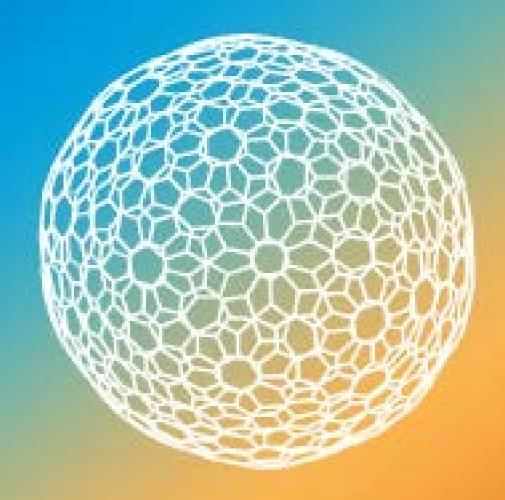
ANNUAL REPORT 2014







Index



Research and Technical Development

Letter from the Director

4

Organisation and People



Severo Ochoa Award

Severo Ochoa Award -Nanodevices for Social Challenges **10**



Research Groups

Atomic Manipulation and Spectroscopy Group

14

Force Probe Microscopy and Surface Nanoengineering Group

18

Inorganic Nanoparticles Group

24

Magnetic Nanostructures Group

30

NanoBioelectronics and Biosensors Group

36

NanoBiosensors and Bioanalytical Applications Group

44

Nanostructured Functional Materials Group

52

Nanostructured Materials for Photovoltaic Energy Group

56



Management and Output



Technical
Development
and Support

Novel Energy-Oriented Materials Group

60

Oxide Nanoelectronics Group

66

Phononic and Photonic Nanostructures Group

70

Physics and Engineering of Nanodevices Group

78

Supramolecular NanoChemistry and Materials Group

82

Theoretical and Computational Nanoscience Group

88

Theory and Simulation Group

94

Electron Microscopy Division

100

Nanofabrication Division

104

Nanomaterials Growth Division

106

Nanoscience Instrument Development Division

110

Core Research Support Facilities

112

Management and Services

116

Scientific Output

118

Projects

121

Finances

122

Facilities and Equipment

125

Technology Transfer

126

Public Outreach

127

Letter from the Director



2014 was a year of growth and intense activity for the Catalan Institute of Nanoscience and Nanotechnology (ICN2).

After the conversion from the former ICN (Institut Català de Nanotecnologia) to the new ICN2 (Institut Català de Nanociència i Nanotecnologia), with the integration of the CSIC groups from the former Centro Mixto CIN2, the process started in 2011 is almost complete. The Board of Trustees of the ICN2 Foundation is formed by the *Generalitat de* Catalunya (Catalan Government), the Consejo Superior de Investigaciones Científicas (CSIC) and the Universitat Autònoma de Barcelona (UAB). Our Patrons are united in their efforts to build a strong centre for research in Nanoscience and Nanotechnology, taking advantage of the strengths of each institution, and enhancing ICN2's scientific potential and impact, financial resources, and competitiveness.

The ICN2 building was officially inaugurated on January 20, 2014, with the presence of **Andreu Mas-Colell** (Minister of Economy and Knowledge of Catalonia, and President of the ICN2 Board of Trustees), **Carmen Vela** (Secretary of State for Research, Development and Innovation of Spain), **Emilio Lora Tamayo** (President of the *Consejo Superior de Investigaciones Científicas*) and **Ferran Sancho** (Rector of the *Universitat Autònoma de Barcelona*). Shortly after, ICN2 received the *Severo Ochoa Excellence Award*, confirming that our efforts were headed in the right direction.

The Severo Ochoa Programme, sponsored by the Spanish Ministry of Economy and Competitiveness (MINECO), aims to identify and support Spanish research centres that are among the world's best in their specialty. This is an outstanding achievement, given the level of competitiveness of these awards,

and will mean a qualitative improvement in the research capabilities of ICN2 and act as a driving force for collaborative activities between the research groups of our Institute, focused on specific, common objectives in "Nanodevices for Societal Challenges in Life, Energy and ICT".

The number of indexed publications (131), with a remarkably high impact factor (5.61), remained notable despite the complexity of the merger process we are completing. ICN2 is strongly involved in the development of one of the European Commission's two FET Flagship Programmes: the Graphene Flagship. In this Annual Report you will also find impressive figures on our success at attracting national and international competitive funding. Additionally, we continued the strategy launched in 2012 to promote technological transfer as a key activity of ICN2. The role and resources of the Technology Transfer Office have been strengthened, which is having a significant impact on the transfer results.

In summary, 2014 was a year of great activity and results for ICN2. Again, our staff have performed exceptionally well in a period of economic hardship and uncertainties. The completion of the institutional changes leading to the conversion to ICN2, the forecast of a brighter economic situation, and the recent attainment of the Severo Ochoa Award are factors that encourage me to be extremely optimistic about the future of our Institute.

I invite you to join me in building this bright future every day, and to participate in this collective journey towards personal and professional growth.

Sincerely,

Prof Pablo Ordejón

Prof Ordejón earned his BSc in Physics (1987) and PhD in Science (1992) at the Universidad Autónoma de Madrid (Spain). 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), where he is currently Research Professor. Since July 2012, he has served as Director of ICN2, where he also leads the Simulation and Theory Research Group.

He has published more than 190 scientific articles, which have received over 17,000 citations (h = 47). Since 2009 he has served as Co-Editor of *EPL* (formerly *Euro Physics Letters*) and since 2004, as Regional Editor of *physica status solidi*. He was in charge of the Condensed Matter Physics area of the Physics Panel of the Spanish National Scientific Evaluation Agency (ANEP), from 2003 to 2006, and 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.

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 is involved in the study of the fundamental properties of materials at the atomistic level. His current interests include, among many others, electronic transport in nanoscale devices and electronic processes at surfaces. He maintains frequent collaborations with industrial laboratories on the simulation of materials processes at the atomic level.

Organisation and People

ORGANISATION

The Institut Català de Nanociència i Nanotecnologia (ICN2) is a non-profit international research institute located in Barcelona, Spain. It was created in 2013, when CSIC joined the Board of Trustees of the former *Institut Català de Nanotecnologia* (ICN), created in 2003 by the Ministry of Universities, Research and Information Society (DIUE) of the Catalan Government and the *Universitat Autònoma de Barcelona* (UAB), and with the incorporation of the CSIC groups from the former *Centro de Investigación en Nanociencia y Nanotecnología* (CIN2), created in 2006 as a joint collaboration between CSIC and ICN.

ICN2 is led by its Director, **Prof Pablo Ordejón**, who reports to the Board of Patrons and is advised by the Scientific Advisory Board, made up of numerous distinguished international scientists.

Research activities are directed by Research Group Leaders - senior scientists of international repute that lead research teams focused on their respective areas of expertise, and that are supported by specialised laboratory engineers and technical and administrative staff.

In 2014, ICN2 comprised 15 Research Groups and 5 Technical Development and Support Divisions and Facilities, covering different areas of nanoscience and nanotechnology.

Research Groups

- Atomic Manipulation and Spectroscopy Group
- Force Probe Microscopy and Surface Nanoengineering Group
- Inorganic Nanoparticles Group
- Magnetic Nanostructures Group
- NanoBioelectronics and Biosensors Group
- NanoBiosensors and Bioanalytical Applications Group
- Nanostructured Functional Materials Group
- Nanostructured Materials for Photovoltaic Energy Group
- Novel Energy-Oriented Materials Group
- Oxide Nanoelectronics Group
- Phononic and Photonic Nanostructures Group
- Physics and Engineering of Nanodevices Group
- Supramolecular NanoChemistry and Materials Group (NANOUP)
- Theoretical and Computational Nanoscience Group
- Theory and Simulation Group

Technical Development and Support

- Electron Microscopy Division
- Nanofabrication Division
- · Nanomaterials Growth Division
- Nanoscience Instrument Development Division
- Core Research Support Facilities

BOARD OF PATRONS

PRESIDENT

Andreu Mas-Colell

Minister of Economy and Knowledge, Generalitat de Catalunya.

