovoltaics: from binary to complex oxide compounds, E-MRS Spring Meeting, Strasbourg (FR), 18-22/06/2018. Mónica Lira-Cantú

Stability of perovskite solar cells, EU Perovskite PV Day, Oxford University (UK), 25-26/06/2018. Mónica Lira-Cantú

Binary and complex metal oxides for stable halide perovskite solar cells, E-MRS Fall Meeting, Warsaw (Poland), 17-20/09/2018. Mónica Lira-Cantú

The role of metal oxides in the stability of halide perovskite solar cells, NanoBio2018, Crete (Greece), 24-28/10/2018. Mónica Lira-Cantú

Binary, doped and complex oxides as transport layers in halide perovskite solar cells, 8th Szeged International Workshop on Advances in Nanoscience (SIWAN8), Szeged, Hungary, 07-10/10/2018. Mónica Lira-Cantú

Metal oxides for stable perovskite solar cells, International Summit on Organic and Perovskite Solar Cell Stability (ISOS-11), Suzhou (China), 21-25/10/2018. Mónica Lira-Cantú

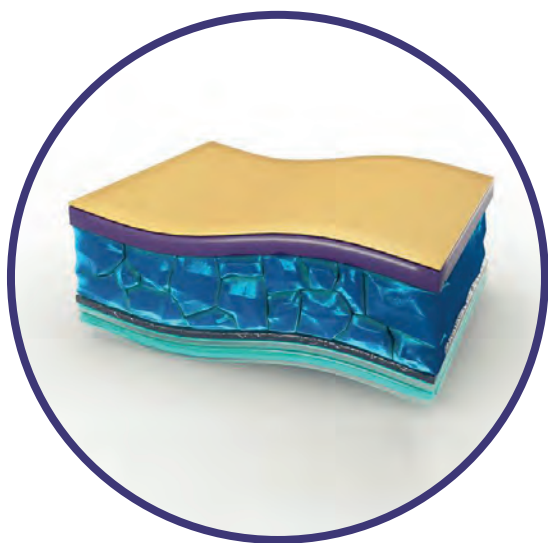
Binary, doped and complex oxides for stable halide perovskite solar cells, Wuhan National Laboratory for Optoelectronics in Huazhong, University of Science and Technology (HUST). 26/10/2018. Mónica Lira-Cantú

Poster

Binary, doped and complex oxides as transport layers in halide perovskite solar cells, HOPV18, Benidorm (Spain), 28-31/05/2018. Mónica Lira-Cantú

Interfacial and doping engineering for stable perovskite solar cells, HOPV18, Benidorm (Spain), 28-31/05/2018. Mónica Lira-Cantú

Printable carbon-based perovskite solar cells employing functionalized oxide interlayers, HOPV18, Benidorm (Spain), 28-31/05/2018. Mónica Lira-Cantú



PARTICIPATED CONGRESSES

NanoBio2018, Crete (Greece), 24-28/09/2018. *Organizer*, Mónica Lira-Cantú

V Congreso Hispano-Luso de Cerámica y Vidrio. LVI Congreso Nacional de la SECV. Barcelona 8-10 October 2018. Monica Lira-Cantu, *Organizer* of the “Ceramic and Glass for Energy” symposium.

International Summit on Organic and Perovskite Solar Cell Stability (ISOS-11), Suzhou (China), 21-25/10/2018. *Organizer*, Mónica Lira-Cantú



THESES

Fernando Echevarria, PhD student 2013-2018, Scholarship: SENEYCYT, Ecuador

Andressa Antunes, PhD student 2014-2018, Sandwich Scholarship, Scholarship: Science without Borders, Brazil



DISSEMINATION CONTRIBUTIONS

Coloquium. Invited, **Festival de la Ciència**, Barcelona (Spain), 09/06/2018. Mónica Lira-Cantú

Los materiales que cambiaron al mundo, La Vanguardia, Barcelona 19/08/2018, Elsa Velasco

Workshop *Nanomaterials para la Energía Fotovoltaica*, at the **Congreso Nacional de Ingeniería Eléctrica y Electrónica del Mayab**. Mérida, Yucatán (Mexico). 16-30 de noviembre 2018.

Energy Focus: Field-effect transistor is powered by solar energy. AR Kirmani, (Lira-Cantu, M). **News MRS Bulletin**

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, inks, etc.) for application in energy storage



GROUP MEMBERS

Gómez Romero, Pedro, CSIC Research Professor and Group Leader

Benages Vilau, Raul, SO Postdoctoral Researcher/ Project Manager

Caban Huertas, Zahilia, Postdoctoral Researcher

González Romero, Carlos, Undergraduate Student

Hernández Cabello, Judith, TFG Student

Hosseinzadeh, Batoul, Visiting Doctoral Student

Israr, Muhammad, Visiting Doctoral Student



GROUP LEADER



CSIC Research Prof. Dr Pedro Gómez-Romero

Prof. Pedro Gómez-Romero completed his BS and Master in Chemistry 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.



Jasso, Kamil, Visiting Doctoral Student
Marchante Fernández, Carlos, Technician.
Master Student
Mollá Romano, Sergio, Postdoctoral
Researcher
Nagar, Bhawna, SO Doctoral Student

Pascual Tudanca, Gonzalo, TFG Student
Rodríguez Laguna, María del Rocío, SO
Doctoral Student
Rueda García, Daniel, Doctoral Student
Zartenaar, Michael Ramón, TFG Student
Zhu, Jun-Jie, Fellowship Doctoral Student

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 2013. 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).

Founder of the spin-off Earthdas for graphene energy storage (2016-).

In 2017 he received the CIDETEC prize for research in electrochemistry.

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



NEW PROJECTS & MILESTONES

This year our group has advanced along the way from materials to devices. Of course, we have maintained our well-established line on hybrid electrode materials, a line which has allowed us to span our collaborations and increase our internationalization with groups from Australia, Germany, Czech Republic, Eslovakia and Brazil. But in addition, we have also focused on the development of hybrid energy storage devices, demonstrating the use of nanocarbons that we have previously developed (N-doped C-NanoPipes) in a hybrid device featuring simultaneously high specific energy (as in batteries) and power (as in supercapacitors).

Graphene and graphene-based materials also keep taking a good share of our time, both at the lab and at the technology transfer bench. Indeed, we have explored several hybrid materials based on graphene (both in solid as well as in nanofluid electrodes), we have worked on printing graphene devices and keep working on the development of graphene-based energy storage devices within the framework of our spin-off Earthdas. And... we have a new breakthrough in this respect. We aim at setting a new standard with our improved and patented Electrochemical Exfoliation technology.

Last, but not least, our work on nanofluids continues along the lines of thermal energy and electrochemical activity, two distinct areas which nevertheless share some common knowledge on which our group is leading.

From hybrid materials to hybrid devices for improved energy storage

The boundaries between batteries and capacitors are quickly blurring. Control over nanostructures is of great importance in the design of high-performance energy storage

devices. We are developing materials with high specific surfaces, as well as ultradispersed molecular materials for application in electrochemical energy storage devices featuring the best properties of batteries (high energy density) and supercapacitors (high specific power). Two of the new materials are novel nanocarbons: i) ultrathin porous carbon nanosheets and ii) N-doped CNPipes, both of which are made through conformal control of nanostructured precursors.

New Nanocarbon materials for energy storage applications

The aforementioned carbon nanopipes 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).

The ultrathin porous carbon nanosheets were prepared from MOF precursors and featured a very high surface area and excellent performance as supercapacitor electrode, a performance that was boosted even further by our approach to hybridize the material with an electroactive component.

Printed graphene devices. From paper to polymers, from supercapacitors to biosensors

This research line, developed within the framework of the SO program in collaboration with A. Merkoçi's group has explored several printing techniques (ink-jet, screenprinting, wax stamping), substrates and graphene hybrid materials leading to the demonstration of low-cost paper-printed supercapacitors with enhanced energy storage thanks to the use of our hybrid (capacitive+faradaic) approach (PhD Thesis Bhawna Nagar).

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. Our graphene nanofluids in organic solvents show a remarkable enhancement of thermal conductivity and specific heat which we are trying to explain through experiment and theory (Research developed within the framework of SO in collaboration with prof. C. Sotomayor's and prof. P. Ordejón's groups)

Graphene and graphene batteries

We are working on various large-scale methods, from mechanical to electrochemical. Electrochemical exfoliation methods, made "our way" have led to a great success (we can prepare high-quality, oxygen-free, few-layer graphene in 3 minutes at 3 Volts) and as a result we have filed a European Patent and will soon publish the results which we believe might set a new standard in the electrochemical exfoliation of graphite.

Our materials can be tailor-made for many different applications, but our favourite, and the one we are developing hard in our recent spinoff (EARTHIDAS), takes the form of fast-charging graphene batteries.



PUBLICATIONS

Towards flexible solid-state supercapacitors for smart and wearable electronics, Dubal D.P., Chodankar N.R., Kim D.-H., Gómez-Romero P. *Chemical Society Reviews*; **47 (6)**: 2065-2129, 2018. 10.1039/c7cs00505a. IF: 40.182

All nanocarbon Li-Ion capacitor with high energy and high power density, Dubal D.P., Gomez-Romero P. *Materials Today Energy*; **8**: 109-117, 2018. 10.1016/j.mtener.2018.03.005.

Battery and supercapacitor materials in flow cells. Electrochemical energy storage in a LiFePO₄/reduced graphene oxide aqueous nanofluid, Rueda-García D., Cabán-Huertas Z., Sánchez-Ribot S., Marchante C., Benages R., Dubal D.P., Ayyad O., Gómez-Romero P. *Electrochimica Acta*; **281**: 594-600, 2018. 10.1016/j.electacta.2018.05.151. IF: 5.116

Design and fabrication of printed paper-based hybrid micro-supercapacitor by using graphene and redox-active electrolyte, Nagar B., Dubal D.P., Pires L., Merkoçi A., Gómez-Romero P. *ChemSusChem*; **11 (11)**: 1849-1856, 2018. 10.1002/cssc.201800426. IF: 7.411

Energy harvesting from neutralization reactions with saline feedback, Lima G., Dubal D.P., Rueda-García D., Gómez-Romero P., Huguenin F. *Electrochimica Acta*; **275**: 145-154, 2018. 10.1016/j.electacta.2018.04.075. IF: 5.116

Hybrid graphene-polyoxometalates nanofluids as liquid electrodes for dual energy storage in novel flow cells, Dubal D.P., Rueda-García D., Marchante C., Benages R., Gómez-Romero P. *Chemical Record*; **18 (7)**: 1076-1084, 2018. 10.1002/tcr.201700116. IF: 4.891

Mechanisms behind the enhancement of thermal properties of graphene nanofluids, Rodríguez-Laguna M.R., Castro-Alvarez A., Sledzinska M., Maire J., Costanzo F., Ensing B., Pruneda M., Ordejón P., Sotomayor Torres C.M., Gómez-Romero P., Chávez-Ángel E. *Nanoscale*; **10 (32)**: 15402-15409, 2018. 10.1039/c8nr02762e. IF: 7.233

Synthesis and characterization of mesoporous FePO₄ as positive electrode materials for lithium batteries, Salamani A., Merrouche A., Telli L., Gómez-Romero P., Huertas Z.C. *Surface Engineering and Applied Electrochemistry*; **54 (1)**: 55-63, 2018. 10.3103/S106837551801012X

Synthesis and characterization of porous sulfur/MWCNTs composites with improved performance and safety as cathodes for Li-S batteries, Fedorkova A.S., Kazda T., Gavalierova K., Gómez-Romero P., Shembel E. *International Journal of Electrochemical Science*; **13 (1)**: 551-562, 2018. 10.20964/2018.01.67. IF: 1.369

Ultrathin hierarchical porous carbon nanosheets for high-performance supercapacitors and redox electrolyte energy storage, Jayaramulu K., Dubal D.P., Nagar B., Ranc V., Tomanec O., Petr M., Datta K.K.R., Zboril R., Gómez-Romero P., Fischer R.A. *Advanced Materials*; **30 (15)**: 1705789, 2018. 10.1002/adma.201705789. IF: 21.950

Unveiling BiVO₄ nanorods as a novel anode material for high performance lithium ion capacitors: Beyond intercalation strategies, Dubal D.P., Jayaramulu K., Zboril R., Fischer R.A., Gomez-Romero P. *Journal of Materials Chemistry A*; **6 (14)**: 6096-6106, 2018. 10.1039/c8ta00549d. IF: 9.931



PROJECTS

NaCarFLOW, Nanofluidos basados en carbonos con microestructura optimizada, funded by MAT2015-68394-R (**MINECO/FEDER, UE**), 01/01/2016 - 31/12/2018, Pedro Gómez Romero

SPS G5148, Development of New Cathodes for Stable and Safer Lithium-Sulfur Batteries, funded by **NATO_REF:SPS G5148**, 15/11/2016 - 15/11/2019, Pedro Gómez Romero

2017 SGR 870, funded by **AGAUR**, 01/01/2017 - 31/12/2020, Pedro Gómez Romero

Flexible Solid-State Supercapacitors for Portable Electronics. DP190101355, funded by **Australian ARC project participation**. 2018. IP Deepak P Dubal (The University of Adelaide, Australia) IP ICN2 Pedro Gomez-Romero

Graphene Powered Mobility (spin-off)
"Almacenamiento de energía mediante baterías de grafeno" *Graphene-based batteries for energy storage*, **R+D Contract with EARTHIDAS**, 2017-2018



TECHNOLOGY TRANSFER

Graphene and Graphitene synthesis, Pedro Gómez-Romero, Daniel Gómez-Casañ. Trade Secret. Deposited Document. CSIC, April 2015. Licenciado a la empresa Earthdas Mayo 2018.

Electrolytic cell and procedure for the preparation of Graphene by means of electrochemical exfoliation (Reactor electroquímico y procedimiento para la obtención optimizada de grafeno mediante exfoliación electroquímica de grafito), Daniel Rueda-García, Pedro Gomez-Romero, **European Patent. 18382798.9-1108**. Filed 12/11/2018



CONTRIBUTIONS

Keynote

Energy Storage. The importance of being Nano, **ICN2 Severo Ochoa International Conference**, Palau de la Música, Barcelona, 15/02/18, Pedro Gómez Romero

Hybrid electrodes and materials for hybrid energy storage, **2nd International Conference on Energy Storage Materials**, Shenzhen, China, 7-10/11/18, Pedro Gómez Romero

Invited

Graphene nanofluids. From electrochemical to thermal applications, **GrapChina 2018**, Xian, China, 19-21/9/18, Pedro Gómez Romero

Graphene nanofluids- from thermal to electrochemical applications, **ImagineNano 2018**, Bilbao, Spain, 13-15/03/18, Pedro Gómez Romero

Hybrid electrodes and materials for hybrid energy storage, **AIMES 2018**, Cancun, Mexico, 30/9/18, Pedro Gómez Romero

Hybrid materials for hybrid energy storage, **E-MRS 2018 Spring Meeting**, Strasbourg, France, 18-22/06/18, Pedro Gómez Romero

On the enhancement of the thermal conductivity of graphene-based nanofluids, **The 18th IEEE International Conference in Nanotechnology**, Cork, Ireland, 23-26/07/18, C.M. Sotomayor Torres; P. Gomez-Romero; E. Chavez-Angel

Poster

Acid-base machine with saline feedback, symposium metal oxides-based nanostructured materials for energy systems and devices, **XVII Brazilian MRS Meeting**, Natal, Brasil, September 16-20/09/18, Gilberto Lima, Fritz Huguenin, Deepak P Dubal, Daniel Rueda-García, Pedro Gómez-Romero



THESES

Carlos Marchante, *Diseño de celdas de flujo y fluidos electroactivos para almacenamiento de energía*, Universitat Autònoma de Barcelona. Master en Nanociència y Nanotecnologia, 07/18, supervised by Pedro Gómez Romero



COURSES

Pedro Gómez Romero, **Energy in transition. A case for Science**, S.O. Summer school in materials for energy. ICMA B, Bellaterra, 17/09/18

Pedro Gómez Romero, **Nanomateriales para un modelo energetico sostenible - De la Nanociencia a la Nanotecnología: luces y sombras del control de la materia a escala atómica**, Cursos de verano Universidad Internacional Menéndez Pelayo, UIMP. Santander, 23-27/07/18



DISSEMINATION CONTRIBUTIONS

Invited conference

De los nanómetros a los teravatios. Retos de los nanomateriales para la energía, **Festival 10alamos9**, Universitat de Barcelona, 13/04/18. Pedro Gómez-Romero

La (re)volución de las baterías: de conejitos que duran y duran a coches de 0 a 100 en 2,7 segundos, **3^{er} Congreso "Som Elèctrics". Congreso sobre el vehículo eléctrico**, Museu de la Ciència i la Tècnica de Terrassa, MNACTEC, Terrassa, Barcelona, 20/04/18. Pedro Gómez-Romero

Nanodiàlogos, **Festival 10alamos9**, Cosmocaixa, Barcelona, 11/04/18. Daniel Rueda

El futuro de la energía y la energía del futuro. Coloquio sobre el futuro de los recursos energéticos, **Exposició "Despres de la fi del mon" CCCB**, Barcelona, 05/04/18. Pedro Gómez-Romero

Graphene and graphene hybrids for energy storage. **Graphene Open Day. BIST, ICFO**, 16/05/18. Pedro Gómez-Romero

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

Catalán Bernabé, Gustau, ICREA Research Professor and Group Leader

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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

The highlight of this year for us was the discovery of bone flexoelectricity and the role that it plays in bone fracture repair [Vasquez-Sancho et al, *Advanced Materials*]. That work resonated with the wider public and motivated a press conference that was well attended and reported. We hope that our discovery will inspire more research on the physical properties of biomaterials and their exploitation for improved therapies. A shout out goes here to Raquel Nuñez, a postdoc now in London who worked with us on experiments with bone cells (work submitted) and to Nathalie Barroca, who is currently working on improved flexoelectric composites for actual medical applications. Stay tuned!

Flexoelectricity has also featured in much of the rest of our research, which includes the first measurement of flexoelectricity in antiferroelectrics [P. Vales et al, *Appl. Phys. Letters*; this research was also highlighted by the MRS Bulletin] and the resolution of a long-standing problem: how (and how well) can piezoelectricity imitate flexoelectricity [A. Abdollahi et al, *Physical Review Letters*].