VICE-PRESIDENT

Emilio Lora Tamayo

President of CSIC (Consejo Superior de Investigaciones Científicas).

SECRETARY

Josep Maria Martorell i Rodon

Director of Research, Ministry of Economy and Knowledge, Generalitat de Catalunya.

MEMBERS

Lluís Calvo

Institutional CSIC Coordinator in Catalonia.

Antoni Castellà Clavé

Secretary for Universities and Research of the Ministry of Economy and Knowledge, Government of Catalonia.

Ferran Sancho Pifarré

Rector of the Universitat Autònoma de Barcelona (UAB).

José Ramón Urquijo Goitia

Vice-President for Organisation and Institutional Relations, CSIC.



SCIENTIFIC ADVISORY BOARD

PRESIDENT

Prof Miquel Salmerón

Principal Researcher, Lawrence Berkeley National Laboratory; Berkeley, California, USA

MEMBERS

Prof Jeff Bokor

Professor, Department of Electrical Engineering and Computer Sciences, University of California, Berkeley; and Deputy Director for Science, The Molecular Foundry, Lawrence Berkeley National Laboratory

Prof Fernando Briones

Professor of Research, Microelectronics Institute of Madrid (IMM - CSIC); Madrid, Spain

Prof Manuel Cardona (He passed away on July 2, 2014. ICN2 mourns him) Co-founder and Emeritus Professor, the Max Planck Institute; Stuttgart, Baden-Württemberg, Germany

Prof Bruno Chaudret

Director, Laboratoire de Physique et Chimie des Nano-Objets (LPCNO); Toulouse, France

Prof Sylvia Daunert

University Research Professor; Distinguished Professor, College of Arts & Sciences; and Gill Eminent Professor of Analytical and Biological Chemistry, University of Kentucky; Lexington, Kentucky, USA

Prof Bengt Kasemo

Professor of Physics, Department of Physics, Chalmers University of Technology; Gothenburg, Sweden.

Prof Jörg P. Kotthaus

Professor of Experimental Physics, Ludwig-Maximilians-Universität München; Munich, Bavaria, Germany

Prof Ernst Meyer

Professor, Institut für Physik, University of Basel; Basel, Switzerland

Prof Anthony Turner

Head of Biosensors & Bioelectronics Centre IFM, Linköping University; Linköping, Sweden

THE ICN2 TEAM

ICN2 is defined by its people. From senior researchers to administration staff, ICN2 personnel work as a team, contributing their creativity, energy, dedication and hard work to further the Institute.

ICN2 prides itself on being an attractor of talent, seeking to provide an environment and an image of excellence that draws

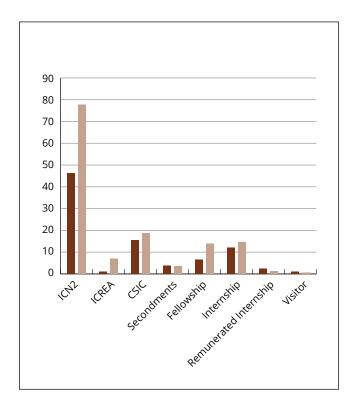
talented scientists, technicians and support personnel from around the world. The Institute has succeeded in this endeavour, as embodied in its highly-qualified scientific staff and demonstrated by its high level of scientific output. Many researchers who have completed a doctoral thesis or post-doctoral stay at ICN2 have moved on to highly prestigious institutes such as Harvard, Yale, the Max Planck institutes, CNRS and CEA. Thus, ICN2 is continuously offering new positions for junior scientists.

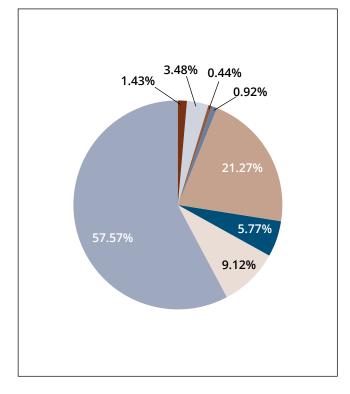
Over the course of 2014, ICN2 engaged an annual average workforce of 226.4 people. Recruitment reached an historic peak, as the Institute fully consolidated its management and administrative teams and met its human resources objectives.

ICN2 is an equal opportunity employer and seeks a workforce diverse in age, culture nationality and gender. By the end of 2014, ICN2 personnel represented multiple nationalities; women comprised an important percentage of all personnel.

	Female	Male	Total
ICN2	46.2	77.8	123.9
ICREA	1	7	8
CSIC	15.6	18.7	34.3
Secondments	3.8	3.6	7.3
Fellowship	6.6	14.0	20.5
Internship	12.1	14.7	26.8
Remunerated Internship	2.5	1.3	3.9
Visitor	1.2	0.4	1.6
Total	88.9	137.5	226.4

Nationalities			
Africa	3.2	1.43%	
Asia	7.9	3.48%	
Australia	1	0.44%	
Central America	2.1	0.92%	
Europe	48.2	21.27%	
North America	13.1	5.77%	
South America	20.6	9.12%	
Spain	130.3	57.57%	
Grand Total	226.4	100.00%	





Research and Technical Development



Severo Ochoa Award -Nanodevices for Social Challenges

The research developed at ICN2 has a big impact on fields such as life sciences (medicine, health, environment), energy and information and communication technologies. This is one of the main reasons why the Spanish Ministry of Economy and Competitiveness acknowledged the Institute in 2014 as a **Severo Ochoa Center of Excellence**. This Programme recognizes the excellence of the scientific contributions of centres, their potential industrial and social impact and their potential for talent attraction. At the time ICN2 received the award, only 18 research centres had been awarded.

The funding provided by the Severo Ochoa award will focus on the Programme on "Nanodevices for Social Challenges". It is largely devoted to the recruitment of staff and the procurement of equipment to support the development of research projects.



CROSS-DISCIPLINARY APPROACHES

The Programme is based on four cross-disciplinary methodological approaches:

Growth and synthesis of nanomaterials

Expertise in growth of thin films, PLD, CVD, ALD, etc. with a broad range of materials, including graphene, metal and multiple component oxides.

Nanofabrication

Expertise in both bottom-up and topdown fabrication, including self-assembly, nanoparticle synthesis, corrosive etching, supramolecular chemistry, screenprinting, nanoimprint lithography, roll-to-roll lithography on flexible substrates, inkjet printing, and rapid prototyping.

Characterisation and metrology

World-class expertise in a very broad range of characterisation techniques, some of them

developed by ICN2 researchers. Experience in nanometrology includes two patent applications, and the plan to establish a dedicated industrial Nanometrology centre with private partners.

Theory and simulation

Expertise includes pioneering developments of tools for atomistic simulations of matter, including electronic and thermal processes in nanodevices, and the structure and properties of nanomaterials.

RESEARCH AREAS

The research will produce specific applications and devices which are able to reach the market, providing new solutions to major social challenges in the following areas:

Biosystems

Expertise in optical and electrochemical biosensing, biofunctionalised inorganic

nanoparticles, supramolecular chemistry, water-surface interactions and characterisation. Related activities include EU projects in point-of-care devices and biosensors, ERC in nanomaterials for diagnostics & therapy, commercialisation with numerous licensed patents and two spin-off companies (biosensing and drug delivery).

Energy

Expertise in materials, capacitors and energy transfer, phononics and photonics, photovoltaics, piezoelectrics, nanofabrication of flexible substrates and thin-film materials, spectroscopy and characterisation, leadership positions in EU projects and platforms (Graphene Flagship, Photonics platform, ERC in piezoelectrics), collaborative prototyping with industry in next-generation photovoltaics, roll-to-roll lithography, and inks for active layers.

Information and communication technologies

Expertise in materials, spintronics, magnetism, graphene, topological isolators, photonics, phononics and heat transfer, nanodevice fabrication and characterisation.

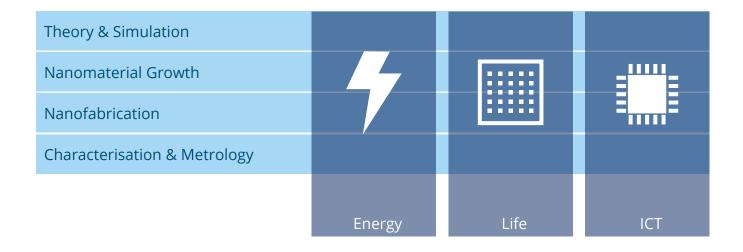
In 2009, the EU identified KETs for their potential impact in strengthening Europe's industrial and innovation capacity. Six KETs were highlighted as key for European sustainable growth: Nanotechnology; Microand Nano-electronics; Advanced Materials; Photonics; Industrial Biotechnology and,

Advanced Manufacturing. In this context, the relevance of the ICN2 Programme on "Nanodevices for Social Challenges" is evident, as it involves virtually all the six KETs.

BEYOND RESEARCH

In addition to the scientific cross-disciplinary goals, ICN2 will carry out a comprehensive **recruiting and training programme** aimed at attracting and developing the professional careers of talented senior and junior researchers associated with the Severo Ochoa Programme (PhD programme; Postdoctoral programme; Visitors programme; ICN2-User Programme Training; Academia Intern Programme; and workshops and seminars). It also includes other ambitious actions such as the creation of a specific Gender action plan and international knowledge dissemination and outreach activities.

An external Scientific and Industrial Advisory Committee (SIAC), appointed by the Director with the advice of the ICN2 Scientific Advisory Board, advises on strategic directions and the progress of the project. The work plan is divided into seven Work Packages, one per Application Area and Cross-Disciplinary Activity. Overall management is carried out by the Project Management Committee, which is formed by one representative of each WP, plus two additional members to follow up dissemination and technology transfer activities.



Research Groups

The research workforce of ICN2 is distributed across 15 highly specialized research groups. Synergies among groups with complementary research lines are stimulated.



- > Atomic Manipulation and Spectroscopy Group
- > Force Probe Microscopy and Surface Nanoengineering Group
- > Inorganic Nanoparticles Group
- > Magnetic Nanostructures Group
- > NanoBioelectronics and Biosensors Group
- > NanoBiosensors and Bioanalytical Applications Group
- > Nanostructured Functional Materials Group
- > Nanostructured Materials for Photovoltaic Energy Group
- > Novel Energy-Oriented Materials Group
- > Oxide Nanoelectronics Group
- > Phononic and Photonic Nanostructures Group
- > Physics and Engineering of Nanodevices Group
- > Supramolecular NanoChemistry and Materials Group
- > Theoretical and Computational Nanoscience Group
- > Theory and Simulation Group

Atomic Manipulation and Spectroscopy Group

Main Research Lines -

- Hybrid interfaces for spintronics: metalorganic networks on metals and topological insulators
- Graphene-based nanostructures: tailoring morphology, edge structure and electronic properties
- Electron scattering in 2D nanostructures and materials with strong spin-orbit interaction



GROUP MEMBERS

Michele Gastaldo, Doctoral Student Sylvie Godey, Technician Aitor Mugarza, Tenure Track and Group Leader Stefano Schirone, FI Doctoral Student Miguel Ángel Valbuena, Postdoctoral Researcher





GROUP LEADER



Dr Aitor Mugarza

Dr Aitor Mugarza earned his BS degree in Physics in 1997 and his PhD in Physics in 2002, both at the University of the Basque Country. After his doctoral studies, he was awarded a Marie Curie fellowship to work as a postdoctoral scientist at the Lawrence Berkeley National Laboratory, USA, and at the Materials Science Institute of Barcelona (ICMAB). He later joined ICN in 2007 with a Ramon y Cajal Fellowship. In 2013, he was appointed Group Leader of the Atomic Manipulation and Spectroscopy Group at ICN2. He is author of 49 articles



NEW PROJECTS & MILESTONES

In 2014 the Atomic Manipulation and Spectroscopy Group focused on three main objectives.

One of the main ongoing research lines has been the study of electronic and magnetic properties of hybrid metalorganic heterostructures. In particular, by combining local probe microscopy and X-ray spectroscopy, we have demonstrated: i) how the molecular charge and spin can be manipulated by selectively doping molecular orbitals; ii) how the momentum of the smallest magnetic objects, single-molecule magnets, can be coupled to ferromagnetic and antiferromagnetic substrates.

Another active field for the group has been the study of **electron scattering on different nanostructured materials**. Here we have focused on the role of order and periodicity of metallic nanostructures, and of the edge structure of graphene nanoislands, on the scattering of surface electrons.

A new project (Covalent Hybrids on Surfaces) was launched, covering research lines dedicated to hybrid organic topological insulator and graphene-based heterostructures, with the incorporation of three new postdoctoral researchers (one a Beatriu de Pinós Fellow), and a doctoral student (Severo Ochoa PhD Fellow).



PUBLICATIONS

Coupling of single, double, and triple-decker metal-phthalocyanine complexes to ferromagnetic and antiferromagnetic substrates, Lodi Rizzini A., Krull C., Mugarza A., Balashov T., Nistor C., Piquerel R., Klyatskaya S., Ruben M., Sheverdyaeva P.M., Moras P., Carbone C., Stamm C., Miedema P.S., Thakur P.K., Sessi V., Soares M., Yakhou-Harris F., Cezar J.C., Stepanow S., Gambardella P., Surface Science: vol. 630, 361-374 (2014). IF: 1.87

Fieldlike and antidamping spin-orbit torques in as-grown and annealed Ta/CoFeB/MgO layers, Avci C.O., Garello K., Nistor C., Godey S., Ballesteros B., Mugarza A., Barla A., Valvidares M., Pellegrin E., Ghosh A., Miron I.M., Boulle O., Auffret S., Gaudin G., Gambardella P., *Physical Review B - Condensed Matter and Materials Physics* (21): vol. 89 (2014). IF: 3.664

Metallic thin films on stepped surfaces: lateral scattering of quantum well states, F Schiller, Z M Abd El-Fattah, S Schirone, J Lobo-Checa, M Urdanpilleta, M Ruiz-Osés, J Cordón, M Corso, D Sánchez-Portal, A Mugarza, J E Ortega, New Journal of Physics: vol. 16 (2014). IF: 3.671

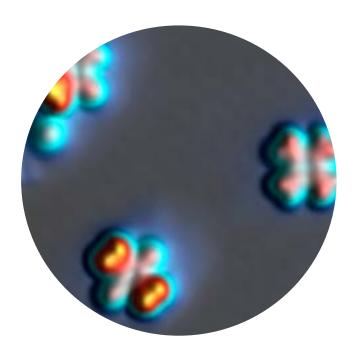
(h-index = 18), and more than 30 invited talks at international conferences, universities and schools since 2007.