In parallel with our flexoelectricity research, Neus Domingo has continued to lead her own research line on scanning probe microscopy and surface physics, while Amador Perez-Tomas has pushed the boundaries on photovoltaics with the invention of a new ferro-photovoltaic device that has been called the *solaristor*: a photoelectric transistor that

powers itself by visible light and that has memory [A. Perez-Tomas et al, *Adv. Func. Mat.*]. This research was also highlighted by the MRS bulletin.

This year we have bid farewell to two new doctors: Kumara Cordero-Edwards and Fabian Vasquez Sancho. May your future careers be as successful as your PhD's!



PUBLICATIONS

A solar transistor and photoferroelectric memory, Pérez-Tomás A., Lima A., Billon Q., Shirley I., Catalan G., Lira-Cantú M. *Advanced Functional Materials*; **28 (17)**: 1707099, 2018. 10.1002/adfm.201707099. IF: 13.325

Flexoelectricity in antiferroelectrics, Vales-Castro P., Roleder K., Zhao L., Li J.-F., Kajewski D., Catalan G. *Applied Physics Letters*; **113 (13)**: 132903, 2018. 10.1063/1.5044724. IF: 3.495

Flexoelectricity in bones, Vasquez-Sancho F., Abdollahi A., Damjanovic D., Catalan G. *Advanced Materials*; **30 (9)**: 1705316, 2018. 10.1002/adma.201705316. IF: 21.950

Interfacial engineering of metal oxides for highly stable halide perovskite solar cells, Mingorance A., Xie H., Kim H.-S., Wang Z., Balsells M., Morales-Melgares A., Domingo N., Kazuteru N., Tress W., Fraxedas J., Vlachopoulos N., Hagfeldt A., Lira-Cantú M. *Advanced Materials Interfaces*; **5 (22)**: 1800367, 2018. 10.1002/admi.201800367.

Local piezoelectric behavior of potassium sodium niobate prepared by a facile synthesis via water soluble precursors, Senes N., Iacomini A., Domingo N., Enzo S., Mulas G., Cuesta-Lopez S., Garroni S. *Physica Status Solidi (A) Applications and Materials Science*; **215 (16)**: 1700921, 2018. 10.1002/pssa.201700921. IF: 1.795

Piezoelectric mimicry of flexoelectricity, Abdollahi A., Vásquez-Sancho F., Catalan G. *Physical Review Letters*; **121 (20)**: 205502, 2018. 10.1103/PhysRevLett.121.205502. IF: 8.839

Substrate dependence of the freezing dynamics of supercooled water films: a high-speed optical microscope study, Pach E., Rodriguez L., Verdaguer A. *Journal of Physical Chemistry B*; **122 (2)**: 818-826, 2018. 10.1021/acs.jpcc.7b06933. IF: 3.146

Wide and ultra-wide bandgap oxides: Where paradigm-shift photovoltaics meets transparent power electronics, Pérez-Tomás A., Chikoidze E., Jennings M.R., Russell S.A.O., Teherani F.H., Bove P., Sandana E.V., Rogers D.J. *Proceedings of SPIE-The International Society for Optical Engineering*; **10533 (105331Q)** 2018. 10.1117/12.2302576.



PROJECTS

ADVISE, Electromecánica de Superficies Avanzada, funded by FIS2015-73932-JIN (**MINECO/FEDER, UE**), 01/12/2016 - 30/11/2019, Neus Domingo

PHABADA, Paredes de Dominio, interfaces y dominios de antifase en Antiferroeléctricos, funded by MAT2016-77100-C2-1-P (**MINECO/FEDER, UE**), 30/12/2016 - 30/12/2016, Gustau Catalán

2016 LLAV 00050, FLEXOFABRIC, funded by **AGAUR**, 26/07/2017 - 26/04/2018, Gustau Catalán

2017 SGR 579, funded by **AGAUR**, 01/01/2017 - 31/12/2020, Gustau Catalán



CONTRIBUTIONS

Invited

*Influence of flexoelectricity on nanomechanical properties of ferroelectrics, **Joint meeting of the European Physics Society (EPS) and the Deutsche Physikalischen Gesellschaft (DPG)**, Germany, 15/3/18. Gustau Catalán*

Flexoelectricity: from nanomechanics to bone healing, Third Seminar on the Mechanics of Multifunctional Materials, Germany, 13/06/18. Gustau Catalán

*Breaking flexoelectrics, **European MRS (E-MRS) Fall Meeting**, Warsaw, Poland, 17/09/18. Gustau Catalán*

*Breaking not-so-bad: fracture flexoelectricity, **25th International Workshop on Oxide Electronics (iWOE 25)**, Les Diablerets, Switzerland, 01/10/18. Gustau Catalán*

*Flexoelectricity: bending induced polarization, from bytes to bones, **13 Simposio en Ciencia de Materiales Avanzados y Nanotecnología (SCIMAN-2018)**, Costa Rica, 10/12/18. Gustau Catalán*

Oral

*In-situ observation of domains across the metal-insulator transition, **European MRS (E-MRS) Fall Meeting 2018**, Warsaw University of Technology, Poland, 17/09/18. Laura Rodríguez, Elena del Corro, José Santiso, Felip Sandiumenge, Gustau Catalan*



PARTICIPATED CONGRESSES

14th International Symposium on Ferroic Domains (ISFD), Barcelona, Spain, 26-28 September, 2018, Gustau Catalán and Neus Domingo, *Conference Chairs*



THESES

Kumara Cordero, *Effect of flexoelectricity on the nano-mechanical properties of ferroelectrics*, supervised by ICREA Prof. Gustau Catalán and Dr Neus Domingo

Fabián Vásquez, *Flexoelectricity in biomaterials*, supervised by ICREA Prof. Gustau Catalán



AWARDS

Laura Rodríguez Domínguez - **Graduate Student Award at the 2018 E-MRS Fall Meeting**, 17-20/09, Warsaw University of Technology, Poland

Dr. Jackeline Narváez Morales - **UAB PhD Special Prize for her thesis** defended on 29 February 2016 and entitled "Flexoelectricity in Single Crystals". 29 November, 2018, UAB, Barcelona, Spain

Phononic and Photonic Nanostructures Group

Main Research Lines

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



GROUP MEMBERS

Sotomayor Torres, Clivia M., ICREA
Research Professor and Group Leader

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Chávez Angel, Emigdio, Postdoctoral Researcher

Colombano Sosa, Martín, SO Doctoral Student

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Florez Peñaloza, Omar Enrique, PreBIST Doctoral 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 46).



Francone, Achille Leo, Postdoctoral Researcher

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Maire, Jeremie, Postdoctoral Researcher

Morales Cuñado, Cristina, Scientific Group Administrator

Navarro Urrios, Daniel, Visiting Postdoctoral Researcher

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 2018 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 (FET)
- ERC panel member
- Evaluator for the Swedish Research Council
- Member of the AENEAS Scientific Community Council

Puertas Pujades, Blanca, Visiting TFG Student

Rodríguez Laguna, María del Rocío, SO Doctoral Student

Sandell, Susanne, Visiting Doctoral Student

Singhal, Dhruv, Visiting Doctoral Student

Sledzinska, Marianna, Specialist Technician

Whitworth, Guy Luke, Postdoctoral Researcher



NEW PROJECTS & MILESTONES

During 2018, five EU 2020 projects were ongoing (**PHENOMEN** All-phononics circuits enabled by opto-mechanics, coordinated by Prof. Sotomayor; **NANOARCHITECTRONICS**, 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, CSA ICT), one Spanish National Plan project **PHENTOM** (Phonon Engineering for Advanced Thermal Management at the Nanoscale and Room Temperature optomechanics), one BIST Ignite project **NANO2DHEAT** (Nanoscale Heat Transport in 2D layered materials), one RIS3CAT Indústrias del futur project (**PLASTFUN**, Pilot plant for plastic parts with advanced functional surfaces).

We passed several milestones in our research endeavours.

Concerning the effect of local resonances and disorder on phonon trapping, their group velocity and confinement, we demonstrated the existence of phononic bandgaps in the range of 2-7 GHz arising from local resonances and Bragg scattering in lithium niobate. We also showed Anderson localisation in optomechanical crystals and that positional

disorder does not affect the lower frequencies of 2D phononic crystals. Taken together, these findings underpin future phonon manipulation for specific functions.

With respect to the thermal conductivity in the nano-scale, we investigated how the suitably designed structures, including feature sizes of 10 nm, with optimised morphology, size and order, enabled the tuning of the thermal conductivity over almost two orders of magnitude. Our studies were based on unsupported silicon membranes, silicon-germanium alloy nanowires and the 2D material MoS₂. Work in progress is looking at energy applications of these findings.

In the exploration of phonon-photon coupling we succeeded in realising a practical phonon source and unveiling a rich set of fundamentally different complex dynamics in structures moving between synchronised and chaotic regimes, of particular interest for secure communications.



PUBLICATIONS

All-optical radio-frequency modulation of Anderson-localized modes, Arregui G.,

Navarro-Urrios D., Kehagias N., Torres C.M.S., García P.D., *Physical Review B*; **98 (18)**: 180202, 2018. 10.1103/PhysRevB.98.180202. IF: 3.813

Composites of laminar nanostructured ZnO and VOx-nanotubes hybrid as visible light active photocatalysts, Benavente E., Navas D.,

Devis S., Segovia M., Sotomayor-Torres C., González G., *Catalysts*; **8 (2)**: 93, 2018. 10.3390/catal8020093. IF: 3.465

Design of a multifunctional nanoengineered PLLA surface by maximizing the synergies between biochemical and surface design bactericidal effects, Nerantzaki M., Kehagias N.,

Francone A., Fernández A., Sotomayor Torres C.M., Papi R., Choli-Papadopoulou T., Bikiaris D.N., *ACS Omega*; **3(2)**: 1509-1521. 2018. 10.1021/acsomega.7b01756

Enhancement photocatalytic activity of the heterojunction of two-dimensional hybrid semiconductors ZnO/V₂O₅, Aliaga J., Cifuentes

N., González G., Sotomayor-Torres C., Benavente E., *Catalysts*; **8 (9)**: 374, 2018. 10.3390/catal8090374. IF: 3.465

Fabrication and replication of re-entrant structures by nanoimprint lithography methods, Kehagias N., Francone A., Guttman

M., Winkler F., Fernández A., Torres C.M.S., *Journal of Vacuum Science and Technology B: Nanotechnology and Microelectronics*; **36 (6)**: 06JF01, 2018. 10.1116/1.5048241

Heterostructured layered hybrid ZnO/MoS₂ nanosheets with enhanced visible light photocatalytic activity, Benavente E., Durán F.,

Sotomayor-Torres C., González G., *Journal of Physics and Chemistry of Solids*; **113**: 119-124, 2018. 10.1016/j.jpcs.2017.10.027. IF: 2.207

Impact of the In situ rise in hydrogen partial pressure on graphene shape evolution during CVD growth of Graphene, Gebeyehu Z.M.,

Arrighi A., Costache M.V., Sotomayor-Torres C.M., Esplandiu M.J., Valenzuela S.O., *RSC Advances*; **8 (15)**: 8234-8239, 2018. 10.1039/c7ra13169k. IF: 2.936

In-line metrology for roll-to-roll UV assisted nanoimprint lithography using diffractometry, Kreuzer M., Whitworth G.L., Francone A.,

Gomis-Bresco J., Kehagias N., Sotomayor-Torres C.M., *APL Materials*; **6 (5)**: 058502, 2018. 10.1063/1.5011740. IF: 4.127

Integrated 3D hydrogel waveguide out-coupler by step-and-repeat thermal nanoimprint lithography: A promising sensor device for water and Ph, Francone A., Kehoe T.,

Obieta I., Saez-Martinez V., Bilbao L., Khokhar A.Z., Gadegaard N., Simao C.D., Kehagias N., Sotomayor Torres C.M., *Sensors (Switzerland)*; **18 (10)**: 3240, 2018. 10.3390/s18103240

Localized thinning for strain concentration in suspended germanium membranes and optical method for precise thickness measurement, Vaccaro P.O., Alonso M.I., Garriga

M., Gutiérrez J., Peró D., Wagner M.R., Reparaz J.S., Sotomayor Torres C.M., Vidal X., Carter E.A., Lay P.A., Yoshimoto M., Goñi A.R. *AIP Advances*; **8 (11)**: 115131, 2018. 10.1063/1.5050674

Mechanisms behind the enhancement of thermal properties of graphene nanofluids, Rodríguez-Laguna M.R., Castro-Alvarez A.,

Sledzinska M., Maire J., Costanzo F., Ensing B., Pruneda M., Ordejón P., Sotomayor Torres C.M., Gómez-Romero P., Chávez-Ángel E., *Nanoscale*; **10 (32)**: 15402-15409. 2018. 10.1039/c8nr02762e. IF: 7.233

Nanocrystalline silicon optomechanical cavities, Navarro-Urrios D., Capuj N.E., Maire J., Colombano M., Jaramillo-Fernandez J., Chavez-Angel E., Martin L.L., Mercadé L., Griol A., Martínez A., Sotomayor-Torres C.M., Ahopelto J., *Optics Express*; **26 (8)**: 9829-9839. 2018. 10.1364/OE.26.009829. IF: 3.356

Optical modulation of coherent phonon emission in optomechanical cavities, Maire J., Arregui G., Capuj N.E., Colombano M.F., Griol A., Martínez A., Sotomayor-Torres C.M., Navarro-Urrios D. *APL Photonics*; **3 (12)**: 126102, 2018. 10.1063/1.5040061

Raman thermometry analysis: Modelling assumptions revisited, Jaramillo-Fernandez J., Chavez-Angel E., Sotomayor-Torres C.M. *Applied Thermal Engineering*; **130**: 1175-1181. 2018. 10.1016/j.applthermaleng.2017.11.033. IF: 3.771



PROJECTS

NEREID, NanoElectronics Roadmap for Europe: Identification & Dissemination, funded by **European Union's Horizon 2020 research and innovation programme** under grant agreement No 685559, 16/11/2015 - 15/12/2018, IP: Clivia M. Sotomayor Torres

PHENOMEN, All-Phononic circuits Enabled by Opto-mechanics, funded by **European Union's Horizon 2020 research and innovation programme** under grant agreement No 713450, 01/09/2016 - 31/08/2019, coordinated by Clivia M. Sotomayor Torres

PHENTOM, Phonon engineering for advanced nanoscale thermal management and room temperature optomechanics, funded by FIS2015-70862-P (**MINECO/FEDER, UE**), 01/01/2016 - 31/12/2018, Clivia M. Sotomayor Torres

NANOARCHITECTONICS, funded by **European Union's Horizon 2020 research and innovation programme** under grant agreement No 737135, 01/01/2017 - 31/12/2018, IP: Clivia M. Sotomayor Torres

FLEXPOL, Antimicrobial FLEXible POLymers for its use in hospital environments, funded by **European Union's Horizon 2020 research and innovation programme** under grant agreement No 721062-1, 01/01/2017 - 31/12/2019, IP: Nikolaos Kehagias

D-SPA, Diamond-based nanomaterials and nanostructures for advanced electronic and photonic Applications, funded by **European Union's Horizon 2020 research and innovation programme** under grant agreement No 734578, 01/04/2017 - 31/03/2021, IP: Nikolaos Kehagias

Europa Investigación, Phonon Engineering in topological phononics for future fault-tolerant information Technology, funded by **Ministerio de Ciencia, Innovación y Universidades - Agencia Estatal de Investigación/ EUIN2017-88879**, 01/01/2017 - 31/12/2018, Clivia M. Sotomayor Torres

2017 SGR 806, funded by **AGAUR**, 01/01/2017 - 31/12/2020, Clivia M. Sotomayor Torres

2DNanoHeat, Nanoscale Heat Transport in 2D layered materials funded by **BIST**, 20/04/2018 - 19/12/2018, Klaas-Jan Tielrooij, Clivia M. Sotomayor Torres, Sergio Valenzuela

PLASTFUN, Planta Pilot de Peces Plàstiques amb Superfícies Funcionals Avançades, funded by **ACCIO**, 01/02/2018 - 31/01/2021, IP: Nikolaos Kehagias



CONTRIBUTIONS

Plenary talk

Towards all-optically driven phononic circuits, **Advanced Architectures in Photonics AAS2018**, United Kingdom, 04/09/18, Clivia Sotomayor Torres

Keynote

Nanophononics: pushing a frontier in nanoscience and nanotechnology, **IEEE Nano 2018**, Cork, Ireland, 24/07/2018, Clivia M. Sotomayor Torres

Phonon-mediated nanoscale thermal transport, **Imaginenano 2018**, Bilbao (Spain), 13-15/03/2018, Clivia M. Sotomayor Torres

Invited

Thermal energy propagation in Si membranes and phononic crystals, **Nanotech Poland 2018** Conference and Exhibition, Adam Mickiewicz University, Poznan, Poland, 8/6/18, Clivia Sotomayor Torres

Phononics: why is it important for Information Technologies?, **2018 Advanced Research Workshop on Future Trends in Microelectronics and NEREID project Meeting**, Italy, 13/06/2018, Clivia Sotomayor Torres

Thermal transport in silicon membranes and phononic crystals: implications for thermoelectrics and thermal rectification, **Edgar Lüscher Seminar 2018**, Klosters (Switzerland), 03-09/02/2018, Clivia M. Sotomayor Torres

Nanophononics: pushing a frontier in nanoscience and nanotechnology, **IEEE Nano 2018**, Cork, Ireland, 24/07/18, Clivia Sotomayor

Towards all-optically driven phononic circuits, **Advanced Architectures in Photonics AAS2018**, United Kingdom, 04/09/18, Clivia Sotomayor

Optomechanical interaction in complex dielectric media, **Piers 2018**, Toyama (Japan), 01/08/2018, David García

Photon-phonon interaction in complex dielectric media, **CEN 2018**, San Sebastián (Spain), 03/10/2018, David García

Amphiphobic nanoimprinted surfaces showing reversible contact angle modification in electrowetting, **EIPBN Conference**, Puerto Rico (USA), 29/05-01/06/2018, Nikolaos Kehagias