His research activity is based on the investigation of the electronic and magnetic properties of matter on the nanoscale, and developing strategies to manipulate them with atomic precision. By combining Scanning Tunnelling Microscopy techniques with Synchrotron Radiation Spectroscopy, he correlates microscopic phenomena to macroscopic observables that are relevant for the understanding and design of new materials and devices. He is currently focusing on novel materials that include molecular nanostructures, graphene, topological insulators and other 2D Dirac materials.

Spin-dependent electron scattering at graphene edges on Ni(111), Garcia-Lekue A., Balashov T., Ollé M., Ceballos G., Arnau A., Gambardella P., Sánchez-Portal D., Mugarza A., *Physical Review Letters* (6): vol. 112 (2014). IF: 7.728

Spin tuning of electron-doped metal-phthalocyanine layers, Sebastian Stepanow, Alberto Lodi Rizzini, Cornelius Krull, Jerald Kavich, Julio C. Cezar, Flora Yakhou-Harris, Polina M. Sheverdyaeva, Paolo Moras, Carlo Carbone, Gustavo Ceballos, Aitor Mugarza, Pietro Gambardella, Journal of the American Chemical Society (14): vol. 136, 5451-5459 (2014). IF: 11.444

Structure and magnetism of Tm atoms and monolayers on W(110), Corneliu Nistor, Aitor Mugarza, Sebastian Stepanow, Pietro Gambardella, Kurt Kummer, José Luis Díez-Ferrer, David Coffey, César de la Fuente, Miguel Ciria, and José I. Arnaudas, *Physical Review B - Condensed Matter and Materials Physics*: vol. 90 (2014). IF: 3.664





PROJECTS

SGR, funded by **AGAUR**, 01/01/2014 - 31/12/2016, Aitor Mugarza

Electron Scattering in materials with strong spinorbit coupling, funded by **AGAUR**, 01/03/2014 - 28/02/2017, Aitor Mugarza

Atomic-scale engineering of unconventional organic superconductors, funded by **AGAUR**, 30/09/2014 - 29/09/2016, Aitor Mugarza

Materiales con efecto espin-orbita amplificados para espintronica, funded by **MINECO**, 01/01/2011 - 30/06/2014, Aitor Mugarza

Híbridos covalentes en superficies (SuperHybrid), funded by **MINECO**, 01/01/2014 - 31/12/2016, Aitor Mugarza



CONTRIBUTIONS

Graphene nanostructures on Ni(111): structural, electronic and scattering properties, Nanospain 2014, organized by Phantoms Foundation, Madrid (Spain), 11-14/03/2014, Mugarza, A. (Invited)

Graphene nanostructures on Ni(111): structural, electronic and scattering properties, **32nd**National Meeting on Condensed Matter
Physics, Sao Paulo (Brazil), 13-17/05/2014,
Mugarza, A. (Invited)

Tuning molecular properties at metallic surfaces, European Conference on Surface Science - ECOSS30, organized by Bilkent University, Ankara (Turkey), 31-08/2014 - 05/09/2014, Mugarza, A. (Invited)

Manipulating the spin by doping single molecules at the metallic interface, Conference on Spintronics and Magnetochemistry on the Atomic and Molecular Level, organized by Laboratory for Micro- and Nanotechnology Paul Scherrer Institut, Switzerland, Ascona (Switzerland), 26-30/10/2014, Mugarza, A. (Invited)

Electron Scattering of Rashba-split states in the BiAg2 surface alloy, Fuerzas y Tunel, 2014, organized by Centro de Física de Materiales (CSIC-UPV/EHU), Donostia, Spain; Centro Nacional de Biotecnología (CNB-CSIC), Madrid, Spain, San Sebastián (Spain), 27-29/08/2014, Schirone, S. (Oral)

Electron Scattering of Rashba-split states in the BiAg2 surface alloy, "Nicolás Cabrera" International Summer School, New Frontiers in to Scanning Force Microscopy:from Ultra-High Vacuum to Biological Material, organized by Instituto Universitario de Ciencias de Materiales Nicolás Cabrera, Madrid (Spain), 14-16/07/2014, Schirone, S. (Poster)



COURSES

Nanoscale Surface Characterisation, in Master's Degree in Nanotechnology & Materials Science, **Universitat Autònoma de Barcelona, Barcelona (Spain)**, 10/2013-01/2014, Dr Aitor Mugarza

Local Probe Microscopies, in Master's Degree in Nanotechnology & Materials Science, **Universitat Autònoma de Barcelona, Barcelona (Spain)**, 10/2014-12/2014, Dr Aitor Mugarza

More information: http://ams.icn.cat/

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 MEMBERS

Carlo Alberto Amadei, CSIC Visiting Doctoral Student Laura Cabezas, CSIC Visiting Student Annalisa Calò, Postdoctoral Researcher María José Esplandiu, CSIC Tenured Scientist Laura Evangelio, CSIC Visiting Doctoral Student Jordi Fraxedas, CSIC Research Scientist and Group Leader Roger Fraxedas, Assistant Armak Karimi González, CSIC Visiting Student
Federico Gramazio, Doctoral Student
Alba Mesa, CSIC Visiting Student
Ramón Pérez, CSIC Visiting Student
Daniel Ruso, CSIC Technician
Sergi Santos, CSIC Visiting Postdoctoral Researcher
Albert Verdaguer, CSIC Tenured Scientist
Oriol Vidal, CSIC Visiting Student



GROUP LEADER



CSIC Research Scientist Dr Jordi Fraxedas

Jordi Fraxedas (Tarragona, 1962) graduated in Physics from the University of Zaragoza (Spain) in 1985 and obtained his PhD (Dr rer. nat.) in 1990 from the University of Stuttgart (Germany). His thesis work was performed at the Max Planck Institut für Festkörperforschung and at the Berliner Speicherring für Synchrotronstrahlung (BESSY), under the supervision of Prof M. Cardona. After a post-doctoral position at the European Synchrotron Radiation Facility (ESRF) in Grenoble (France) and an Established Researcher position at the European Laboratory



NEW PROJECTS & MILESTONES

The Group participates in several projects at the European and Spanish level. Within the EU FP7 the Group is involved in advanced AFM instrumentation and in directed self-assembly of block co-polymers in collaboration with leading European universities and companies. In the first case, a prototype of an AFM head is being designed which should be able to be operated in industrial environments with a robot arm at high speed (3 MHz) and providing real-time information on the mechanical properties of surfaces of industrial interest (plastic injection, solar cells, etc.). In the second case the

interfacial mechanisms of self-assembly are being investigated at the fundamental level in order to better address the future use of new smaller polymers.

At the Spanish level the Group participates in two projects focused on the **tailoring of the affinity of water to surfaces and to micro/nanofluidics using carbon-based materials** (nanotubes and graphene), respectively. The main objective is to be able to control the dynamics of water at different interfaces, i.e., structuring water as ice at temperatures above 0 degrees C and inducing mass transport via electrokinetic processes.



for Particle Physics (CERN) in Geneva (Switzerland), he joined the Solid State Research Institute of Barcelona (ICMAB) of the Spanish Research Council (CSIC) in 1995 and worked as a *Chercheur associé* at the Centre National de la Recherche Scientifique (CNRS) in 2002.

His research activity is focused on interfacial phenomena and surface science. He has coauthored more than 100 peer-reviewed scientific articles and published the books entitled *Molecular Organic Materials: From Molecules to Crystalline Solids* (Cambridge University Press, 2006) and *Water at Interfaces: A Molecular Approach* (Taylor and Francis CRC (2014)).



PUBLICATIONS

A nanoscopic approach to studying evolution in graphene wettability, Chia-Yun Lai, Tzu-Chieh Tang, Carlo A. Amadei, Alexander J. Marsdend, Albert Verdaguer, Neil Wilson, Matteo Chiesa, *Carbon*: vol. 80, 784-792 (2014). IF: 6.16

Bioinspired catechol-terminated self-assembled monolayers with enhanced adhesion properties, Guardingo M., Bellido E., Miralles-Lluma R., Faraudo J., Sedó J., Tatay S., Verdaguer A., Busqué F., Ruiz-Molina D., *Small* (8): vol. 10, 1594-1602 (2014). IF: 7.514

Electrocatalytic tuning of biosensing response through electrostatic or hydrophobic enzyme – graphene oxide interactions, Luis Baptista-Pires, B. Pérez-López, Carmen C. Mayorga-Martínez, Eden Morales-Narváez, Neus Domingo, María José Esplandiu, Francesc Alzina, C.M. Sotomayor Torres, A. Merkoçi, *Biosensors and Bioelectronics*: vol. 61, 665-662 (2014). IF: 6.451

Four molecular superconductors isolated as nanoparticles, De Caro D., Faulmann C., Valade L., Jacob K., Chtioui I., Foulal S., de Caro P., Bergez-Lacoste M., Fraxedas J., Ballesteros B., Brooks J.S., Steven E., Winter L.E., *European Journal of Inorganic Chemistry* (2014). IF: 2.965

Hydrophobic coating of mica by stearic acid vapor deposition, Sauthier G., Segura J.J., Fraxedas J., Verdaguer A., Colloids and Surfaces A: *Physicochemical and Engineering Aspects*: vol. 443, 331-337 (2014). IF: 2.354

Influence of the relative molecular orientation on interfacial charge-transfer Excitons at donor/acceptor Nanoscale heterojunctions, Aghamohammadi M., Fernández A., Schmidt M., Pérez-Rodríguez A., Goni A.R., Fraxedas J., Sauthier G., Paradinas M., Ocal C., Barrena E., Journal of Physical Chemistry C (27): vol. 118, 14833-14839 (2014). IF: 4.835

Sequential tasks performed by catalytic pumps for colloidal crystallisation, Afshar Farniya A., Esplandiu M.J., Bachtold A., *Langmuir* (39): vol. 30, 11841-11845 (2014). IF: 4.384

Sub-10 nm resistless nanolithography for directed self-assembly of block copolymers,

M. Fernández-Regulez, L. Evangelio, M. Lorenzoni, J. Fraxedas and F. Pérez-Murano, *ACS Applied Materials & Interfaces* (23): vol. 6, 21596-21602 (2014). IF: 5.9

Synthesis of polydopamine at the femtoliter scale and confined fabrication of Ag nanoparticles on surfaces, Guardingo M., Esplandiu M.J., Ruiz-Molina D., *Chemical Communications* (83): vol. 50, 12548-12551 (2014). IF: 6.718

Unlocking higher harmonics in atomic force microscopy with gentle interactions, Santos S., Barcons V., Font J., Verdaguer A., *Beilstein Journal of Nanotechnology* (1): vol. 5, 268-277 (2014). IF: 2.332

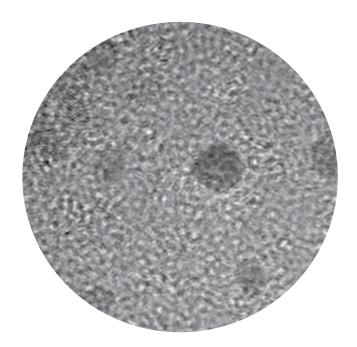
Water adsorption on etched hydrophobic surfaces of L-, D- and DL-valine crystals, Segura J.J., Verdaguer A., Fraxedas J., *Surface Science*: vol. 621, 191-196 (2014). IF: 1.87



Nanoscòpia i Nanoenginyeria de Superfícies, funded by AGAUR, 01/01/2014 - 31/12/2016, Iordi Fraxedas

Automated In-line Metrology for Nanoscale Production (AIM4NP), funded by EC, 01/03/2013 - 28/02/2016, Jordi Fraxedas

Afinidad y estructura del agua interfacial sobre superficies nanoestructuradas en condiciones ambientales (NANEAU), funded by MINECO, 01/01/2013 - 31/12/2015, Albert Verdaguer





CONTRIBUTIONS

Confocal Fluorescence Microscopy: the use of ion fluorescent probes for studing micro/ nanoactuators propelled by catalytical reactions, **31st Leica Workshop**, organized by Leica. Barcelona (Spain), Esplandiu, M. José (Invited)

Controlling water freezing on surfaces, CECAM-ETHZ. Zurich (Switzerland), 02-04/04/2014, Verdaguer, A. (Invited)

Development and performance analysis of catalytic micropumps, International Workshop on Micro and Nanomachines (MNM2014), organized by Center for Integrated Nanotechnologies, USA; Columbia University, USA; Max Planck Institute for Intelligent Systems, Germany. Hannover (Germany), 02-05/07/2014, Esplandiu, M. José (Invited)

Optimizing the performance of catalytic micropumps: a theoretical approach, International Workshop on Micro and Nanomachines (MNM2014), organized by Center for Integrated Nanotechnologies,

USA; Columbia University, USA; Max Planck Institute for Intelligent Systems, Germany. Hannover (Germany), 02-05/07/2014, Esplandiu, M. José (Invited)

Agua interfacial: ¿estructurada o estructurante? Ciencia y Tecnología del Siglo XXI, organized by Universidad de Granada. Granada (Spain), 11/11/2014, Jordi Fraxedas (Invited)

Neutral amphiphilic molecules as structuring agents for the growth of nanocrystals or nanoparticles of molecule-based superconductors, VI Journées Franco-Catalanes de Chimie Moléculaire, Toulouse (France), 01/2014, D. de Caro; K. Jacob; S. Foulal; I. Chtioui; C. Faulmann; L. Valade; J. Fraxedas (Oral presentation)

Euro AFM Forum 2014, organized by Third Institute of Physics - Biophysics, Göttingen; The Institute for Materials Physics - Georg-August University Göttingen. Göttingen (Germany), 17-19/03/2014 (Oral presentation)

Room temperature ice water films induced by surfaces: BaF2 and CaF2 lattice mismatch,

WaterEurope, organized by CNRS and
UPMC, Paris, France and EPFL, Lausanne,
Switzerland; University of Barcelona,
Spain;Universitat Politècnica de CatalunyaBarcelona Tech, Spain. Zaragoza (Spain), 1214/06/2014, A. Verdaguer, J. Fraxedas (Oral presentation)

Water-induced surface passivation of amino acids, WaterEurope, organized by CNRS and UPMC, Paris, France and EPFL, Lausanne, Switzerland; University of Barcelona, Spain; Universitat Politècnica de Catalunya-Barcelona Tech, Spain. Zaragoza (Spain), 12-14/06/2014, J. Fraxedas; A. Verdaguer; E. Barrena; C. Ocal (Oral presentation)

Water footprints in tip-sample force reconstruction for dynamic atomic force microscopy in ambient conditions, **5th Multifrequency AFM Conference**, organized by Instituto de Ciencias de Materiales, CSIC. Madrid (Spain), 16-18/06/2014, Verdaguer, A. (Oral presentation)

Room temperature Ice Films Induced by Structural Lattice Mismatch: BaF2 and CaF2,

The 45th Annual Conference of the British Association for Crystal Growth, organized by British Association for Crystal Growth. Leeds, United Kingdom, 13-15/07/2014, Verdaguer, A. (Oral presentation)

Attractive Tip-sample Force Reconstruction For Dynamic Atomic Force Microscopy in Ambient Conditions, Fuerzas y Túnel, 2014, organized by Centro de Física de Materiales (CSIC-UPV/EHU), Donostia, Spain; Centro Nacional de Biotecnología (CNB-CSIC), Madrid, Spain. San Sebastián (Spain), 27-29/08/2014, Verdaguer, A. (Oral presentation)