Combining top-down bottom-up nanomanufacturing techniques for the fabrication of dynamic and reversible, **MNE Conference**, Copenhagen (Denmark), 24-27/09/2018, Nikolaos Kehagias

Real-time diffractometry for roll-to-roll nanoimprinting quality control, **EOSAM European Optical Society Biennial Meeting**, Delft (The Netherlands), 08-12/10/2018, Nikolaos Kehagias

On the enhancement of the thermal conductivity of graphene-based nanofluids, **18th IEEE**

International conference on nanotechnology, Cork (Ireland), 23-26/07/2018, Emigdio Chávez

Thermal and acoustic properties of nanostructures, **XVII International Materials Research Congress**, Cancun (Mexico), 19-24/08/2018, Emigdio Chávez

Oral

Phonons in nanocrystalline Si: a thermal, structural and optomechanical study, **IEEE Eurotherm 111, Nanoscale and Microscale Heat Transfer VI**, Levi, Finland, 02-07/12/2018, Clivia M. Sotomayor Torres

Coupled phonons, photons and RF read-out for phononic circuits, **IEEE Ultrasonics International Conference 2018**, Kobe, Japan, 25/10/2018, Clivia M. Sotomayor Torres

Self-assembled SiO₂ microspheres for broadband radiative cooling, **EMN Meeting on Structure and Dynamics of Nanoscale Solids**, Berlin (Germany), 15-20/07/2018, J. Jaramillo-Fernández

Self-assembled opal-based structures for broadband radiative cooling, **EMRS Fall Meeting**, Warsaw (Poland), 09/2018, J. Jaramillo-Fernández

Poster

Thermal conductivity of MoS₂ membranes, **34th Int. Conf. Physics Semiconductors**, Montpellier, France, 31/07/18, Clivia Sotomayor



PARTICIPATED CONGRESSES

Eurotherm 108-Nanoscale and Microscale Heat Transfer VI, Levi, Finland, 3-7 December 2018, **Scientific Committee**, Clivia M Sotomayor Torres

34th Int. Conference on the Physics of Semiconductors, Montpellier, 29 July - 3 August 2018, **International Advisory Program Committee**, Clivia M Sotomayor Torres



THESES

Arindom Chatterjee, *Thermoelectric performance of layered cobaltate epitaxial films deposited by pulsed laser evaporation*, supervised by ICREA Prof. Clivia M. Sotomayor Torres and CSIC Researcher Jose Santiso



AWARDS

ICREA Prof. Clivia M. Sotomayor Torres appointed **new board member of the Danish National Research Foundation**



DISSEMINATION CONTRIBUTIONS

Invited conference

Manifestacions de l'energia i el seu ús per a un futur verd, Cicle Dilluns de Ciència, Residència d'Investigadors CSIC Barcelona, 05/11/18.

Emigdio Chávez

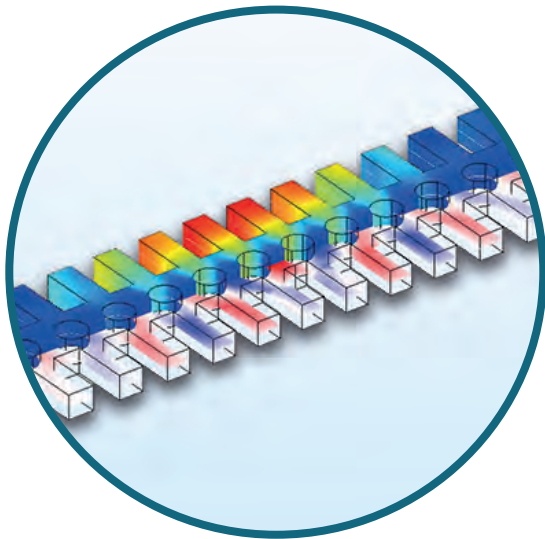
Girls Science & tech Sabadell, Nano Workshop, Biblioteca Vapor Badia, Sabadell, Barcelona, 17/11/18. Juliana Jaramillo

You Tube video of the EU H2020 FET Open project PHENOMEN, EU ICT event, 04/12/2018, Vienna. [youtube.com/watch?v=uFvb_QhBv0I](https://www.youtube.com/watch?v=uFvb_QhBv0I)

Invited seminar

Thermal energy propagation in Si membranes and phononic crystals, Physics Dept. seminar, Exeter University, UK, 12/10/2018, Clivia M. Sotomayor Torres.

Nanoscale heat transfer in Si membranes and phononic crystals, University of Wuppertal, Wuppertal, Germany, 15 October 2018, Clivia M. Sotomayor Torres



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 he 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 60 articles (*Nature*, *Science*, *Reviews of Modern Physics*, *Nature Materials*, *Nature Physics*, *Nature Nanotechnology*, *Physical Review Letters*, among others), four patents, and five books or book chapters.



GROUP MEMBERS

Valenzuela, Sergio Osvaldo, ICREA
Research Professor and Group Leader

Arrighi, Aloïs Jean Guillaume, SO Doctoral
Student

Barrera Català, Aleix, Visiting Degree Student

Batlle Porro, Sergi, Visiting TFG Student

Benítez Moreno, Luís Antonio, Doctoral
Student

Bonell, Frédéric, Postdoctoral Researcher

Costache, Marius Vasile, Senior Researcher

Fernández Aguirre, Iván, Doctoral Student

Figuroa García, Adriana Isabel,
Postdoctoral Researcher

Forn Díaz, Pol, Visiting PostDoctoral
Researcher

Galceran Vercher, Regina, Postdoctoral
Researcher

Gebeyehu, Zewdu Messele, Doctoral
Student

López Muñoz, David, Visiting Doctoral
Student

Savero Torres, Williams Fernando,
Postdoctoral Researcher

Sierra García, Juan Francisco, Postdoctoral
Researcher

Svetlík, Josef, Fellowship Master Student

Timmermans, Matias, Postdoctoral
Researcher

Warren, Christopher, Visiting Technician



NEW PROJECTS & MILESTONES

In 2018 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. The group has continued to make progress 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 conversion 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. A collaboration is also established with researchers at the Barcelona Supercomputing Center on quantum computation regarding to quantum annealing.

The group also carried out research on hybrid magnon-phonon-photon systems.

Regarding new funding the group has been awarded a FET-PROACTIVE project on Topological Matter that will be coordinated by ICREA Prof. S. O. Valenzuela, and a project by KAUST on 2D materials, both scheduled to start during 2019.



PUBLICATIONS

A barrier to spin filters, Sergio O. Valenzuela, Stephan Roche, *Nature Electronics*; **1(6)**: 328-329. 2018. 10.1038/s41928-018-0089-x.

Bottom-up synthesis of multifunctional nanoporous graphene, Moreno C., Vilas-Varela M., Kretz B., Garcia-Lekue A., Costache M.V., Paradinas M., Panighel M., Ceballos G., Valenzuela S.O., Peña D., Mugarza A. *Science*; **360 (6385)**: 199-203. 2018. 10.1126/science.aar2009. IF: 41.058

Impact of the: In situ rise in hydrogen partial pressure on graphene shape evolution during CVD growth of graphene, Gebeyehu Z.M., Arrighi A., Costache M.V., Sotomayor-Torres C.M., Esplandiú M.J., Valenzuela S.O. *RSC Advances*; **8 (15)**: 8234-8239. 2018. 10.1039/c7ra13169k. IF: 2.936

Strongly anisotropic spin relaxation in graphene-transition metal dichalcogenide heterostructures at room temperature, Benítez L.A., Sierra J.F., Savero Torres W., Arrighi A., Bonell F., Costache M.V., Valenzuela S.O. *Nature Physics*; **14 (3)**: 303-308. 2018. 10.1038/s41567-017-0019-2. IF: 22.727

Thermoelectric spin voltage in graphene, Sierra J.F., Neumann I., Cuppens J., Raes B., Costache M.V., Valenzuela S.O. *Nature Nanotechnology*; **13 (2)**: 107-111. 2018. 10.1038/s41565-017-0015-9. IF: 37.490



PROJECTS

SpinBound, Exploring the spin physics at the boundaries of materials with strong spin orbit interaction, funded by **European Union's Horizon 2020 research and innovation programme** under grant agreement N° 306652, 01/02/2013-31/01/2018, Sergio Valenzuela

2DMD, Heteroestructuras Basadas en Materiales Bidimensionales para Dispositivos de Electrónica Avanzada, funded by MAT2016-75952-R (**MINECO/FEDER, UE**), 30/12/2016-29/12/2019, Sergio Valenzuela

Red Española de Espintrónica, funded by **Ministerio de Ciencia, Innovación y Universidades - Agencia Estatal de Investigación/MAT2017-90771-REDT**, 01/07/2018-30/06/2020, Sergio Valenzuela

2017 SGR 827, funded by **AGAUR**, 01/01/2017-31/12/2020, Sergio Valenzuela

EEBB-I-18-13041, Estancia en Pennsylvania State University 4 meses funded by EEBB-I-18-13041 (**MINECO**), 01/06/2018-31/12/2018, IP: Zewdu Messele Gebeyehu

GRAPHENE CORE 2, Graphene Flagship Core Project 2, funded by **European Union's Horizon 2020 research and innovation programme** under grant agreement N° 785219, 01/04/2018-31/03/2020, IP: Stephan Roche, José A. Garrido, Arben Merkoçi, Sergio O. Valenzuela

GRAPHENE CORE 1, Graphene-based disruptive technologies, funded by **European Union's Horizon 2020 research and innovation programme** under grant agreement No 696656, 01/04/2016-31/03/2018, IP: Stephan Roche, José A. Garrido, Sergio O. Valenzuela

2DNanoHeat, Nanoscale Heat Transport in 2D layered materials funded by **BIST**, 20/04/2018 - 19/12/2018, Klaas-Jan Tielrooij, Clivia M. Sotomayor Torres, Sergio Valenzuela



CONTRIBUTIONS

Invited (selection)

Insights into topological insulator thin films using synchrotron radiation techniques, **X GEFES (Division de Física de la Materia Condensada de la Real Sociedad Española de Física)**, Valencia, Spain, 24-26/01/18, A. I. Figueroa

Experimental graphene spintronics, Kick-off meeting SP2: Spanish Network for 2D Materials, Madrid, Spain, 04/18, Juan F. Sierra

NanoEngineering Flagship, Paris, France, 01/06/18, Sergio Valenzuela

Spin transport in Graphene, Comarruga, Tarragona, Spain, 04/06/18, Sergio Valenzuela

Spin and hot electron transport in graphene based devices, **Nano2018**, Hong-Kong, China, 26/06/18, Sergio Valenzuela

Current challenges in experimental graphene spintronics, **2nd ELECFI International Workshop**, Zaragoza, Spain, 06/18, Juan F. Sierra

Proximity effects in Graphene, San Sebastian, Spain, 16/07/18, Sergio Valenzuela

Spin and hot electron transport in graphene, Buenos Aires, Argentina, 20/09/18, Sergio Valenzuela

Spintronics in 2D materials, **ESONN School**, Cargese, France, 14/09/18, Sergio Valenzuela

Spin orbit torques in topological insulators, Buenos Aires, Argentina, 21/09/18, Sergio Valenzuela

Magnon-heat interaction in magnetic nanostructures, **Magnetodynamics workshop 2018**, Kista- Stockholm, Sweden, 04/10/18, M.V. Costache

Spin and hot carrier transport in graphene,
Condensed Matter Physics Center (IfiMAC) seminar series, Madrid, Spain, 29/11/18, Juan F. Sierra

Oral (selection)

Strongly anisotropic spin relaxation in graphene-transition metal dichalcogenide heterostructures at room temperature, **Graphene 2018**, Dresden, Germany, 26-29/06/18, L. Antonio Benítez, Juan F. Sierra, Williams Savero Torres, Aloïs Arrighi, Frederic Bonell, Marius V. Costache and Sergio O. Valenzuela

Metal-organic topological insulator heterostructure with robust interfacial properties, **Fuerzas y Tunel 2018**, Jaca, Spain, 27-29/06/19, Marc González Cuxart

Thermoelectric spin voltage in graphene, **Graphene Conference 2018**, Dresden, Germany, 06/18, Juan F. Sierra, I Neumann, J Cuppens, B Raes, M. V Costache, S. O Valenzuela

Insights into magnetic proximity effects at topological insulators/magnetic insulator interfaces using x-ray magnetic circular dichroism, **JEMS 2018 - The Joint European Magnetic Symposia**, Mainz, Germany, 03-07/09/18. A. I. Figueroa, F. Bonell, M. G. Cuxart, M. Valvidares, A. Mugarza, and S. O. Valenzuela

Spin-orbit torque-ferromagnetic resonance with topological insulators, **JEMS 2018 - The Joint European Magnetic Symposia**, Mainz, Germany, 03-07/09/18, F. Bonell, M. Goto, S. Miwa, J.F. Sierra, M.V. Costache, Y. Suzuki, S.O. Valenzuela

Strongly anisotropic spin relaxation in graphene-transition metal dichalcogenide heterostructures at room temperature, **JEMS 2018 - The Joint European Magnetic Symposia**, Mainz, Germany, 03-07/09/18, L. Antonio Benítez, Juan F. Sierra, Williams Savero Torres, Aloïs Arrighi, Frederic Bonell, Marius V. Costache and Sergio O. Valenzuela

Spin precession and spin Hall effect in monolayer graphene/Pt nanostructures, **JEMS 2018 - The Joint European Magnetic Symposia**, Mainz, Germany, 03-07/09/18, W. Savero Torres, J.F. Sierra, L. A. Benitez, F. Bonell, M.V. Costache & S.O. Valenzuela

Thermoelectric spin voltage in graphene, **JEMS 2018 - The Joint European Magnetic Symposia**, Mainz, Germany, 03-07/09/18, Juan F. Sierra, I. Neumann, J. Cuppens, B. Raes, M. V. Costache, S. O. Valenzuela

Poster

Metal-organic topological insulator heterostructure with robust interfacial properties, **Novel 2D materials explored via scanning probe microscopy & spectroscopy**, Donostia, Spain, 25-29/06/18, Cuxart, Marc G., Valbuena, Miguel A., Moreno, César, Bonell, Frédéric, Robles, Roberto, Cruz, Jorge, Imaz, Inhar, Nistor, Corneliu, Gargiani, Pierluigi, Ordejon, Pablo, Gambardella, Pietro, Valenzuela, Sergio O., Mugarza, Aitor

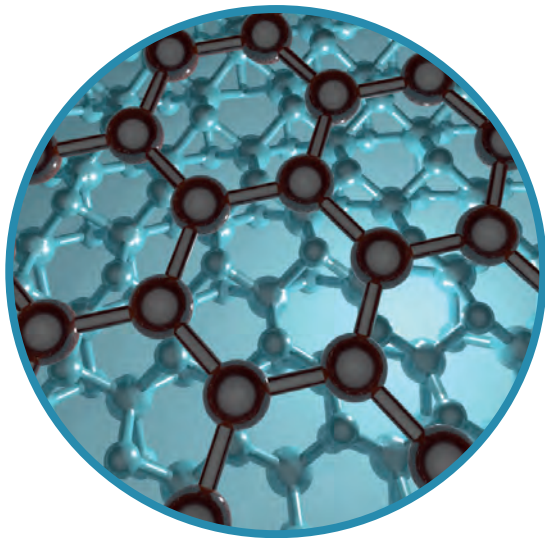


EDITORIAL CONTRIBUTIONS

Juan Sierra, **editorial board member**, *Journal of Physics: Materials* (IOP Science Group)

Juan Sierra, **guest editor**, *Special Issue "Topological Matter"*, *Journal of Physics: Materials*

F. Casoli, MV Costache and M. Miron, **guest editor**, *focus issue on "Spin-Dependent Phenomena In New Materials: From 2D Materials To Topological Insulators And Beyond"* for *JPhys Materials*.



DISSEMINATION AND EVENT ORGANIZATION

Nano Workshop, Girls Science & tech Sabadell Biblioteca Vapor Badia, Sabadell, Barcelona, 17/11/18, Round table moderator of the Celebrating Women in Science, Adriana Figueroa, Regina Galcerán

Celebrating Women in Science, ICN2, Bellaterra, Barcelona, Spain, 13/02/18, A. I. Figueroa

Entrevistes a joves nanotecnòlegs: La nanotecnologia mola, NanoEduca closure event, Barcelona, Spain, 09/05/18, A. I. Figueroa

Què és la nanoescala i com ens afecta?, **Science & Tech Girls Vallès**, Sabadell, Barcelona, Spain, 17/11/18, A. I. Figueroa, J. Jaramillo and R.

Magnetism and spin transport in topological materials, JEMS 2018 - The Joint European Magnetic Symposia, Mainz, Germany, 03-07/09/18, L. Vila and M.V. Costache. Sergio O. Valenzuela as *member of the program committee*

JEMS 2018 - The Joint European Magnetic Symposia, Mainz, Germany, 03-07/09/18,

The BIST PostDoc Day #2, an event organized by postdocs that seeks to foster interaction and create new collaborations among **BIST institutes** (200 participants anticipate), Barcelona, Spain, 22/10/18, MV Costache

Commercialising spintronic devices which exploit graphene and related materials, Interview to Prof. Stephan Roche and Dr. Regina Galceran in *SciTechEuropa*, 28/10/18, **Graphene Flagship** article page 82-85

Intro to the nanoscience talk, St. Peter School students, ICN2, 23/02/18, Marc Gonzalez Cuxart

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

Maspoch Comamala, Daniel, ICREA Research Professor and Group Leader

Albalad Alcalá, Jorge, Doctoral Student

Çamur, Ceren, Doctoral Student

Avcı, Civan, Doctoral Student

Bermejo Gijón-Bonales, Natalia, Visiting TFG Student

Boix i Soler, Gerard, Doctoral Student

Broto Ribas, Anna, Research Assistant

Cano Sarabia, Antonia, Senior Researcher

Carné Sánchez, Arnau, Postdoctoral Researcher

Fernández De Retana Alda, Sofia, Visiting Doctoral Student

García Jimeno, Sonia, Postdoctoral Researcher

Garzón Tovar, Luís Carlos, Doctoral Student

Ghasempour, Hossein, Fellowship Doctoral Student

Grancha Marco, Thais María, Postdoctoral Researcher

Guillerm, Vincent, Postdoctoral Researcher

Imaz, 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 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.



Liu, Yang, Fellowship Doctoral Student

Mendoza Valentí, Paula, Visiting TFG Student

Navalón López, María, Visiting TFG Student

Ortín Rubio, Borja, Research Assistant

Pérez Carvajal, Javier, Postdoctoral Researcher

Puga Aranda, Rosa, Scientific Group Administrator

Rodríguez Muguruza, Asier, Visiting Master Student

Rodríguez Vidal, Silvia, Visiting Senior Researcher

Ruiz García, Marta, Visiting Doctoral Student

Ruiz Martínez, Cristina, Visiting Master Student

Sanmartí Espinal, Marta, Technician

Suárez del Pino, José Antonio, Technician

Troyano Prieto, Javier, Postdoctoral Researcher

Xu, Heng, Doctoral Student

Yang, Yunhui, Fellowship Doctoral Student

Yazdi, Amirali, SO Doctoral Student

Zarekarizi, Farnoosh, Fellowship Doctoral Student

In 2014 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 124 papers and six 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 16 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 2018 two important projects of the ICN2 Supramolecular NanoChemistry and Materials Group or “NANOUP” has come to an end. On one hand, the MOFCAS project to develop multifunctional composites based on MOFs as advanced sorbents for biomedical and energy-related applications. Led by Prof. Maspoch, this three-year project began in 2016, supported by the Spanish Ministry of Economy, Industry and Competitiveness under its National Programme for Research Aimed at the Challenges of Society. On the other hand, the European H2020 project ProDIA has also finished. As part of this project, the group has scaling-up the production of nanoporous materials for use in industrial adsorption processes via spray drying technique. The group has also continued working on the ERC Consolidator Grant project, InanoMOF, achieving the development of several functional nanoMOF@INP composites. This year, has started the new project H2020 GENESIS, a European project that aims developing and upscaling the most promising membrane materials for CO₂ capture and demonstrate their performance, durability and reliability in industrial environments.

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

A CO₂ optical sensor based on self-assembled metal-organic framework nanoparticles,

Chocarro-Ruiz B., Pérez-Carvajal J., Avci C., Calvo-Lozano O., Alonso M.I., Maspoch D., Lechuga L.M. *Journal of Materials Chemistry A*; **6 (27)**: 13171-13177. 2018. 10.1039/c8ta02767f. IF: 9.931

A self-folding polymer film based on swelling metal-organic frameworks,

Troyano J., Carné-Sánchez A., Pérez-Carvajal J., León-Reina L., Imaz I., Cabeza A., Maspoch D. *Angewandte Chemie-International Edition*; **57(47)**: 15420-15424. 2018. 10.1002/anie.201808433. IF: 12.102

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Avci-Camur C., Troyano J., Pérez-Carvajal J., Legrand A., Farrusseng D., Imaz I., Maspoch D. *Green Chemistry*; **20 (4)**: 873-878. 2018. 10.1039/c7gc03132g. IF: 8.586

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Qian W., González-Campo A., Pérez-Rodríguez A., Rodríguez-Hermida S., Imaz I., Wurst K., Maspoch D., Ruiz E., Ocal C., Barrera E., Amabilino D.B., Aliaga-Alcalde N. *Chemistry-A European Journal*; **24 (49)**: 12950-12960. 2018. 10.1002/chem.201802031. IF: 5.160

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Avci-Camur C., Perez-Carvajal J., Imaz I., Maspoch D. *ACS Sustainable Chemistry and Engineering*; **6 (11)**: 14554-14560. 2018. 10.1021/acssuschemeng.8b03180. IF 6.140

Phosphatidylserine-liposomes promote tolerogenic features on dendritic cells in human type 1 diabetes by apoptotic mimicry, Rodriguez-Fernandez S., Pujol-Autonell I., Brianso F., Perna-Barrull D., Cano-Sarabia M., Garcia-Jimeno S., Villalba A., Sanchez A., Aguilera E., Vazquez F., Verdaguer J., MasPOCH D., Vives-Pi M. *Frontiers in Immunology*; **9**: 253, 2018. 10.3389/fimmu.2018.00253. IF: 5.511

Photothermal activation of metal-organic frameworks using a uv-vis light source, Espín J., Garzón-Tovar L., Carné-Sánchez A., Imaz I., MasPOCH D. *ACS Applied Materials and Interfaces*; **10 (11)**: 9555-9562, 2018. 10.1021/acsami.8b00557. IF: 8.097

Postsynthetic selective ligand cleavage by solid-gas phase ozonolysis fuses micropores into mesopores in metal-organic frameworks, Guillerm V., Xu H., Albalad J., Imaz I., MasPOCH D. *Journal of the American Chemical Society*; **140 (44)**: 15022-15030, 2018. 10.1021/jacs.8b09682. IF: 14.357

Purification of Uranium-based endohedral metallofullerenes (EMFs) by selective supramolecular encapsulation and release, Fuertes-Espinosa C., Gómez-Torres A., Morales-Martínez R., Rodríguez-Fortea A., García-Simón C., Gándara F., Imaz I., Juanhuix J., MasPOCH D., Poblet J.M., Echegoyen L., Ribas X. *Angewandte Chemie-International Edition*; **57 (35)**: 11294-11299, 2018. 10.1002/anie.201806140. IF: 12.102

Reversible thermochromic polymeric thin films made of ultrathin 2D crystals of coordination polymers based on Copper(I)-Thiophenolates, Troyano J., Castillo O., Martínez J.I., Fernández-Moreira V., Ballesteros Y., MasPOCH D., Zamora F., Delgado S. *Advanced Functional Materials*; **28 (5)**: 1704040, 2018. 10.1002/adfm.201704040. IF: 13.325

Self-assembly of polyhedral metal-organic framework particles into three-dimensional ordered superstructures, Avci C., Imaz I., Carné-Sánchez A., Pariente J.A., Tasios N., Pérez-Carvajal J., Alonso M.I., Blanco A., Dijkstra M., López C., MasPOCH D. *Nature Chemistry*; **10 (1)**: 78-84, 2018. 10.1038/NCHEM.2875. IF: 26.201

Sequential deconstruction-reconstruction of metal-organic frameworks: an alternative strategy for synthesizing (multi)-layered ZIF composites, Avci C., Yazdi A., Tarrés M., Bernoud E., Bastús N.G., Puentes V., Imaz I., Ribas X., MasPOCH D. *ACS Applied Materials and Interfaces*; **10 (28)**: 23952-23960, 2018. 10.1021/acsami.8b05098. IF: 8.097

Single-crystal-to-single-crystal postsynthetic modification of a metal-organic framework via ozonolysis, Albalad J., Xu H., Gándara F., Haouas M., Martineau-Corcós C., Mas-Ballesté R., Barnett S.A., Juanhuix J., Imaz I., MasPOCH D. *Journal of the American Chemical Society*; **140 (6)**: 2028-2031, 2018. 10.1021/jacs.7b12913. IF: 14.357

Squaramide-IRMOF-16 analogue for catalysis of solvent-free, epoxide ring-opening tandem and multicomponent reactions, Vignatti C., Luis-Barrera J., Guillerm V., Imaz I., Mas-Ballesté R., Alemán J., MasPOCH D. *ChemCatChem*; **10 (18)**: 3995-3998, 2018. 10.1002/cctc.201801127. IF: 4.674

The photothermal effect in MOFs: Covalent post-synthetic modification of MOFs mediated by UV-Vis light under solvent-free conditions, Espín J., Garzón-Tovar L., Boix G., Imaz I., MasPOCH D. *Chemical Communications*; **54 (33)**: 4184-4187, 2018. 10.1039/c8cc01593g. IF: 6.290

Zigzag ligands for transversal design in reticular chemistry: unveiling new structural opportunities for metal-organic frameworks, Guillerm V., Grancha T., Imaz I., Juanhuix J., MasPOCH D. *Journal of the American Chemical Society*; **140 (32)**: 10153-10157, 2018. 10.1021/jacs.8b07050. IF: 14.357



BOOKS

P. Cortés, M. Cano-Sarabia, J. Colom, J. Otero, D. Maspoch, M. Llagostera. **Nano/Micro Formulations for Bacteriophage Delivery**. *Springer Book in Phage Therapy 2018*, Springer.



PROJECTS

InanoMOF, Multifunctional micro- and nanostructures assembled from nanoscale metal-organic frameworks and inorganic nanoparticles, funded by **European Union's Horizon 2020 research and innovation programme** under grant agreement No 615954, 01/04/2014 - 31/03/2019, Daniel Maspoch

ProDIA, Production, control and Demonstration of structured hybrid nanoporous materials for Industrial adsorption Applications, funded by **European Union's Horizon 2020 research and innovation programme** under grant agreement No 685727, 01/11/2015 - 31/10/2018, IP: Daniel Maspoch

MOFCAS, Composites multifuncionales basados en redes metalorgánicas (MOFs) como sorbentes avanzados para aplicaciones biomédicas y energéticas, funded by MAT2015-65354-C2-1-R (**MINECO/FEDER, UE**), 01/01/2016 - 31/12/2018, Daniel Maspoch, Inhar Imaz

GENESIS, High performance MOF and IPOSS enhanced membrane systems as next generation CO2 capture technologies, funded by **European Union's Horizon 2020 research and innovation programme** under grant agreement No 760899-2, 01/01/2018 - 31/12/2021, IP: Daniel Maspoch

2017 SGR 328, funded by **AGAUR**, 01/01/2017 - 31/12/2020, Daniel Maspoch



CONTRIBUTIONS

Invited

Phosphatidylserine-liposomes promote tolerogenic features on dendritic cells in human type 1 diabetes by apoptotic mimicry, **XXIX Congreso de la Sociedad Española de Diabetes**, Oviedo, Spain, 18/04/18, Daniel Maspoch

Self-assembly of polyhedral metal-organic framework particles into three-dimensional ordered superstructures, **docMOF 2018: 1st European Doctoral Symposium on Metal-Organic Frameworks**, Germany, 30/04/18, Daniel Maspoch

Ozonolysis as a solid-gas post-synthetic tuning of porosity in Metal-Organic Frameworks, **IREC Barcelona**, Spain, 12/06/18, Daniel Maspoch

Controlling the interaction between magnetic molecules and topological surface states via ligand chemistry, **Fuerzas y Túnel 2018 Conference**, Spain, 27/06/18, Daniel Maspoch

MOFs and MOF-based composites generated by Spray-Drying, **43rd International Conference on Coordination Chemistry ICC2018**, Sendai, Japan, 28/07/18, Daniel Maspoch

Mesoscale Assembly of MOF particles into three-dimensional ordered superstructures, **43rd International Conference on Coordination Chemistry ICC2018**, Sendai, Japan, 28/07/18, Daniel Maspoch

Composite salt in porous metal-organic frameworks for adsorption heat transformation, **1st European symposium of sorption science**, Austria, 05/09/18, Daniel Maspoch

Synthesis of MOFs and MOF-based nanocomposites using spray-drying, **e-MRS fall Meeting**, Poland, 17/09/18, Daniel Maspoch

Controlling the interaction between magnetic molecules and topological surface states via ligand chemistry, **10th Microencapsulation Training School**, Norway, 18/09/18, Daniel Maspoch

Ozonolysis in Metal-Organic Frameworks: post-synthetic modification and mesopore creation by clip-off chemistry, **Novel Porous Materials Symposium**, Australia, 07/12/18, Daniel Maspoch

A brief history of the spray-drying synthesis of MOFs and MOF-based composites: from the lab to scale-up production, **6th international conference on Metal-Organic Frameworks and open frameworks compounds**, New Zealand, 12/12/18, Daniel Maspoch

Transferring the breathing behaviour of flexible MOF crystals to macroscopic soft materials, **6th international conference on Metal-Organic Frameworks and open frameworks compounds**, New Zealand, 12/12/18, Daniel Maspoch

Ozonolysis in Metal-Organic Frameworks: post-synthetic modification and mesopore creation by clip-off chemistry, **6th international conference on Metal-Organic Frameworks and open frameworks compounds**, New Zealand, 12/12/18, Daniel Maspoch



PARTICIPATED CONGRESSES

ICCC2018, Symposium 22. *MOFs as Scaffolds for Nanomaterials Synthesis and Encapsulation*, Sendai (Japan), 28/07-04/08/18



THESES

Luis Carlos Garzón, *Confining reactions in a droplet: synthesis of MOFs, COFs and Composites using spray drying*, 19/07/18, supervised by ICREA Prof. Daniel Maspoch and Dr Inhar Imaz

Jordi Espin, *The photothermal effect in MOFs*, 26/10/18, supervised by ICREA Prof. Daniel Maspoch and Dr Inhar Imaz

Amirali Yazdi, *Nanoengineering composites made of metal- and covalent-organic frameworks and inorganic nanoparticles using encapsulation techniques*, 30/11/18, supervised by ICREA Prof. Daniel Maspoch, Dr Inhar Imaz and ICREA Prof. Victor F. Puntes

Civan Avci, *Zeolitic Imidazolate Framework-8: Control of particle size, and shape and its self-assembly*, 19/12/18, supervised by ICREA Prof. Daniel Maspoch and Dr Inhar Imaz



AWARDS

Civan Avci - **Best Oral Presentation Award** - 1st European Doctoral Symposium on Metal-Organic Frameworks (docMOF 2018), 29/4/18 - 2/5/18, Raitenhaslach, Germany

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' 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 200 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 the Habilitation to supervise PhD students from the Université Joseph Fourier (Grenoble, France) in 2004, since which time he has supervised more than ten PhD students and about 25 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, since 2011 he has been actively involved in the European Graphene Flagship project as deputy leader of the spintronics work Package, and will become the WP leader from April 2020 .



GROUP MEMBERS

Roche, Stephan, ICREA Research Professor and Group Leader

Antidormi, Alejandro, Senior Postdoctoral Researcher

Cummings, Aron William, Senior Researcher

De Moraes Araujo, Bruna Gabrielly, Doctoral Student

García Aguilar, Jose Hugo, Postdoctoral Researcher

Pezo López, Armando Arquímedes, Fellowship Doctoral Student

Power, Stephen, Postdoctoral Researcher

Song, Kenan, SO Doctoral Student

Vila Tusell, Marc, Doctoral Student



NEW PROJECTS & MILESTONES

In 2018 the group published the following four publications of note:

Ballistic tracks in graphene nanoribbons

In collaboration with an experimental group in Germany (Technische Universität Chemnitz), and the Danish Graphene Center from DTU we have theoretically analyzed unprecedented results obtained and asymmetric terminations at opposite ribbon edges due to the underlying SiC structure morphology. Our findings demonstrate a precise control of transport through multiple, independent, ballistic tracks in graphene-based devices, opening intriguing pathways for quantum information device concepts.

Origin of nonlocal resistance in multiterminal graphene on hexagonal-boron-nitride: Fermi surface edge currents rather than Fermi sea topological valley currents

Combining ab initio with quantum transport calculations, we have demonstrated that G/hBN wires with zigzag edges host low-energy dispersive edge states that are absent in theories based on the simplistic Hamiltonian, and are strongly resilient to disorder effects. Such edge states resolve the long-standing puzzle of why the highly insulating state of G/hBN is rarely observed and allow to conclude that intriguing non local resistance signals obtained in experiments are unrelated to Fermi sea topological valley currents conjectured for gapped Dirac spectra, as wrongly proposed by some theory.

Tailoring emergent spin phenomena in Dirac material heterostructures

Together with an experimental group in Chalmers University of Technology, We have investigated the spin transport properties of heterostructures combining graphene with

topological insulators (TIs) in van der Waals heterostructures, and have demonstrated the emergence of a strong proximity-induced spin-orbit coupling in graphene. By performing spin transport and precession measurements supported by ab initio simulations, we discover a strong tunability and suppression of the spin signal and spin lifetime due to the hybridization of graphene and TI electronic bands. The enhanced spin-orbit coupling strength is estimated to be nearly an order of magnitude higher than in pristine graphene. These findings in graphene-TI heterostructures could open interesting opportunities for exploring exotic physical phenomena and new device functionalities governed by topological proximity effects.

Spin Proximity Effects in Graphene/Topological Insulator Heterostructures

Enhancing the spin-orbit interaction in graphene, via proximity effects with topological insulators, could create a novel 2D system that combines nontrivial spin textures with high electron mobility. To engineer practical spintronics applications with such graphene/topological insulator (Gr/TI) heterostructures, an understanding of the hybrid spin-dependent properties is essential. However, to date, despite the large number of experimental studies on Gr/TI heterostructures reporting a great variety of remarkable (spin) transport phenomena, little is known about the true nature of the spin texture of the interface states as well as their role on the measured properties. By using ab initio simulations and tight-binding models, we have determined the precise spin texture of electronic states in graphene interfaced with a Bi₂Se₃ topological insulator. Our calculations predict the emergence of a giant spin lifetime anisotropy in the graphene layer, which should be a measurable hallmark of spin transport in Gr/TI heterostructures and suggest novel types of spin devices.