AFM nanolithography for block co-polymer directed self-assembly, ECOSS-30, 30th European Conference on Surface Science, organized by Bilkent University. Ankara (Turkey), 31/08/2014 - 05/09/2014, L. Evangelio; M. Fernández-Regulaz; J. Fraxedas; F. Pérez-Murano (Oral presentation)

Creation of chemical guiding patterns for directed self-assembly of block co-polymers by AFM lithography, SPIE Advanced Lithography, San Diego (USA), 23/02/2014 -27/07/2014, F. Pérez-Murano; M. Fernández-Regulez; L. Evangelio; J. Fraxedas (Poster)

Automated In-line Metrology for Nanoscale Production - aim4np, ECOSS-30, 30th European Conference on Surface Science, organized by Bilkent University. Ankara (Turkey), 31/08/2014 - 05/09/2014, J. Fraxedas; U. Staufer; R. Munnig Schmidt; J. Spronck; E. Rull Trinidad; R. Deng, G. Schitter; M. Thier; R. Hainisch; R. Saathof; F. Pérez-Murano; A. Verdaguer; A. Blümel; E. J. W. List-Kratochvil; R. Koops; M. van Veghel; R. Sum; A. Lieb; W. Schott; D. Dontsov; T. Sulzbach; W. Engl; C. Penzkofer; C. Colominas; K. Fluch; A. García-Granada; J. M. Puigoriol-Forcada (Poster)



BOOKS

Water at Interfaces: A Molecular Approach.

J. Fraxedas. USA: CRC Press / Taylor and Francis, FL. 2014.



COURSES

Chemistry for Specific Materials, included in the Master Universitari en Química Industrial i Introducció a la Recerca Química. **Universitat Autònoma de Barcelona, Barcelona (Spain)**, 28/10/2014



THESES 2014

Doctorand: Ali Afshar Farinya

Title: Development and Performance Analysis

of Autonomous Catalytic Micropumps

Defense Date: 41774

Director: Dr María José Esplandiu

Inorganic Nanoparticles Group

Main Research Lines

- Design and development of synthetic strategies for the production of complex nanoparticles
- Functionalisation with specific relevant (bio)molecules
- The study of their physicochemical and fundamental properties



GROUP MEMBERS

Martí Busquets, Doctoral Student Eudald Casals, Laboratory Engineer Sarah Deville, Visiting Doctoral Student Agnieszka Dybowska, Visiting Doctoral Student Víctor F. Puntes, ICREA Research Professor and Group Leader Neus Gómez, Ramón y Cajal Postdoctoral Researcher Cecilia López, Group Project Manager Jedrzej Rafal Malec, CSIC Visiting Student Katia Maltoni, Visiting Senior Researcher Florind Merkoçi, Technician Laura Moreno, Visiting Student

Javier Patarroyo, Doctoral Student Rozhin Penjweini, Visiting Doctoral Student Ariadna Peral, Group Project Manager Jordi Piella, Doctoral Student Joana Ribeiro, Visiting Postdoctoral Researcher Sofia Rubio, Doctoral Student Ngoc Tran Thi Thanh, Doctoral Student Jonathan Yeung, Visiting Student Tetyana Yudina, Doctoral Student Yiayuan Zhao, Visiting Doctoral Student Mirjam Zimmerman, Visiting Doctoral Student



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; nanotoxicology and nanosafety; and myriad applications for sectors including medicine and the environment.

Prof 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 Magnetoresistance



NEW PROJECTS & MILESTONES

In 2014 the Inorganic Nanoparticles Group completed several of its ongoing projects, such as NanoTOES - Nanotechnology: Training of Experts in Safety, and began many new ones, such as Framework to respond to regulatory needs of future nanomaterials and Markets from European Union - FP7.

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



in granular alloys. He then spent more than 3 years at the University of California, Berkeley, and the Lawrence Berkeley National Laboratory (LBNL), in the groups of 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 University of Barcelona, and in 2005 obtained an ICREA Professorship at ICN to create the Inorganic Nanoparticles Group, which he presently heads.

By the end of 2013, Prof Puntes held 110 peer-reviewed publications and over 6,000 total citations. He is also well-known for his work in science communication for the general public, his industrial and commercial efforts, and for his endeavours linking science and art.

By the end of 2014, Prof Puntes held 110 peer-reviewed publications and over 7,000 total citations.

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

I. Design and development of synthetic strategies for the production of complex nanoparticles (focusing on complex multicomponent and hollow nanoparticles comprising different families of metal, metal oxides, semiconductor oxides and semiconductors).

II. Functionalisation with specific relevant (bio) molecules and

III. The study of their physicochemical and fundamental properties. As a result, we design new drug-delivery platforms, advanced catalysts to improve energy-chemical processes, optimize NP's features to enhance the production of hydrogen or boost the 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.



PUBLICATIONS

Common Strategies and Technologies for the Ecosafety Assessment and Design of Nanomaterials Entering the Marine Environment, Corsi, I., Cherr, GN., Lenihan, HS., Labille, J., Hassellov, M., Canesi, L., Puntes, V. F., et al., *ACS Nano* (10): vol. 8, 9694-9709 (2014). IF: 12.033

Gene expression profiles reveal distinct immunological responses of cobalt and cerium dioxide nanoparticles in two in vitro lung epithelial cell models, Verstraelen, S., Remy, S., Casals, E., De Boever, P., Witters, H., Gatti, A., Puntes, V.F., Nelissen, I., *Toxicology Letters* (3): vol. 228, 157-169 (2014). IF: 3.355

Interaction of differently functionalized fluorescent silica nanoparticles with neural stem- and tissue-type cells, Izak-Nau E., Kenesei K., Murali K., Voetz M., Eiden S., Puntes V.F., Duschl A., Madarasz E., *Nanotoxicology* (suppl. 1): vol. 8, 138-148 (2014). IF: 7.336

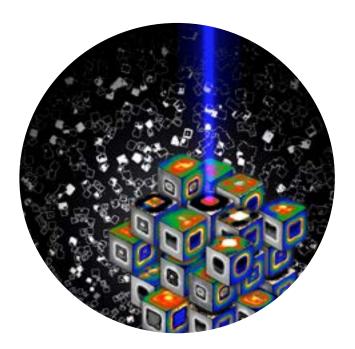
Little Adjustments Significantly Improve the Turkevich Synthesis of Gold Nanoparticles, Schulz, F., Homolka, T., Bastús, NG., Puntes, V.F., Weller, H., Vossmeyer, T., *Langmuir* (35): vol. 30, 10779-10784 (2014). IF: 4.384

Nanoparticles for Imaging, Sensing, and Therapeutic Intervention, Bogart, LK., Pourroy, G., Murphy, CJ., Puntes, V. F., Pellegrino, T., Rosenblum, D., Peer, D., Lévy, R., *ACS Nano* (4): vol. 8, 3107-3122 (2014). IF: 12.033

Optimising the use of commercial LAL assays for the analysis of endotoxin contamination in metal colloids and metal oxide nanoparticles, Li, Y., Italiani, P., Casals, E., Tran, N., Puntes, V.F., Boraschi, D., *Nanotoxicology*: vol. 14, 1-12 (2014). IF: 7.336

Programmed iron oxide nanoparticles disintegration in anaerobic digesters boosts biogas production, Casals, E., Barrena, R., García, A., González, E., Delgado, L., Busquets Fité, M., Font, X., Arbiol, J., Glatzel, P., Kvashnina, K., Sánchez, A., Puntes, V. F., *Small* (14): vol. 10, 2801-2808 (2014). IF: 7.514