PUBLICATIONS

1D ferromagnetic edge contacts to 2D

graphene/h-BN heterostructures, Karpiak B., Dankert A., Cummings A.W., Power S.R., Roche S., Dash S.P. *2D Materials*; **5 (1)**: 014001, 2018. 10.1088/2053-1583/aa8d2b. IF: 7.042

A barrier to spin filters, Sergio O. Valenzuela, Stephan Roche, *Nature Electronics*; **1(6)**: 328-329. 2018. 10.1038/s41928-018-0089-x

Ballistic tracks in graphene nanoribbons, Aprojanz J., Power S.R., Bampoulis P., Roche S., Jauho A.-P., Zandvliet H.J.W., Zakharov A.A., Tegenkamp C. *Nature Communications*; **9 (1)**: 4426 2018. 10.1038/s41467-018-06940-5. IF: 12.353

Charge and spin transport anisotropy in nanopatterned Graphene, Gregersen S.S. Garcia J.H., Jauho A.P., Roche S. and Power S.R., *Journal of Physics: Materials*; **1(1)**: 015005. 2018

Conductance quantization suppression in the quantum Hall regime, Caridad J.M., Power S.R., Lotz M.R., Shylau A.A., Thomsen J.D., Gammelgaard L., Booth T.J., Jauho A.-P., Bøggild P. *Nature Communications*; **9(1)**: 659, 2018. 10.1038/s41467-018-03064-8. IF: 12.353

Effect of the channel length on the transport characteristics of transistors based on boron-doped graphene ribbons, Marconcini P., Cresti A., Roche S. *Materials*; **11 (5)**: 667, 2018. 10.3390/ma11050667. IF: 2.467

Finite-size correction scheme for supercell calculations in Dirac-point two-dimensional materials, Rocha C.G., Rocha A.R., Venezuela P., Garcia J.H., Ferreira M.S. *Scientific Reports*; **8 (1)**: 9348, 2018. 10.1038/s41598-018-27632-6. IF: 4.122

Large spin relaxation anisotropy and valley-Zeeman spin-orbit coupling in WSe₂ / graphene/ h -BN heterostructures, Zihlmann S., Cummings A.W., Garcia J.H., Kedves M., Watanabe K., Taniguchi T., Schönenberger C., Makk P. *Physical Review B*; **97 (7)**: 075434, 2018. 10.1103/PhysRevB.97.075434. IF: 3.813

Origin of nonlocal resistance in multiterminal graphene on hexagonal-boron-nitride: Fermi surface edge currents rather than Fermi sea topological valley currents, J. M. Marmolejo-Tejada, J. H. García, M. Petrović, P.-H. Chang, X.-L. Sheng, A. Cresti, P. Plecháč, S. Roche, B. K. Nikolic. *Journal of Physics: Materials*; **1**, 015006. 2018. 10.1088/2515-7639/aad585. IF: 0

Proximity-induced spin-orbit coupling in graphene/Bi_{1.5}Sb_{0.5}Te_{1.7}Se_{1.3} heterostructures, Jafarpisheh S., Cummings A.W., Watanabe K., Taniguchi T., Beschoten B., Stampfer C. *Physical Review B*; **98 (24)**, 2018. 10.1103/PhysRevB.98.241402. IF: 3.813

Quantum Hall effect in graphene with interface-induced spin-orbit coupling, Cysne T.P., Garcia J.H., Rocha A.R., Rappoport T.G. *Physical Review B*; **97 (8)**: 085413, 2018. 10.1103/PhysRevB.97.085413. IF: 3.813

Sensing ion channel in neuron networks with graphene field effect transistors, Veliev F., Cresti A., Kalita D., Bourrier A., Belloir T., Briançon-Marjollet A., Albrieux M., Roche S., Bouchiat V., Delacour C. *2D Materials*; **5 (4)**: 045020, 2018. 10.1088/2053-1583/aad78f. IF: 7.042

Shubnikov-de Haas oscillations in the anomalous Hall conductivity of Chern insulators, Canonico L.M., García J.H., Rappoport T.G., Ferreira A., Muniz R.B. *Physical Review B*; **98 (8)**: 085409, 2018. 10.1103/PhysRevB.98.085409. IF: 3.813

Spin proximity effects in graphene/topological insulator heterostructures, Song K., Soriano D., Cummings A.W., Robles R., Ordejón P., Roche S. *Nano Letters*; **18 (3)**: 2033-2039. 2018. 10.1021/acs.nanolett.7b05482. IF: 12.080

Spin transport in graphene/transition metal dichalcogenide heterostructures, Garcia J.H., Vila M., Cummings A.W., Roche S. *Chemical Society Reviews*; **47 (9)**: 3359-3379. 2018. 10.1039/c7cs00864c. IF: 40.182

Tailoring emergent spin phenomena in Dirac material heterostructures, Khokhriakov D., Cummings A.W., Song K., Vila M., Karpiak B., Dankert A., Roche S., Dash S.P. *Science Advances*; **4 (9)**: aat9349, 2018. 10.1126/sciadv.aat9349. IF: 11.511

Unequivocal signatures of the crossover to Anderson localization in realistic models of disordered quasi-one-dimensional materials, Alejandro Lopez-Bezanilla, Luis S. Froufe-Pérez, Stephan Roche, and Juan José Sáenz, *Phys. Rev. B*; **(98)**: 235423



PROJECTS

MANSPINDIRAC, Spin Manipulation in Dirac Matter, funded by FIS2015-67767-P (**MINECO/FEDER, UE**), 01/01/2016 - 31/12/2018, Stephan Roche and Aron Cummings

2017 SGR 692, funded by **AGAUR**, 01/01/2017 - 31/12/2020, Stephan Roche

GRAPHENE CORE 2, Graphene Flagship Core Project 2, funded by **European Union's Horizon 2020 research and innovation programme** under grant agreement No 785219, 01/04/2018 - 31/03/2020, IP: Stephan Roche, José A. Garrido, Arben Merkoçi, Sergio Valenzuela

GRAPHENE CORE 1, Graphene-based disruptive technologies, funded by **European Union's Horizon 2020 research and innovation programme** under grant agreement N° 696656, 01/04/2016 - 31/03/2018, IP: Stephan Roche, José A. Garrido, Sergio Valenzuela



CONTRIBUTIONS

Invited

2D materials for Spin/Valleytronics: Theoretical Perspective, **IMAGINENANO - NANOSPAIN 2018**, Bilbao, Spain, 14/03/18, Stephan Roche

Real space computational approaches for exploring charge/spin/thermal transport in materials with billions of atoms, **First-Principles Modelling & Quantum Transport Simulations of 2D Materials Workshop/ Spring Lane Building, Campus West**, University of York, United Kingdom, 12/06/18, Stephan Roche

2D materials for spintronics and valleytronics, **GRAPHENE WEEK 2018**, San Sebastián, Spain, 10/09/18, Stephan Roche

Foresight on spintronics and valleytronics using 2D materials, **GRAPCHINA 2018**, Xian, China, 17/09/18, Stephan Roche

Simulation of graphene-based materials for spintronics applications, **NANOBIO 2018**, Herakliom, Greece, 23/09/18, Stephan Roche

Spin-orbitronics in graphene/transition metal dichalcogenide heterostructures, **GDR GRAPHENE AND CO - MEETING ANNUEL**, Sète, France, 09/10/18, Stephan Roche

Spintronics in graphene, Sète, France, 15/10/18, Stephan Roche

Simulation of realistic models of graphene based materials, **Graphene Institute**, Beijing, China, 25/10/18, Stephan Roche

Spintronics and valleytronics in graphene,
Workshop EU Flagship, Sendai, Japan,
10/11/18, Stephan Roche

Charge, thermal and spin transport in graphene composites & polycrystalline heterostructures,
1and2DM International Conference, Japan,
22/12/18, Stephan Roche

Spin transport in graphene interfaced with high spin-orbit materials, **Graphene for US Conference**, New York, USA, 22/02/18, Aron Cummings

Spin transport in graphene interfaced with strong spin-orbit materials, **New Trends in Topological Insulators Conference**, Luxembourg City, Luxembourg, 18/07/18, Aron Cummings

Quantum transport simulation of graphene non-local spin valves, **IMAGINENANO - NANOSPAIN 2018**, Bilbao, Spain, 15/03/18, Marc Vila

Poster

Giant spin lifetime anisotropy in graphene/TMDC heterostructures, **Graphene Conference**, Dresden, Germany, 28/06/18, Aron Cummings

Quantum transport simulation of graphene non-local spin valves, **Graphene 2018**, Dresden, Germany, 28/06/18, Marc Vila

Anisotropic spin transport in graphene interfaced with topological insulators, **GDR Graphene and Co Annual Meeting**, Sète, France, 9/10/18, Aron Cummings



THESES

Kenan Song, *Theoretical study of disorder and proximity effects in three dimensional models of topological insulators*, 13/7/18, supervised by ICREA Prof. Stephan Roche and Prof. Pablo Ordejón



PARTICIPATED CONGRESSES

GRAPHENE 2018 (June26-29,Dresden Germany), Stephan Roche, *member of organizing committee*

3rd EU-Japan Flagship Workshop on Graphene and Related 2D Materials, Stephan Roche, *member of organizing committee*

Trends in Nanotechnologies, TNT2018 (3-7/09/2018, Lecce, Italy), Stephan Roche, *member of scientific committee*

NanoPortugal2018, Stephan Roche, *member of scientific committee*



AWARDS

S. Roche: **Editor in Chief position** at *Journal of Physics: materials*

Marc Vila: **Graphene Flagship Mobility grant for a 2-month stay in Japan**



DISSEMINATION CONTRIBUTIONS

Harvesting the manifold quantum degrees of freedom in Dirac fermions and their interlinking for controlling the transport mechanisms and information processing, **Invited Seminar at ICFO**, Castelldefels, Barcelona, 08/02/18, Stephan Roche

Coordinator and speaker of Nanoscience and Nanotechnology talks, **Barcelona Pint of Science**, Casa Orlandai, Barcelona, 14-16/03/18, Marc Vila

Theory and Simulation Group

Main Research Lines

- Development of theoretical methods, numerical algorithms and simulation tools: towards massive HPC facilities
- Codes: SIESTA development and its connection with other codes and informatic infrastructures like AiIDA
- First-principles simulations at the nanoscale
- Physical properties and chemical processes in materials



GROUP MEMBERS

Ordejón Rontomé, Pablo, CSIC Research Professor and Group Leader and Director

Akhtar, Arsalan, Doctoral Student

Alonso Pruneda, José Miguel, CSIC Tenured Scientist

Canadell Casanova, Enric, Visiting Senior Researcher

Costanzo, Francesca, Postdoctoral Researcher

Cuadrado Del Burgo, Ramón, Postdoctoral Researcher

Dewandre, Antoine, Visiting doctoral student

Dikan, Vladimir, Doctoral Student

Febrer Calabozo, Pol, Master Student

Grillet, Corentin, Postdoctoral Researcher

Guarda Pincheira, Fabián Adolfo, Visiting Undergraduate Student

Guster, Ionel-Bogdan, Doctoral Student

Iguaz Juan, Joaquim, Undergraduate Student (TFG)

Illera Robles, Sergio, Postdoctoral 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 25,000 citations (h-index of 56). He was co-editor of *EPL* (formerly *Euro Physics Letters*) from 2010 to 2015, and is member of the Editorial



Martínez Balagué, Pau, Visiting TFG Student

Monteiro Campos de Melo, Pedro

Miguel, Visiting Postdoctoral Researcher

Pilo González, Jorge, Fellowship Postdoctoral Researcher

Popescu, Bogdan Stefan, Postdoctoral Researcher

Robles Rodríguez, Roberto, SO Senior Postdoctoral Researcher

Sabadell Rendón, Albert, Visiting Master Student

Verstraete, Matthieu, Visiting Senior Researcher

Wittemeier, Nils, Doctoral Student

Zanolli, Zeila, Ramon y Cajal Senior Postdoctoral Researcher

Boards of the *physica status solidi* journals since 2004 and *Nanomaterials* since 2018. 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 received the Narcis Monturiol medal from the Catalan Government in 2018.

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 spinoff company SIMUNE.



NEW PROJECTS & MILESTONES

In 2018 we have continued to focus our efforts on work related to the MaX Centre (www.max-centre.eu), one of the eight European Centres of Excellence in HPC Applications supported by the EU under its 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 was initially based on the collaboration of 13 teams, including five research groups, like the ICN2 Theory and Simulation Group, which focuses on enhancing the capabilities of the SIESTA package and develop new methodologies for industrial applications of simulation tools in materials science. After a first period of three years (2015-2018), the grant has been renewed for the 2018-2021 period, with an increased budget and the incorporation of new groups and codes to the team.

We have continued improving the modularity and efficiency of the SIESTA and its modules (including TranSIESTA for the computation of electronic transport processes in nanodevices). In June 2018 we participated in the organisation of a Hackathon at the Barcelona Supercomputing Center, under the umbrella of MaX activities, for the development of the MaX codes (including SIESTA). 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 implementation and parallelisation of the Density Functional Perturbation Theory for the calculation of the phonon excitations in materials.

The group has continued its participation in NFFAEurope (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 users' projects. Up to date, our group has been awarded with eight user's projects, three of them having been carried out in 2018.

In 2018 we hosted three visiting international PhD students who came to learn about the techniques developed in the group.

On the science side of things, in 2018 we made progress in the following research lines:

Thermal transport in Nanofluids:

Our group established a fruitful collaboration with the Novel Energy-Oriented Materials Group (Prof. P. Gomez) and the Phononic and Photonic Nanostructures Group (Prof. Clivia Sotomayor-Torres) to understand their exciting experimental results on the thermal properties of graphene-dispersed nanofluids. This collaboration produced a joint publication in the *Nanoscale* journal, in which our group was able to determine the effect of the presence of the graphene flakes on the structure of the fluid, demonstrating the formation of layers in the liquid close to the graphene surface.

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. A joint publications with the ICN2 experimental group of Dr. D. Ruiz has been produced in this topic on the spin states of 2D coordination polymers.

Understanding the properties of 2D materials:

A major advance has been made in this field during 2018, with several articles being published on the explanation of the existence of Charge Density Waves in 2D transition metal dichalcogenides like TiSe_2 , TiTe_2 and NbSe_2 . Other work in 2D materials includes spin-proximity effects in graphene/topological insulator heterostructures, and the optical properties of MoS_2 under pressure.

Understanding oxygen diffusion in

Yttria-stabilized Zirconia: We started a collaboration with an industrial group on the understanding of the microscopic processes related to oxygen transport in materials used for gas sensing for the automotive industry. Our work has studied the mobility of oxygen in these materials by means of atomistic simulations, helping to determine the effect of the interfaces between the material and the metallic electrodes, a key factor of device performance.



PUBLICATIONS

A liquid-liquid transition in supercooled aqueous solution related to the HDA-LDA transition, Woutersen S., Ensing B., Hilbers M., Zhao Z., Austen Angell C. *Science*; **359 (6380)**: 1127-1131. 2018.
10.1126/science.aao7049. IF: 41.058

A multiscale model of the effect of Ir thickness on the static and dynamic properties of Fe/Ir/Fe films, Cuadrado R., Oroszlány L., Szunyogh L., Hrkac G., Chantrell R.W., Ostler T.A. *Scientific Reports*; **8 (1)**: 3879, 2018.
10.1038/s41598-018-21934-5. IF: 4.122

Addressing the environment electrostatic effect on ballistic electron transport in large systems: A QM/MM-NEGF approach, Feliciano G.T., Sanz-Navarro C., Coutinho-Neto M.D., Ordejón P., Scheicher R.H., Rocha A.R. *Journal of Physical Chemistry B*; **122 (2)**: 485-492. 2018.
10.1021/acs.jpcc.7b03475. IF: 3.146

First principles analysis of the CDW instability of single-layer 1T- TiSe_2 and its evolution with charge carrier density, Guster B., Canadell E., Pruneda M., Ordejón P. *2D Materials*; **5 (2)**: 25024, 2018. 10.1088/2053-1583/aab568. IF: 7.042

Hybrid quantum anomalous Hall effect at graphene-oxide interfaces, Zanolli Z., Niu C., Bihlmayer G., Mokrousov Y., Mavropoulos P., Verstraete M.J., Blügel S. *Physical Review B*; **98 (15)**: 155404, 2018.
10.1103/PhysRevB.98.155404. IF: 3.813

Mechanisms behind the enhancement of thermal properties of graphene nanofluids, Rodríguez-Laguna M.R., Castro-Alvarez A., Sledzinska M., Maire J., Costanzo F., Ensing B., Pruneda M., Ordejón P., Sotomayor Torres C.M., Gómez-Romero P., Chávez-Ángel E. *Nanoscale*; **10 (32)**: 15402-15409. 2018.
10.1039/c8nr02762e. IF: 7.233

Optical and electronic properties of 2H-MoS₂ under pressure: Revealing the spin-polarized nature of bulk electronic bands, Mauro Brotons-Gisbert, Alfredo Segura, Roberto Robles, Enric Canadell, Pablo Ordejón, and Juan F. Sánchez-Royo *Physical Review Materials*; **2 (5)**: 54602. 2018.

10.1103/PhysRevMaterials.2.054602. IF: 0.000

Site-resolved contributions to the magnetic-anisotropy energy and complex spin structure of Fe/MgO sandwiches, Cuadrado R., Oroszlány L., Deák A., Ostler T.A., Meo A., Chepulskii R.V., Apalkov D., Evans R.F.L., Szunyogh L., Chantrell R.W. *Physical Review Applied*; **9 (5)**: 054048, 2018. 10.1103/

PhysRevApplied.9.054048. IF: 4.782

Spin proximity effects in graphene/topological insulator heterostructures, Song K., Soriano D., Cummings A.W., Robles R., Ordejón P., Roche S. *Nano Letters*; **18 (3)**: 2033-2039. 2018.

10.1021/acs.nanolett.7b05482. IF: 12.080

Spin-Crossover in an exfoliated 2D coordination polymer and its implementation in thermochromic films, Salvio Suárez-García, Nayarassery N. Adarsh, Gábor Molnár, Azzedine Bousseksou, Yann Garcia, Marinela M. Dîrtu, Javier Saiz-Poseu, Roberto Robles, Pablo Ordejón, and Daniel Ruiz-Molina *ACS Applied Nano Materials*; **1 (6)**: 2662-2668. 2018.

10.1021/acsanm.8b00341 .

Structure evolution of mononuclear tungsten and molybdenum species in the protonation process: Insight from FPMD and DFT calculations, Zhang N., Yi H., Zeng D., Zhao Z., Wang W., Costanzo F. *Chemical Physics*; **502**: 77-86. 2018.

10.1016/j.chemphys.2018.01.009. IF: 1.707

Implementatio of Non-Collinear spin-constrained DFT calculations in SIESTA with a fully relativistic Hamiltonian, Cuadrado R., Pruneda M., García A., Ordejón P., *J. Phys. Materials* **1** 015010 (2018).

2x2 charge density wave in single-layer TiTe₂, Guster B., Robles R., Pruneda M., Canadell E., Ordejón P., *2D Materials* **6** 015027 (2018).

10.1088/2053-1583/aaf20b



PROJECTS

2017 SGR 1506, funded by **AGAUR**, 01/01/2017 - 31/12/2020, Pablo Ordejón

MaX, Materials design at the eXascale. European Centre of Excellence in materials modelling, simulations, and design funded by **European Union's Horizon 2020 research and innovation programme** under grant agreement No 824143, 01/12/2018 - 30/11/2021, IP: Pablo Ordejón

MaX, Materials Design at the eXascale funded by **European Union's Horizon 2020 research and innovation programme** under grant agreement No 676598, 01/09/2015 - 31/08/2018, IP: Pablo Ordejón

SIESTA, SIESTA and the Theory of Instabilities and Transport in Functional and Low-Dimensional Materials funded by FIS2015-64886-C5-3-P (**MINECO/FEDER, UE**), 01/01/2016 - 31/12/2018, Pablo Ordejón and Miguel Pruneda

PRX17/00600, Desarrollo de nuevas herramientas computacionales para el estudio de nanomateriales en SIESTA (ESTANCIA de 3 meses en Universidad de Berkeley) funded by PRX17/00600 (**MECD**), 03/05/2018 - 31/07/2018, Miguel Pruneda

NFFA-Europe, Nanoscience foundries and fine analysis-Europe, funded by **European Union's Horizon 2020 research and innovation programme** under grant agreement No 654360, 01/09/2015 - 31/08/2019, IP: Pablo Ordejón /Gustavo Ceballos/ José Santiso /Jordi Braxedas

First principles engineering of novel nanomaterials for spintronics applications, Ramon y Cajal fellowship, RYC-2016-19344, Spanish **MINECO**, 01/06/2018 - 31/05/2023, Zeila Zanolli



TECHNOLOGY TRANSFER

An auto-electrical and electronic components manufacturer for the automotive market, NDA with **FAE - Francisco Albero S.A.U.**, based at Barcelona



CONTRIBUTIONS

Invited

On the enhancement of thermal properties of graphene nanofluids, **MaX International Conference**, ICTP-Trieste, Italy, 01/18, Pablo Ordejón

Layered and 2D materials: electronic properties and structural instabilities from first principles, **Nanospain 2018**, Bilbao, Spain, 03/18, Pablo Ordejón

Layered and 2D materials: electronic properties and structural instabilities from first principles, **1st SP2 Network Workshop**, Madrid, Spain, 04/18, Pablo Ordejón

Layered and 2D materials: electronic properties and structural instabilities from first principles, **Nanotech France 2018**, Paris, France, June 2018, Pablo Ordejón

Theoretical methods, numerical algorithms and simulation tools for materials design, **European Materials Society Fall Meeting**, Warsaw, Poland, 09/18, Pablo Ordejón

Charge density waves in transition metal dichalcogenides, **International Workshop Game of Materials**, Dubrovnik, Croatia, 10/18, Pablo Ordejón

Spintronics by design: playing with interfaces, **HPC computing for next generation nanomaterials & nanodevices engineering**, ICN2, Barcelona, Spain, 30-31/05/18, Z. Zanolli

Spintronics at the interface, **MaX International Conference Materials Design Ecosystem at the Exascale: High-Performance and High-Throughput Computing**, ICTP, Trieste, Italy, 29-31/01/18, Z. Zanolli

Poster

SIESTA interface to AiiDA, **Materials Design Ecosystem at the Exascale: High-Performance and High-Throughput Computing**, The Abdus Salam International Centre for Theoretical Physics (Trieste), 28-31/01/18, Vladimir Dikan, Alberto García, Victor M. Garcia-Suarez, Emanuele Bosoni, Pablo Ordejón

Spin-Orbit implementation by means of fully separable Kleinman-Bylander pseudopotential formalism under atomic orbital basis in SIESTA code, Conference on the **Materials Design Ecosystem at the Exascale: High-Performance and High-Throughput Computing**, Trieste, Italy, 29-31/01/18, R. Cuadrado, J. I. Cerdá, M. Pruneda, A. García, P. Ordejón

Hybrid quantum anomalous hall effect at graphene-oxide interfaces, **TransIESTA workshop**, DTU Nanotech, Denmark, 20-23/11/18, Z. Zanolli

Electronic and transport properties of double-walled carbon nanotubes, **TranSIESTA workshop**, DTU Nanotech, Denmark, 20-23/11/18, N. Wittemeier and Z. Zanolli

Electronic and transport properties of double-walled carbon nanotubes, **ETSF workshop**, Milan University, Italy, 10-14/09/18, N. Wittemeier, M. J. Verstraete, L. Henrard, P. Lambin, R. Mazzarello, Z. Zanolli

Charge density waves in 2D materials, **Kick-off Meeting of the Spanish Network for the 2D Materials**, ICMM-CSIC, Madrid, Spain, 04/18, Bogdan Guster, Enric Canadell, Miguel Pruneda and Pablo Ordejón

Coexistence of distinct 3x3 structural distortions in the charge density wave state in NbSe₂, **Novel 2D materials explored via scanning probe microscopy & spectroscopy (2DSPM)**, San Sebastian, Spain, 06/18, Bogdan Guster, Paul Dreher, Carmen Rubio-Verdú, Roberto Robles, Javier Zaldívar-Fernández, Deung-Jang Choi, Miguel Pruneda, Pablo Ordejón, J. Silva-Guillén, José I. Pascual, Miguel M. Ugeda, Enric Canadell

Oral

DFT and electron holography, Non-equilibrium real-time dynamics on TMDs: photoluminescence and Kerr signals, **ETSF workshop**, Milan University, Italy, 10-14/09/18, P. Melo, M. J. Verstraete, Z. Zanolli

Ab initio photoluminescence in 2D materials, **15th ETSF Young Researchers' Meeting**, Max Plank Institute for the Structure and Dynamics of Matter, Hamburg, Germany, 04-08/06/18, P. Melo, M. J. Verstraete, Z. Zanolli

Interplay of magnetization between graphene and magnetoelectric multiferroics, **HPC meets materials**, University of Namur, Belgium, 25/05/18, Z. Zanolli

Interplay of magnetization between graphene and magnetoelectric multiferroics, **DPG Spring Meeting**, Berlin, Germany, 11-18/03/18, Z. Zanolli

Ab initio photoluminescence in 2D materials, **DPG Spring Meeting, Focus Session: Frontiers of Electronic-Structure Theory**, Berlin, Germany, 11-18/03/18, P. Melo, A. Marini, M. J. Verstraete, Z. Zanolli

Quantitative agreement between electron-optical phase images of WSe₂ and simulations based on electrostatic potentials that include bonding effects, **APS March Meeting**, Los Angeles, USA, 04-09/03/18, M. J. Verstraete, S. Borghardt, Z. Zanolli, F. Winkler, J. Barthel, A. H. Tavabi, R. E. Dunin-Borkowski, B. Kardynal

Charge density waves in 2D materials, **Graphene2018 International Conference**, Dresden Germany, 06/18, Bogdan Guster, Enric Canadell, Miguel Pruneda, Pablo Ordejón



PARTICIPATED CONGRESSES

2018 Max Hackathon, UPC, Barcelona, July 16-20/07/18.

23rd ETSF Workshop: Interdisciplinary views on quantum many-body theory, 11-14/09/18, Milan, Italy, Zeila Zanolli

The Platform for Advanced Scientific Computing (PASC) Conference, *Papers program committee co-chair for Chemistry and Materials*, editions: 2019 (Zurich, CH), 2020 (CH), Zeila Zanolli



COURSES

Dr. Ramón Cuadrado, *Spin-Orbit Coupling in SIESTA: Magnetism and other capabilities*, **Open Knowledge Workshop at ICN2** (20/21/22 - 06/18)



AWARDS

Dr Zeila Zanolli is elected **board member and treasurer of the Young Academy of Europe Board** at the **2018 Annual General Assembly**, held this year in Barcelona on 28 and 29 November.

Dr Zeila Zanolli is awarded the **MaX EU Centre of Excellence Prize** for her work on Ab initio design of new materials for spintronics applications, in recognition of frontier research in computational materials science.

Dr. Zeila Zanolli is elected **member of the steering committee of the European Theoretical Spectroscopy Facility (ETSF)**, a research network of about 200 researchers in Europe and in the United States focusing on theoretical and computational methods for studying electronic and optical properties of materials.

Prof. Pablo Ordejón receives the **Medalla Narcís Monturiol al mèrit científic i tecnològic**. The Narcís Monturiol awards recognises the outstanding contributions of nineteen researchers and one institution to several fields of science and technology in Catalonia



THESES

Kenan Song, *Theoretical study of disorder and proximity effects in three dimensional models of topological insulators*, 13/7/18, supervised by ICREA Prof. Stephan Roche and Prof. Pablo Ordejón



DISSEMINATION CONTRIBUTIONS

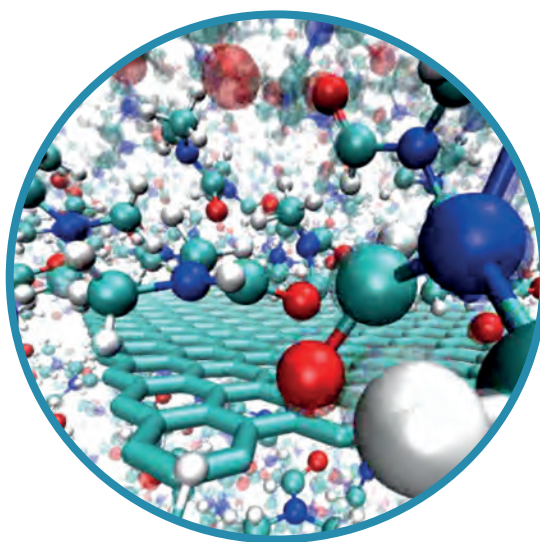
P. Ordejón: Presentación en el II Forum Gadea-Ciencia: Física y Ciencias del Universo, 26/10/2018, Madrid.
<https://gadeaciencia.org/events/ii-forum-gadea-ciencia>

Z. Zanolli: new media science dissemination accounts on

Twitter: [@zeilazanolli](https://twitter.com/zeilazanolli)

YouTube: Spintronics by Design
<https://www.youtube.com/channel/UCaAlZzO9yuZN9av1dwsRSBQ>

Website and web-blog:
<http://zeilazanolli.wordpress.com>



Ultrafast Dynamics in Nanoscale Systems Group

Main Research Lines

- Heat and charge transport in systems based on 2D materials
- Ultrafast optoelectronic techniques
- Photodetection and terahertz technologies
- Nanofabrication of systems based on 2D materials



GROUP MEMBERS

Tielrooij, Klaas-Jan, RyC and Group Leader
Saleta Reig, David, Research Assistant

Xiaoyu Jia, visiting PhD Student

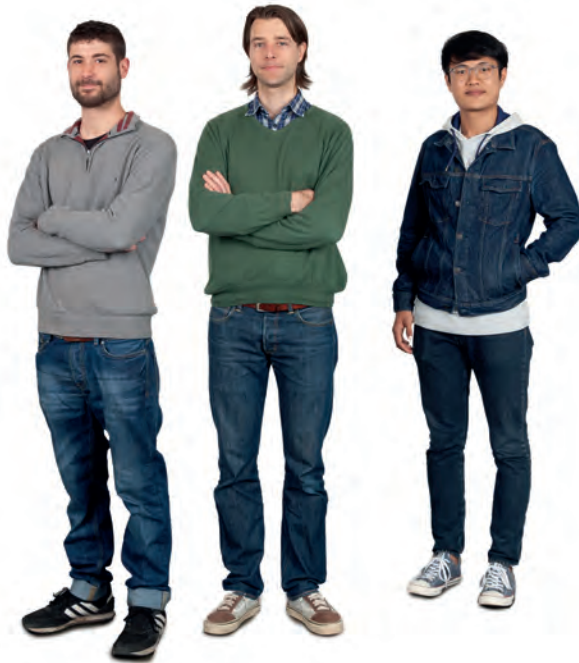


GROUP LEADER



RyC Dr Klaas-Jan
Tielrooij

Klaas-Jan Tielrooij joined the ICN2 in October 2018, starting the ICN2 Ultrafast Dynamics in Nanoscale Systems Group. In July 2018, he was awarded a visiting professorship at the Graduate School of Excellence Material Science in Mainz (Germany). Before coming to the ICN2, he was a research fellow at fellow-BIST institute ICFO in Barcelona. He obtained his Ph.D. at the University of Amsterdam (Netherlands) in December 2010. He was awarded an ERC Starting Grant in 2018. Other recognitions include the FOM Physics Thesis Prize 2011. He has more than 35 peer-reviewed publications, of which 13 in *Nature* and *Science* and family, and over 4,300 citations. His H-index is currently 24 (8 years after Ph.D.)



NEW PROJECTS & MILESTONES

Dec 2018: Start of ERC StG project “CUHL - Controlling Ultrafast Heat in Layered materials” (ERC-2018-STG-804349)

July 2018: Visiting professorship at Graduate School of Excellence “Material Science in Mainz” (Germany)



CONTRIBUTIONS

Invited

A graphene story from lab to industry, **Johannes Gutenberg University**, Mainz (Germany), 28/11/18, Klaas-Jan Tielrooij

Graphene hot electrons to detect light and more, **GDR Graphene and Co annual meeting 2018**, Sète (France), 15-19/10/18, Klaas-Jan Tielrooij



PROJECTS

CUHL, Controlling Ultrafast Heat in Layered materials, funded by **European Union’s Horizon 2020 research and innovation programme** under grant agreement N° 804349, 01/12/2018 - 30/11/2023, Klaas-Jan Tielrooij

2DNanoHeat, Nanoscale Heat Transport in 2D layered materials funded by **BIST**, 20/04/2018 - 19/12/2018. IP: Klaas-Jan Tielrooij (*from ICFO*), Clivia M. Sotomayor Torres, Sergio Valenzuela



DISSEMINATION CONTRIBUTIONS

Premio Nobel de Fisica 2018: el empuje de la luz, **Gadea Ciencia (2018)**, Klaas-Jan Tielrooij, 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.136**
- Electron Microscopy Unit **p.138**
- Nanomaterials Growth Unit **p.142**

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.146**
- Photoemission Spectroscopy (XPS&UPS) Facility **p.148**
- Molecular Spectroscopy and Optical Microscopy Facility **p.149**
- X-Ray Diffraction Facility **p.150**
- Mechanical Workshop Facility **p.152**
- Biolab Facility **p.153**

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 Mago, Gustavo,
Head of Research Support
Division and Unit Leader



Maymó i Camos, Marc,
Research Engineer



UNIT LEADER

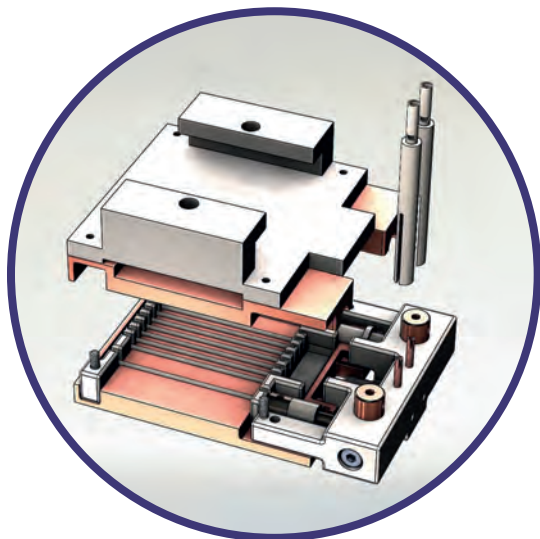
Dr Gustavo Ceballos earned his degree in chemistry at the *Universidad Central de Venezuela* in 1989. He obtained his PhD in 1996 at the *Institut für Physikalische und Theoretische Chemie der Universität Bonn* (Germany). In 1997 he moved to the *Institut für Experimentalphysik der Freie Universität 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-INFN* (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 2018 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

Bottom-up synthesis of multifunctional nanoporous graphene, Moreno C., Vilas-Varela M., Kretz B., Garcia-Lekue A., Costache M.V., Paradinas M., Panighel M., Ceballos G., Valenzuela S.O., Peña D., Mugarza A. *Science*; **360 (6385)**: 199 - 203. 2018. 10.1126/science.aar2009. IF: 41.058

On-surface synthesis of superlattice arrays of ultra-long graphene nanoribbons, Moreno C., Paradinas M., Vilas-Varela M., Panighel M., Ceballos G., Peña D., Mugarza A. *Chemical Communications*; **54 (68)**: 9402 - 9405. 2018. 10.1039/c8cc04830d. IF: 6.290



PROJECTS

NFFA-Europe, Nanoscience foundries and fine analysis-Europe, funded by **European Union's Horizon 2020 research and innovation programme** under grant agreement No 654360, 01/09/2015 - 31/08/2019, IP: Pablo Ordejón /Gustavo Ceballos/ José Santiso /Jordi Fraxedas



TECHNOLOGY TRANSFER

A nanoporous graphene structure and method for preparation thereof, **EU patent application** (Application number: EP18382088.5)



THESES

Michele Gastaldo, *Tailoring the structural and electronic properties of graphene by bottom-up methods*, supervised by ICREA Prof. Aitor Mugarza and Dr. Gustavo Ceballos

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, Specialist 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 72 peer-reviewed articles with about 1300 citations.



NEW PROJECTS & MILESTONES

In 2018 the Electron Microscopy Unit was granted with an infrastructure project by the Spanish Ministry, which allowed the acquisition of an state-of-the-art EDX detector system for the FEI Magellan 400L XRSEM. Installation and initial tests took place from June-September, being completely operative at the lasts months of the year. The recently attached X-Max Ultim Extreme EDX (Oxford Instruments) converts this microscope in a unique tool at the forefront of nanocharacterisation, as it allows an ultrafast compositional nanoanalysis and mapping with an unprecedented sensitivity and energy resolution, even for light elements such as lithium.

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* and at the *Universitat Catalana d'Estiu* (UCE).

The Unit also devoted efforts to the NFFA-Europe infrastructure project, providing access and to our electron microscopy facilities to a number of researchers from other institutions.

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 shown the laser-assisted synthesis of tubular van der Waals heterostructures templated by carbon nanotubes.