Synthesis of highly monodisperse citratestabilized silver nanoparticles of up to 200 nm: Kinetic control and catalytic properties, Bastús, NG., Merkoçi, F., Piella, J., Puntes, V. F., Chemistry of Materials (9): vol. 26, 2836-2846 (2014). IF: 8.535





PROJECTS

SGR, funded by **AGAUR**, 28/09/09 - 30/04/2014, Víctor F. Puntes

SGR, funded by **AGAUR**, 01/01/2014 - 31/12/2016, Víctor F. Puntes

NanoTOES—Nanotechnology: Training Of Experts in Safety (NANOTOES), funded by **EC**, 01/11/10 - 28/02/2015, Víctor F. Puntes

A pan-European infrastructure for quality in nanomaterials safety testing (QNANO), funded by **EC**, 01/02/11 - 31/01/2015, Víctor F. Puntes

Developing New Strategies for the Production of Viable Hybrid Nanocrystals with Applicability in Energy Conversion and (Photo)catalysis (MINE), funded by **EC**, 01/12/2012 - 30/11/2015, Neus Gómez Bastús

Assessment and mitigation of nano-enabled product risks on human and environmental health: Development of new strategies and creation of a web-based guidance tool for nanotech industries (GUIDEnano), funded by EC, 01/11/2013 - 30/04/2017, Víctor F. Puntes

Framework to respond to regulatory needs of future nanomaterials and markets (FutureNanoNeeds), funded by **EC**, 01/01/2014 - 31/12/17, Víctor F. Puntes

Cerium Oxide nanoparticles as a new therapeutic tool for tissue regeneration in liver diseases, funded by **La Marató TV3**, 14/01/2013 - 13/01/2016, Víctor F. Puntes

Synthesis of metal-semiconductor hybrid nanocrystals for energy conversion and catalysis, funded by **MINECO**, 01/01/2012 - 14/12/2014, Víctor F. Puntes

Desarrollo de Estrategias para Síntesis de Nanocristales Inorgánicos Multi-componente Complejos con Propiedades Físico-Químicas Ajustables (TUNANOCRYSTAL), funded by **MINECO**, 01/01/2013 - 31/12/2015, Víctor F. Puntes



CONTRIBUTIONS

Nanoceria, NaNaX 6 Nanoscience with nanocrystals, organized by University of Linz & Gme; ETH Zurich; CEA Grenoble; City University of Hong Kong, Bad Hofgastein (Austria), 18-23/05/2014, Puntes, V. (Invited)

Nanoceria for nanomedicine, **E-MRS 2014 Spring Meeting**, organized by E-MRS. Lille (France), 26-30/05/2014, Puntes, V. (Invited)

Hi ha nous escenaris per a la construcció del coneixement?, FIET: Fòrum Internacional d'Educació i Tecnologia, organized by Grup de recerca ARGET. URV. Tarragona (Spain), 25-28/06/2014, Puntes, V. (Invited)

Nanotechnology in Health: Gold Nanoparticles as Radiotherapy Enhancers, Radio Oncology Department, organized by Radio Oncology Department. Lausanne (Switzerland), 23-24/01/2014, Puntes, V. (Invited Seminar)

Nanoparticle properties and their interactions with the environment, Putting environmental realism into nanosafety assessment, organized by QualityNano NanoFATE & NAnoMILE. Birmingham (United Kingdom), 04-07/03/2014, Puntes, V. (Invited talk)

Application of inorganic nanoparticles in medicine, II Reunión de Jóvenes Investigadores en Coloides e Interfases, organized by Universidad de Granada. Granada (Spain), 27-30/04/2014, Puntes, V. (Invited talk)

Nanoparticles synthesis and reactivity, Lecture at Nanoscience Ile-de-France Summer School, organized by Nanoscience Ile-de-France Summer School. Etiolles (France), 23-25/06/2014, Puntes, V. (Invited talk)

Nanocrystals as reagents: building the next generation of nanoparticles, New frontiers of nanomaterial technologies for applications in biology and medicine, organized by DSCTM, IC, CN2, IIT, (ISOF)-CNR, Università degli di Studi di Bari, OPAL, Tirana University. Tirana (Albania), 10-11/07/2014, Puntes, V. (Invited talk)

Medical Nanochemistry, the use of reactive inorganic nanoparticles in medicine, **14th Nanomedicine Symposium**, organized by CEN, Centro Europeo Nanomedicina, Politecnico di Milano, IRCCS. Milan (Italy), 13-14/11/2014, Puntes, V. (Invited talk)



Chemistry for Specific Materials, included in Màster Universitari en Química Industrial i Introducció a la Recerca Química, **Universitat Autònoma de Barcelona, Spain**, 28/10/2013

More information:

http://www.inorganicnanoparticles.net/

Magnetic Nanostructures Group

Main Research Lines

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



GROUP MEMBERS

Sebastià Agramunt, Postdoctoral Researcher Alejandro Gómez, Beatriu de Pinós Postdoctoral Researcher Pau Güell, Master Student Mark Laver, Visiting Researcher

José Francisco López-Barberá, CSIC Visiting Postdoctoral Researcher

Enric Menéndez, Visiting Researcher Josep Nogués, ICREA Research Professor

and Group Leader





GROUP LEADER



ICREA Prof Josep Nogués

Prof Nogués earned his BSc from the Universitat Autònoma de Barcelona (UAB), in Spain, in 1986. After obtaining his PhD at the Royal Institute of Technology in Stockholm, Sweden, in 1993, he moved to the University of California San Diego for post-doctoral studies. In 1997 he returned to UAB. He is currently an ICREA Research Professor and Group Leader of ICN's Magnetic Nanostructures Group. Prof Nogués has published over 210 articles (including 8 reviews), and has more than 11,500 citations and an h-index of 45. He has authored two patents and given over 160 invited talks.



NEW PROJECTS & MILESTONES

In 2014, the Group continued working on the study of exchange coupling in core/shell nanoparticles and magnetic nanostructures in the context of various ongoing projects (MAGTUNE, ONDA and COEFNANO). Moreover, the Group advanced in the study of magnetic nanowires to be used for molecule manipulation within the MANAQA project.

It also started working on novel nanoparticles and nanostructures for biomedical application in the framework of THERANANO (Multifunctional magnetic and magnetoplasmonic theranostic nanostructures). The aim of the project is designing bottom-up and top-down hybrid magnetic nanostructures for diverse biomedical applications (hyperthermia or multimode imaging).



PUBLICATIONS

A combinatorial study of the mechanical and magnetic properties of a gradually nitrided austenitic stainless steel single crystal, Menéndez E., Templier C., Abrasonis G., López-Barberá J.F., Nogués J., Temst K., Sort J., *CrystEngComm* (17): vol. 16, 3515-3520 (2014). IF: 3.858

Direct evidence for an interdiffused intermediate layer in bi-magnetic coreshell nanoparticles, Juhin A., López-Ortega A., Sikora M., Carvallo C., Estrader M., Estradé S., Peiro F., Baró M.D., Sainctavit P., Glatzel P., Nogués J., *Nanoscale* (20): vol. 6, 11911-11920 (2014). IF: 6.739

Green electrochemical template synthesis of CoPt nanoparticles with tunable size, composition, and magnetism from microemulsions using an ionic liquid (bmimPF6), Serra A., Gómez E., López-Barberá J.F., Nogués J., Valles E., *ACS Nano* (5): vol. 8, 4630-4639 (2014). IF: 12.033

Interdependence between training and magnetisation reversal in granular Co-CoO exchange bias systems, Menéndez E., Dias T., Geshev J., López-Barberá J.F., Nogués J., Steitz R., Kirby B.J., Borchers J.A., Pereira L.M.C., Vantomme A., Temst K., *Physical Review B - Condensed Matter and Materials Physics* (14): vol. 89 (2014). IF: 3.664