PUBLICATIONS

An in operando study of chemical expansion and oxygen surface exchange rates in epitaxial GdBaCo₂O_{5.5} electrodes in a solid-state electrochemical cell by time-resolved X-ray diffraction, Chatterjee A., Caicedo J.M., Ballesteros B., Santiso J. *Journal of Materials Chemistry A*; **6 (26)**: 12430-12439. 2018. 10.1039/c8ta02790k. IF: 9.931

Comparative study of shortening and cutting strategies of single-walled and multi-walled carbon nanotubes assessed by scanning electron microscopy, Kierkowicz M., Pach E., Santidrián A., Sandoval S., Gonçalves G., Tobías-Rossell E., Kalbáč M., Ballesteros B., Tobias G. *Carbon*; **139**: 922-932. 2018. 10.1016/j.carbon.2018.06.021. IF: 7.082

Determination of the length of single-walled carbon nanotubes by scanning electron microscopy, Sandoval S., Kierkowicz M., Pach E., Ballesteros B., Tobias G. *MethodsX*; **5**: 1465-1472. 2018. 10.1016/j.mex.2018.11.004

Encapsulation of cationic iridium(iii) tetrazole complexes into a silica matrix: Synthesis, characterization and optical properties, Zanoni I., Fiorini V., Rosado M., Ballesteros B., Androulidaki M., Blosi M., Ortelli S., Stagni S., Dondi M., Costa A.L. *New Journal of Chemistry*; **42 (12)**: 9635-9644. 2018. 10.1039/c8nj01514g. IF: 3.201

Epoxidation of carbon nanocapsules: Decoration of single-walled carbon nanotubes filled with metal halides, D'Accolti L., Gajewska A., Kierkowicz M., Martincic M., Nacci A., Sandoval S., Ballesteros B., Tobias G., Da Ros T., Fusco C. *Nanomaterials*; **8(3)**: 137. 2018. 10.3390/nano8030137. IF: 3.504

Facile synthesis of nanoparticles of the molecule-based superconductor κ -(BEDT-TTF)₂Cu(NCS)₂ [Synthèse aisée de nanoparticules du supraconducteur moléculaire κ -(BEDT-TTF)₂Cu(NCS)₂], Cormary B., Faulmann C., de Caro D., Valade L., de Caro P., Ballesteros B., Fraxedas J. *Comptes Rendus Chimie*; **21 (9)**: 809-813. 2018. 10.1016/j.crci.2018.07.006. IF: 1.877

Optimisation of growth parameters to obtain epitaxial Y-doped BaZrO₃ proton conducting thin films, Magrasó A., Ballesteros B., Rodríguez-Lamas R., Sunding M.F., Santiso J. *Solid State Ionics*; **314**: 9-16. 2018. 10.1016/j.ssi.2017.11.002. IF: 2.751

Protein-corona-by-design in 2D: A reliable platform to decode bio-nano interactions for the next-generation quality-by-design nanomedicines, Mei K.-C., Ghazaryan A., Teoh E.Z., Summers H.D., Li Y., Ballesteros B., Piasecka J., Walters A., Hider R.C., Mailänder V., Al-Jamal K.T. *Advanced Materials*; **30 (40)**: 1802732. 2018. 10.1002/adma.201802732. IF: 21.950

Selective laser-assisted synthesis of tubular Van der Waals heterostructures of single-layered Pbl₂ within carbon nanotubes exhibiting carrier photogeneration, Sandoval S., Kepić D., Pérez Del Pino Á., György E., Gómez A., Pfanmoeller M., Tendeloo G.V., Ballesteros B., Tobias G. *ACS Nano*; **12 (7)**: 6648-6656. 2018. 10.1021/acsnano.8b01638. IF: 13.709



PROJECTS

2017 SGR 327 funded by **AGAUR**, 01/01/2017 - 31/12/2020, IP: Belén Ballesteros

Adquisición de un sistema de detección de Energía Dispersiva de Rayos X de última generación para el microscopio de ultra-alta resolución Magellan 400L, funded by **FEDER/ Ministerio de Ciencia, Innovación y Universidades - Agencia Estatal de Investigación/EQC2018-004582-P**, 01/01/2018 - 31/12/2019, Belén Ballesteros



CONTRIBUTIONS

Invited

Electron microscopy studies of tubular van der Waals heterostructures, 2nd ELECMI

International Workshop, Zaragoza,
11-13/06/18, Belén Ballesteros



COURSES

Winterschool on Microscopy within the **BIST Master of Multidisciplinary Research in Experimental Sciences**, 01/18

Nanotecnologia i Reptes Socials. Fundació Universitària Bages-UManresa. Manresa,
04-05/18

Ciència i Tecnologia. Universitat Catalana d'Estiu. Manresa, 07/18



AWARDS

An image by *Marcos Rosado*, SEM image of a nanoplankton from the north Pacific Ocean, wins the **December Thermo Fisher Scientific image contest**



DISSEMINATION CONTRIBUTIONS

Festival 10 alamos9 - Nanocentros en la Calle,
visit at ICN2 Electron Microscopy Unit hosted
by Belén Ballesteros and Marcos Rosado

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 (metal-insulating transitions, ferroelectric, ferromagnetic, oxide ionic conducting, thermoelectric, transparent conducting, resistive switching, etc.)
- MOCVD growth of 2D layers of transition metal dichalcogenides
- Structural characterisation by RHEED and advanced XRD, and 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 Sômiya 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 (I²CNER, 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 23.



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
(also in Oxide nanophysics group)



Chatterjee, Arindom,
PhD Student and presently
research assistant



Rubio Lorente, Carlos,
Technician



Sakai, Jo,
Visiting Professor
(also in Oxide nanophysics group)



NEW PROJECTS & MILESTONES

Our unit produces films by means of a pulsed laser deposition technique, and works in close collaboration with many ICN2 research groups, as well as with external collaborators. Our unit carries out advanced structural characterisation of thin films, primarily by X-ray diffraction as well as working 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 phenomena, such as oxygen exchange kinetics. For this purpose we have

developed a time-resolved XRD technique that monitors the subtle chemical expansion produced in transition metal oxide thin films when changing their oxygen stoichiometry. We aim to perform in-situ and in-operando characterisation by XRD in different solid state electrochemical devices. These studies have also been extended to in-situ structural studies of ferroelectric materials, and resistive switching.

In 2018 we have also continued to develop a thin film MOCVD process for the growth of high-quality ultrathin transition metal dichalcogenides, starting with MoS₂, in collaboration with the ICN2 group led by Prof. José A. Garrido. During 2019 there are plans to scale this process up for 2" wafers.



PUBLICATIONS

Atomic resolution imaging and quantitative elemental mapping of the misfit dislocation core phase in multicomponent oxides, Bagués N., Santiso J., Esser B.D., Williams R.E.A., McComb D.W., Konstantinovic Z., Balcells L., Sandiumenge F., *Microscopy and Microanalysis*; **24 (S1)**, 24-25. 2018. doi.org/10.1017/S1431927618000612

An in operando study of chemical expansion and oxygen surface exchange rates in epitaxial $\text{GdBaCo}_2\text{O}_{5.5}$ electrodes in a solid-state electrochemical cell by time-resolved X-ray diffraction, Chatterjee A., Caicedo J.M., Ballesteros B., Santiso J. *Journal of Materials Chemistry A*; **6 (26)**: 12430-12439. 2018. 10.1039/c8ta02790k. IF: 9.931

Growth and structural characterization of strained epitaxial $\text{Hf}_{0.5}\text{Zr}_{0.5}\text{O}_2$ thin films, L. Torrejón, E. Langenberg, C. Magén, A. Larrea, J. Blasco, J. Santiso, P. A. Algarabel, J. A. Pardo, *Physical Review Materials*; **2 (1)**: 13401. 2018. 10.1103/PhysRevMaterials.2.013401

Optimisation of growth parameters to obtain epitaxial Y-doped BaZrO_3 proton conducting thin films, Magrasó A., Ballesteros B., Rodríguez-Lamas R., Sunding M.F., Santiso J. *Solid State Ionics*; **314**: 9-16. 2018. 10.1016/j.ssi.2017.11.002. IF: 2.751

Substrate dependence of the freezing dynamics of supercooled water films: a high-speed optical microscope study, Pach E., Rodriguez L., Verdaguer A., *Journal of Physical Chemistry B*; **122 (2)**: 818-826. 2018. 10.1021/acs.jpcc.7b06933. IF: 3.146

The misfit dislocation core phase in complex oxide heteroepitaxy, Bagués N., Santiso J., Esser B.D., Williams R.E.A., McComb D.W., Konstantinovic Z., Balcells L., Sandiumenge F. *Advanced Functional Materials*; **28 (8)**: 1704437, 2018. 10.1002/adfm.201704437. IF: 13.325



PROJECTS

DAFNEOX, Designing Advanced Functionalities through controlled NanoElement integration in OXide thin films, **European Union's Horizon 2020 research and innovation programme** under grant agreement No 645658, 01/07/2015 - 30/06/2019, IP: José Santiso

SURKINOX, Designing rules for enhancing SURface KINetics in functional OXides for clean energy technologies, PCIN-2016-026 (**MINECO**), 01/05/2016 - 30/04/2019, IP: José Santiso

FUN-TO-BE: FUNDamental aspects of Thin film growth of Oxide heterostructures controlling their resistive switching BEhaviour, Référence 261091, PICS 2015. **Proyecto de cooperación CNRS-CSIC, approved CNRS-CSIC**, 1/01/2016- 31/12/2018: IPs: José Santiso (ICN2-CSIC) and Mónica Burriel (LMGP Grenoble-CNRS)

NFFA-Europe, Nanoscience foundries and fine analysis-Europe, funded by **European Union's Horizon 2020 research and innovation programme** under grant agreement No 654360, 01/09/2015 - 31/08/2019, IP: Pablo Ordejón /Gustavo Ceballos/ José Santiso /Jordi Fraxedas



CONTRIBUTIONS

Invited

Misfit dislocations in complex oxide epitaxial thin films, **E-MRS Spring Meeting 2018**, Symposium R: Solid State Ionics: Advanced Functional Materials for solid State devices. Session: Interface & Surface Phenomena (III). Strasbourg (France), 18-22/06/18, José Santiso, Núria Bagués, Bryan D. Esser, Robert E.A. Williams, Dave W. McComb, Zorica Konstantinovic, Lluís Balcells, and Felip Sandiumenge

Time resolved X-ray diffraction for oxygen surface exchange determination, Workshop on Ion conducting ceramic electrochemical devices: how interfaces and surfaces affect performance and lifetime, **FOXCET-SURKINOX joint meeting**, 19-20/04/18, University of Oslo (Norway), José Santiso, Arindom Chatterjee, Jose Manuel Caicedo, Jessica Padilla, Anna Magrasó

Oral

In-situ observation of domains across the metal-insulator transition of VO₂ thin films, **E-MRS Fall Meeting 2018**, Symposium P: SEMICONDUCTORS AND ELECTRONIC MATERIALS: Epitaxial oxide films for electronic applications, Warsaw (Poland), September 17-20/09/18, Laura Rodríguez, Gustau Catalan, José Santiso, Felip Sandiumenge

LaNiO₃ thin films: influence of the deposition technique and growth parameters on the film quality, **E-MRS Spring**, Jun 2018, Strasbourg, France, 2018, Maas K., Boudard M., Rafhay Q., Jimenez C., Rapenne L., Roussel H., Roussel H., Caicedo J.M., Santiso J., Burriel M.



COURSES

XRD Advanced characterisation, **Master Nanotechnology UAB**, course 2017-2018, theoretical and practical case studies. José Santiso



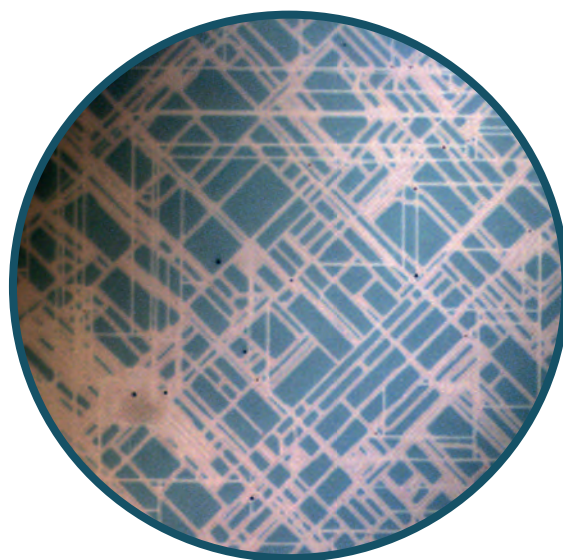
THESES

Arindom Chatterjee, *Thermoelectric performance of layered cobaltate epitaxial films deposited by pulsed laser evaporation*, supervised by ICREA Prof. Clivia Sotomayor and CSIC Researcher Jose Santiso



AWARDS

Laura Rodríguez Domínguez receives a **Graduate Student Award at the 2018 E-MRS Fall Meeting**, *In-situ observation of domains across the metal-insulator transition of VO₂ thin films*, Warsaw University of Technology, 17-20/09/18



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



Borrísé, Xavier, Research
Engineer



AVAILABLE TECHNIQUES

- Electron-beam lithography (EBL)
- Focused ion beam (FIB)
- Direct write laser UV lithography (DWL)
- UV mask aligner
- Thermal and UV-nanoimprint lithography (NIL)
- E-beam evaporation
- ICP-RIE plasma dry etching
- Plasma cleaning
- Wedge bonding
- Spin coating
- Optical microscopy
- Atomic force microscopy (AFM)
- 3D optical profiler
- Stylus profilometer



NEW PROJECTS & MILESTONES

In 2018 work in relation to the Nanofabrication Facility has been focused on the setup and commissioning stage of a new environmentally-controlled area within the main ICN2 building. This included the installation of new equipment that will boost existing nanofabrication services at the ICN2. With a focus on dry etching and photolithography processes (and combined with the existing thin film 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.



PUBLICATIONS

Arrays of suspended silicon nanowires defined by ion beam implantation: Mechanical coupling and combination with CMOS Technology, Llobet J., Rius G., Chuquitarqui A., Borrísé X., Koops R., Van Veghel M., Perez-Murano F. *Nanotechnology*; **29 (15)**: 155303, 2018.
10.1088/1361-6528/aaac67. IF: 3.404

Design, fabrication, and characterisation of wire grid polarizers for the deep UV spectral range, Rodríguez-De Marcos L., Ong Bin L., Citra Asmara T., Heussler S.P., Guerrero A., Mas R., Borrísé X., Breese M.B.H., Rusydi A. *Proceedings of SPIE - The International Society for Optical Engineering*; **10691**: 1069124. 2018.
10.1117/12.2314459

Geometric frustration in a hexagonal lattice of plasmonic nanoelements, Conde-Rubio A., Rodríguez A.F., Borrísé X., Perez-Murano F., Batlle X., Labarta A. *Optics Express*; **26 (16)**: 20211 - 20224. 2018.
10.1364/OE.26.020211. IF: 3.356



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



PUBLICATIONS

Characterization of carbon-contaminated B4C-Coated optics after chemically selective cleaning with low-pressure RF plasma, Moreno Fernández H., Rogler D., Sauthier G., Thomasset M., Dietsch R., Carlino V., Pellegrin E. *Scientific Reports*; **8 (1)**: 1293, 2018. 10.1038/s41598-018-19273-6. IF: 4.122

Control of the polarization of ferroelectric capacitors by the concurrent action of light and adsorbates, Liu F., Fina I., Sauthier G., Sánchez F., Rappe A.M., Fontcuberta J. *ACS Applied Materials and Interfaces*; **10 (28)**: 23968 - 23975. 2018. 10.1021/acsami.8b05751. IF: 8.097



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

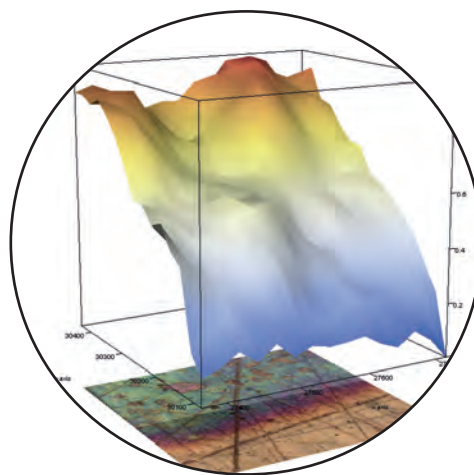


Saiz, Javier, Research Technician of the Molecular Spectroscopy and Optical Microscopy Facility



AVAILABLE TECHNIQUES

- FT-IR spectroscopy
- UV-Vis spectroscopy
- FT-IR and Vis-NIR microspectroscopy
- Dynamic light scattering and zeta potential
- Optical-Fluorescence microscopy
- Static contact angle



X-Ray Diffraction Facility

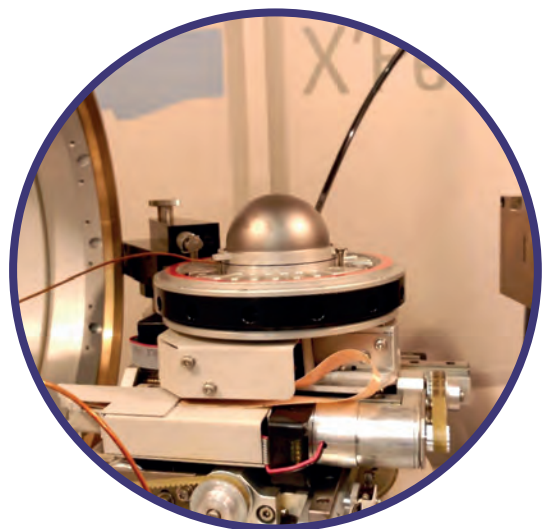
This facility is equipped with two advanced X-ray diffractometers (X'Pert MPD and MRD from PANalytical). These pieces of equipment are used to perform X-ray diffraction (XRD) analysis of nanopowders and thin films, and by doing so support the research activities of ICN2 groups and the surrounding research 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)
- In-situ thin films characterization applying:
 - Gas exchanges at elevated temperatures (redox kinetics, oxide ionic materials).
 - Applied voltage bias (piezoelectric, ferroelectric, electrostriction, resistive switching).
 - Exchange between wet and dry atmosphere (water uptake, protonic conducting materials).
 - Simultaneous atmosphere exchange and electrical conductivity.
 - LED illumination at RT (photo-activated phase transitions, photostriction,...)



Mechanical Workshop

The main objective of the Mechanical Workshop is to assist ICN2 researchers with the production and development of mechanical components. If capacity allows, tasks are also carried out for customers outside.

The facility is equipped with state of the art CNC machine tools, conventional lathes and milling machines and welding and fabrication equipment. We are further equipped with a CAD/CAM package to enhance the design and manufacturing capabilities.

The Workshop is characterized by flexibility, quality and cooperation, and the tasks are carried out by a highly qualified staff. The staff is available to assist the researchers in the design assessment and feasibility, the material selection and the sourcing of associated components.



FACILITY MEMBERS



León, Rafael, Severo Ochoa
Mechanical Workshop Technician



AVAILABLE TECHNIQUES

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



Biolab Facility

2018 the ICN2 initiated the construction of a dedicated BSL-2 BioLab facility, with the support of the FEDER CENanoTech project, that will address the current growing interest in the experimentation combining of life sciences with phenomena taking place at the nano and micro scales and will enable substantial advances in the research work of ICN2 groups in this field. The lab space has been conditioned and some important equipment has been acquired and installed. By the end of 2018 the institute started the process of hiring a dedicated technician who will be in charge of the day by day activity of the lab.



AVAILABLE TECHNIQUES

- CO₂ Incubators
- Biological Safety Cabinets (class I and class II)
- Benchtop microcentrifuges
- Tabletop autoclave
- Inverted phase contrast microscope
- Refrigerators and freezer



Strategy Development Office



Strategy Development Office

The ICN2 Strategy Development Office works to provide a response to the different challenges faced by the institute on the short and long term. It works in close collaboration with both the research community and the administrative departments, bringing insights and strategic manpower to hot topics like research data management and ongoing initiatives to support the ICN2 in becoming a world-leading research institution. Several of its members are devoted exclusively to the business development of in-house technologies.



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

Benítez, Núria, Strategy Development

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

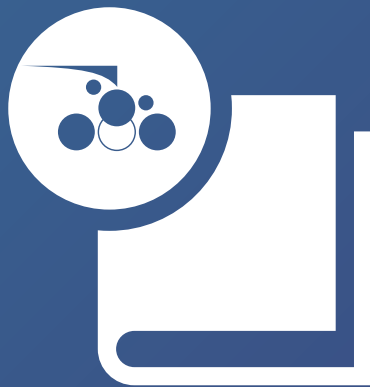
Pons, Nadia, Business Development Officer

Reverter Cendros, Jordi, IP & Technology
Transfer

Spinato, Cinzia, Business Development

Tienda, Dulce, Strategy Development

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 a fluent communication and adaptation of the service to their specific needs. 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.



HEALTH AND SAFETY AREA

During 2018 the new Health & Safety Area has supported ICN2's research and organization community in proactively controlling chemical, biological, and physical hazards in managing their safety activities in a complex and diverse research environment.

The Area has developed new lab safety programs (Biosafety and Laser Safety) and performed more than 100 hazard corrections and 10 safety inspections. Last year 366 safety-related courses were completed and we have currently a 91% compliance in safety training.

Regarding sustainability, ICN2 recalls the importance of environment respect promoting recycle with new green points around the building and sharing sustainable initiatives among its community.

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.

Among others projects, during 2018 it implemented the new Firewall and VPN, the new System for WebAdmin ticketing, the new Netapp Cabin as a new Backup System and the deployment of the new General Data Protection Regulation (GDPR).

MAINTENANCE AND SERVICES

The ICN2 Maintenance and Services Department manages two buildings facilities and plays a key role in the configuration of new spaces.

One is the main building (ICN2 building) with a constructed area of 6,565 m² distributed in 50 laboratories devoted to research, 13 shared spaces (e.g.: warehouses, meeting rooms, dining room) and 14 common laboratories that offer a transversal support to the research activity. Among these, we can highlight a Biological Room and a Nano-manufacturing Room, which came into service in 2018.

The second one (CM3 module) offers 560 m² of useful area, divided into 9 research laboratories, 43 work places and 4 shared infrastructure spaces.

The Maintenance and Services Department members work to keep over 40 laboratories in optimal conditions. The department also oversees management of external service providers such as those involved in cleaning, gardening, reception, security, courier and post.

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 coordinates graphic design tasks to ensure that the quality of visual support material is on a par with the science being developed, as well as writing support for 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. Regarding transparency and accountability, it has an active role in institutional reporting as well as in the implementation of the Open Science requirements regarding data and publications.



Events and Dissemination



- > Science and Industry **p.166**
- > Public Outreach and Education Sector **p.170**
- > Community-Building **p.176**
- > Media Impact **p.178**

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

Severo Ochoa International Conference

February 2018, Palau de la Música



- The ICN2 paid homage to its Severo Ochoa accreditation and grant, together with international collaborators and research leaders in nanoscience and nanotechnology.
- The program was grouped into three thematic areas, Life, Energy and ICT, largely representing the main areas of application of the centre's Severo Ochoa research programme "Nanodevices for social challenges", which ended in 2018.

Stability of Emerging Photovoltaics from Fundamental to Applications (SEPV2018)

February 2018, Barcelona

- A four-day conference with around 100 attendees and talks from the main world leaders in the emerging field of photovoltaics.
- It was the closing act of a four-year COST Action coordinated by Prof. Mónica Lira to pool existing and generate new fundamental knowledge and expertise in a bid to reinstate Europe's competitiveness in photovoltaics manufacturing.



HPCnano workshop

June 2018, ICN2, UAB Campus

- The High Performance Computing for Next Generation Nanomaterials and Nanodevice Engineering (HPCnano) workshop brought together over 30 young researchers willing to apply supercomputing technologies in nanomaterials, molecular electronics and nanodevices.
- Sponsored by the Spanish Supercomputing Network (RES), it aimed to provide introductory knowledge on how high performance computing can be harnessed to solve a range of complex problems.



14th International Symposium of Ferroic Domains

September 2018, Casa Convalescència, Barcelona

- This Symposium is a highly specialised event to discuss phenomena with implications for fundamental physics and electronic applications. It gathered around 100 experts.
- Held every two years since 1989, in 2018 the event was organised by ICREA Prof. Gustau Catalán, leader of the ICN2 Oxide Nanophysics Group, and Dr Neus Domingo, senior researcher in this group and head of the ICN2 Advanced Atomic Force Microscopy Platform.



BrainCom Summer School

September 2018, Casa Convalescència, Barcelona

- Braincom is a collaborative European research project led by ICN2 to drive the development of neural interfaces able to record and interpret brain activity at source.
- On October 2018 project partners came to Barcelona for a dedicated summer school.



Workshop on Bio-inspired Adhesives and Functional Coatings based on Catechols

October 2018, ICN2, UAB Campus

- The two-day event brought together key representatives of the international biomimicry community to discuss state of the art and future directions in this vibrant field.
- The event, which gathered over 50 experts, was organised by the ICN2 Nanostructured Functional Materials Group in the framework of its participation in the European Network of Bioadhesives (ENBA).



ICN2 Workshop on Research, Strategy and Innovation

November 2018, Castelldefels

- As part of ongoing actions to boost networking in research support, the ICN2 Strategy Development Office organised an international networking and training action.
- Around 60 research professionals attended the event, including some key voices within the European research management community.



ICN2 BOOTH AT TRADE SHOWS AND FAIRS

Mobile World Congress (MWC)

February 2018, Fira de Barcelona

- For the third time in a row, the MWC offered a selection of the most promising applications based on 2D materials like graphene in the Graphene Flagship's Graphene Experience Zone.
- As a Flagship research partner and field leader in graphene technologies, the ICN2 was there to showcase its brain implant technologies, being developed under the H2020 BrainCom project to restore speech, and more generally as part of the ICN2 Severo Ochoa research programme.



Graphene 2018

June 2018, Germany

- ICN2 was involved in the event with organisational, institutional and scientific efforts to share the latest advances in graphene research.
- Those who dropped by the ICN2 booth learned from members of the ICN2 Strategy Development Office and numerous ICN2 researchers about brain implants to restore speech and nanoporous graphene, among other breakthroughs.



Graphene Week 2018

September 2018, Donostia

- Graphene Week is the Graphene Flagship International Conference.
- The program includes some ICN2 researchers and their innovations were exhibited at the Flagship's booth.



CAREERS FAIRS

University of Barcelona Careers Fair (Fira d'Empreses)

May 2018, UB Faculty of Physics, Barcelona

- The ICN2 was among the over 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 2018. Details can be found in the group sections. In total our researchers participated in 172 international conferences in 2018, giving a total of 216 talks (168 as invited speakers) and 39 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 2018 NanoEduca was awarded with the Catalan National Scientific Communication Award (Premi Nacional de Comunicació Científica). The programme includes the NanoKit, distributed to schools throughout Catalonia via the Catalan Ministry of Education, a yearly contest for schools and educational courses to train high school teachers.

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).



GSMA-mSchools

A collaboration with GSMA-mSchools allowed the creation of the first NanoEduca digital educational content. The materials were presented in an interactive workshop with high school teachers at YoMo 2018.

Students learn how to measure hydrophobicity and how to use it everyday life applications. They can access an online tutorial, which includes educational content about nanoscience, and use their mobile phones to identify urban elements that may benefit from superhydrophobic coatings (against graffiti, to protect surfaces...).



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 were the coordinators of the third edition of these series of events devoted to Physics.

Over the course of the year, 25 outstanding students to are invited to interact with researchers from the ICN2, IFAE, UAB, ICMAB, Alba Synchrotron 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.



EVENTS AIMED AT A YOUNG PUBLIC

Youth Mobile Festival (YoMo)

February 2018, La Farga de l'Hospitalet, Barcelona

- This event is held in parallel to the Mobile World Congress and aimed at a young public and the education community.
- As part of a BIST institutional stand, the ICN2 put on a show of scientific experiments designed to convey the impact of the nanoscale in everyday life, with particular emphasis on applications



aimed at the transport and storage of energy.

- Along with the GSMA's mSchools initiative and fellow members of NanoEduca, the ICN2 organised the YoMo "Dive into graffiti" workshop. The session looked at fun ways to bring the concept of hydrophobicity to the classroom and explore the applications of super hydrophobic materials in the urban setting.

Festival 10alamos9

April 2018, Barcelona, UAB Campus and other venues

- In its third edition, the 10alamos9 Festival of Nanoscience and Nanotechnology was back with over 100 activities to choose from across numerous locations in Spain.
- The festival kicked off at UAB Campus in Bellaterra with a tour of the different research facilities and a workshop involving ICN2 group leaders Prof. Laura Lechuga, Prof. Pedro Gómez and ICREA Prof. Victor Puntes, joined by fellow ICN2 professionals Daniel Rueda, Àlex Argemí and Ana de la Osa.
- The ICN2 coordinated the activities on the UAB Campus with the participation of the UAB, ICMAB and CNM-CSIC, in an educational activity funded by the Spanish Foundation for Science and Technology (FECYT).



NanoEduca Schools Contest

May 2018, Universitat de Barcelona

- As a key 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

June 2018, Parc de la Ciutadella de Barcelona

- The ICN2 was at the 2018 Barcelona Science Fair together with collaborating institutions such as the UAB, ICMAB, UB, ACCC and IFAE.
- 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.
- The event paid homage to the figure of Prof. Richard Feynman in the context of the celebrations of the 100 anniversary of his birth.



Science Week

December 2018, Barcelona and Sabadell

The ICN2 was involved in a series of celebrations during the 2018 Science Week, including the final event of the Feynman Total series of events at the Vil·la Urània Civic Center in Barcelona; The first edition of the Science&Tech Girls Vallès held at the Vapor Badia Library (in collaboration with the Societat Catalana de Nancociència i Nanotecnologia, SCN2); and outreach events with researchers such as Miguel Angel Moreno and Dr. César Moreno.



OTHER OUTREACH

CSIC Science Mondays (*Lunes de Ciencia*)

January 2018, 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.

Nano2All Stakeholders Debate

February 2018, Barcelona Institute of Science and Technology (BIST)

- 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, two 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.



Researcher's Night

September 2018, CosmoCaixa, Barcelona

- The European Researchers' Night is a Europe-wide effort to boost public awareness of the positive role of research in society.
- The 2018 program at CosmoCaixa included a series of events at CosmoCaixa, with a specific area devoted to nanoscience and nanotechnology. Many coordinated institutions, including the ICN2, made it possible.
- The ICN2 led a workshop for kids and their families and offered a visit to the traveling exhibit Dimensió Nano.



Feynman Total: Celebrating 100 years of Prof. Richard Feynman's birth

All year, different locations

- The ICN2 was involved in the organization of a series of events celebrating the figure of Prof. Richard Feynman, together with institutions such as Universitat de Barcelona (UB), Societat Catalana de Nanociència i Nanotecnologia (SCN2), and Institut de Ciència de Materials de Barcelona (ICMAB).
- Members of the ICN2 participated in talks, workshops and the design of dissemination materials to bring this brilliant physicist closer to Catalan society.



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 2018 we hosted Prof. Omar M. Yaghi, the James and Neeltje Tretter Chair Professor of Chemistry at the University of California, Berkeley. Widely known for the discovery and development of several classes of new materials, Prof. Yaghi pioneered the new field of reticular chemistry, which he defines as “stitching molecular building blocks into extended structures by strong bonds”. Invited by ICREA Prof. Daniel Maspoch, he gave a talk with the title “Reticular Chemistry” that attracted researchers from the ICN2 but also from other research centers and Departments of the UAB Campus.

The full lecture can be found on the ICN2 YouTube channel.

COFFEE WITH PABLO

In 2018 the “Coffee with Pablo” initiative launched by the Human Resources Department consolidated as an informal channel for internal communication. This event, held twice a-year, allows 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 2018 one such coffee session was held.

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 2018 a total of 38 seminars were held, delivered by researchers from centres in the United States (6), Europe (16), Spain (11) and the rest of the world (5).



OPEN KNOWLEDGE PROGRAMME

The ICN2 Open Knowledge Programme was developed as a forum for the exchange of knowledge, experiences and skills among ICN2 colleagues. Coordinated by Human Resources, the individual programmes are created by the various ICN2 groups/departments, and address a broad topic from different angles. The talks tend to be highly specialised, while also offering an overview of the topic for researchers in other fields and advanced science graduates.

On June 2018 the eighth edition of the Open Knowledge Programme was held, promoted by Dr Ramón Cuadrado from the ICN2 Theory and Simulation Group. The event was organized in the context of the the MaX Center of Excellence in “Materials Design at the Exascale” program. This series of interactive talks were entitled “Spin-Orbit Coupling in SIESTA: Magnetism and Other Capabilities”.

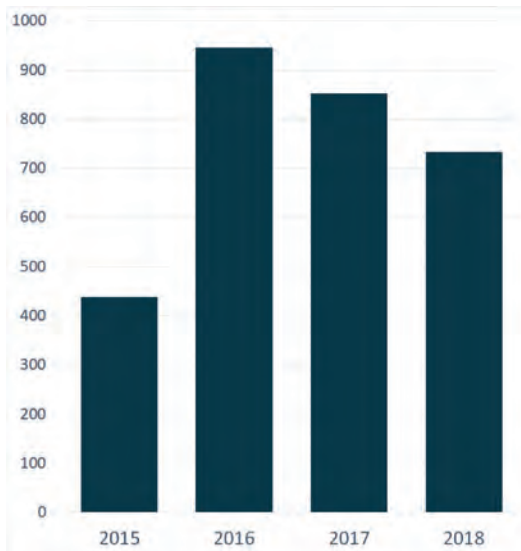
Media Impact

In 2018 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 journalistic online impacts per year



El ICN2 diseña implantes de grafeno para restaurar la capacidad de hablar

Buscan captar la señal en el cerebro y descodificarla en un sintetizador de voz

MAITE BUIS
Barcelona

Investigadores del Institut Català de Nanociència i Nanotecnologia (ICN2), en col·laboració amb el projecte European, han desenvolupat un dispositiu que captura la senyal del cervell i la descodifica en un sintetizador de veu. El dispositiu està dissenyat per captar la senyal elctrica que es genera al cervell quan una persona intenta parlar, i la descodifica en un sintetizador de veu que pot ser utilitzat per persones amb discapacitats de parla.



Los nuevos sensores, flexibles y ultra delgados, se exhiben en el pabellón del grafeno del ICN2

El ICN2 diseña implantes de grafeno para restaurar la capacidad de hablar. Buscan captar la señal en el cerebro y descodificarla en un sintetizador de voz. Los nuevos sensores, flexibles y ultra delgados, se exhiben en el pabellón del grafeno del ICN2.

Los nuevos sensores, flexibles y ultra delgados, se exhiben en el pabellón del grafeno del ICN2.



El ICN2 crea cinco 'spin off' desde 2014

Innovació El centro de investigación hace balance del programa Severo Ochoa del Ministerio de Economía

El Institut Català de Nanociència i Nanotecnologia (ICN2) ha creat cinc empreses spin off des de 2014, segons el balanç del programa Severo Ochoa del Ministeri d'Economia.

El balanç del programa Severo Ochoa del Ministeri d'Economia mostra que el ICN2 ha creat cinc empreses spin off des de 2014.

El colador atòmic que multiplica les possibilitats del grafè

El nou material podria servir per fer diàlisi, sequenciar l'ADN, purificar l'aigua i substituir el silici als xips

ELABORACIÓ BARCELONA

El grafè és el material de les últimes possibilitats i aplicacions. És un material que pot servir per fer diàlisi, sequenciar l'ADN, purificar l'aigua i substituir el silici als xips.

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Los nuevos productos de ICN2

Los nuevos productos de ICN2. Los nuevos productos de ICN2.

Los nuevos productos de ICN2. Los nuevos productos de ICN2.

José A. Garrido INVESTIGADOR DEL ICN2

El Institut Català de Nanociència i Nanotecnologia (ICN2) ha dissenyat implants que captan senyals de los centros cerebrales del habla y las envían a un dispositivo externo, un avance para que algunas personas puedan volver a hablar. PÁGINA 45



Fracturas eléctricas

Las microfibras deosas generan un voltaje que guía a las células cargadas de la reparación. El descubrimiento podría servir para el desarrollo de mejores prótesis

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Annual Report 2018

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Marketing and Communication Department

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