One-pot electrosynthesis of multi-layered magnetic metallopolymer nanocomposites, Ozkale B., Pellicer E., Zeeshan M.A., López-Barberá J.F., Nogués J., Sort J., Nelson B.J., Pane S., *Nanoscale* (9): vol. 6, 4683-4690 (2014). IF: 6.739

Oxide wizard: An EELS application to characterize the white lines of transition metal edges, Yedra L., Xuriguera E., Estrader M., López-Ortega A., Baró M.D., Nogués J., Roldán M., Varela M., Estradé S., Peiró F., *Microscopy and Microanalysis* (3): vol. 20, 698-705 (2014). IF: 2.161

Structural determination of Bi-doped magnetite multifunctional nanoparticles for contrast imaging, Laguna-Marco M.A., Piquer C., Roca A.G., Boada R., Andrés-Vergés M., Veintemillas-Verdaguer S., Serna C.J., ladecola A., Chaboy J., *Physical Chemistry Chemical Physics* (34): vol. 16, 18301-18310 (2014). IF: 4.198



PROJECTS

Understanding the Properties of Advanced Multifunctional Materials for Technological Applications, funded by **AGAUR**, 07/01/2013 -06/01/2015

Coupling effects in magnetic systems of reduced dimensionality (COEFNANO), funded by **EC**, 01/01/2013 - 31/12/2016

Ordered hetero- and Nano-structures with Epitaxial Dielectrics for magnetic and electronics Applications (ONDA), funded by **EC**, 15/06/2010 - 14/06/2014

Magnetic nano actuators for quantitative analysis, funded by **EC**, 01/08/2012 - 31/07/2015

Modulación de las propiedades magnéticas de nanopartículas y estructuras litografiadas, mediante parámetros intrínsecos y extrínsecos (MAGTUNE), funded by **MINECO**, 01/01/2011 - 30/06/2014

Nanoestructuras magnéticas y magnetoplasmónicas teranósticas (THERANANO), funded by **MINECO**, 01/01/2014 - 31/12/2016

Magneto-optical mechanical nanoresonators, funded by **MINECO**, 01/09/2014 - 31/08/2015



CONTRIBUTIONS

Antiferromagnetic coupling in ferrimagnetic hard-soft core/shell nanoparticles, Materials Research Society Spring Meeting, organized by MRS. San Francisco (USA), 21/04/2014 - 25/01/2014, J. Nogués; M. Estrader; A. López-Ortega; S. Estradé; I. Golosovsky; G. Salazar-Álvarez; M. Vasilakaki; K.N. Trohidou; M. Varela; D.C. Stanley; M. Sinko; M.J. Pechan; D. J. Keavney; F. Peiró; S. Suriñach; M.D. Baró (Invited)

Antiferromagnetic coupling in ferrimagnetic hard-soft core/shell nanoparticles,

Encontro Nacional de Fisica da Materia Condensada, organized by UFBAC. Costa do Sauipe (Brazil), 12-16/05/2014, J. Nogués; M. Estrader; A. López-Ortega; S. Estradé; I. Golosovsky; G. Salazar-Álvarez; M. Vasilakaki; K.N. Trohidou; M. Varela; D.C. Stanley; M. Sinko; M.J. Pechan; D. J. Keavney; F. Peiró; S. Suriñach; M.D. Baró (Invited)

Size-dependent magnetism in FeO/Fe3O4 core/shell nanoparticles, International Union of Materials Research Societies – International Conference on Electronic Materials (IUMRS-ICEM), organized by MRS-T, Taiwan. Taipei (Taiwan), 10-14/06/2014, A.G. Roca; M. Estrader; A. López-Ortega; G. Salazar-Álvarez; S. Estradé; E. Winkler; I.V. Golosovsky; M. Vasilakaki; K.N. Trohidou; J.S. Ardisson; W. Macedo; F. Peiró; S. Suriñach; R.D. Zysler; M.D. Baró; J. Nogués (Invited)

Antiferromagnetic coupling in ferrimagnetic hard-soft core/shell nanoparticles,

Collaborative Conference on 3D & Materials Research, organized by Seoul National University; Korea Advanced Institute of Science and Technology, Gwangju Institute of Science & Technology. Incheon (Korea), 23-27/06/2014, M. Estrader; S. Estradé; F. Peiró; A. López-Ortega; I. Golosovsky; G. Salazar-Álvarez; M. Vasilakaki; K.N. Trohidou; M.A. Roldán; M. Varela; D.C. Stanley; M. Sinko; M.J. Pechan; D. J. Keavney; M. Laver; K. Krycka; J.A: Borchers; S. Suriñach; M.D. Baró; J. Nogués (Invited)

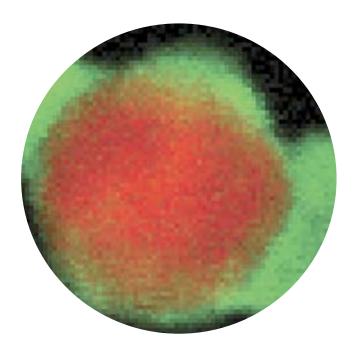
Semiconductor 3D ordered mesoporous architectures prepared by nanocasting: (i) oxide diluted magnetic semiconductors and (ii) photoluminiscent antidots. Prospects and new challenges, Collaborative Conference on 3D & Materials Research, organized by Seoul National University; Korea Advanced Institute of Science and Technology, Gwangju Institute of Science & Technology, Incheon (Korea), 23-27/06/2014, J. Sort; E. Menéndez; M. Guerrero; J. Fornell; E. Rossinyol; M. Roldán; O. Castell; S. Suriñach; M.D. Baró; A. Vantomme; K. Temst; J. Nogués; E. Pellicer (Invited)

Evidence of an interfacial antiferromagnetic coupling in ferrimagnetic hard-soft core/shell nanoparticles, ISMANAM. Cancun (Mexico), 30/06/2014 - 04/07/2014, M. Estrader; S. Estradé, F. Peiró, A. López-Ortega; I. Golosovsky; G. Salazar-Álvarez; M. Vasilakaki; K.N. Trohidou; M.A. Roldán; M. Varela; D.C. Stanley; M. Sinko; M.J. Pechan; D. J. Keavney; S. Suriñach; M.D. Baró; J. Nogués (Invited)

Antiferromagnetic coupling in ferrimagnetic hard-soft core/shell nanoparticles,

International Union of Materials Research Societies – International Conference in Asia (IUMRS_ICA), organized by MRS-J. Fukuoka (Japan), 24-30/08/2014, M. Estrader; S. Estradé; F. Peiró; A. López-Ortega; I. Golosovsky; G. Salazar-Álvarez; M. Vasilakaki; K.N. Trohidou; M.A. Roldán; M. Varela; D.C. Stanley; M. Sinko; M.J. Pechan; D. J. Keavney; M. Laver; K.L. Krycka; J.A. Borchers; S. Suriñach; M.D. Baró; J. Nogués (Invited)

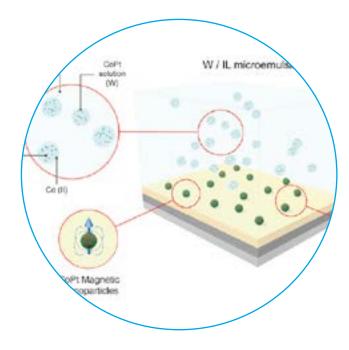
Antiferromagnetic coupling in ferrimagnetic hard-soft core/shell nanoparticles, European Materials Research Society, organized by E-MRS. Warsaw (Poland), 15-19/09/2014, M. Estrader, S. Estradé, F. Peiró, A. López-Ortega, I. Golosovsky, G. Salazar-Álvarez, M. Vasilakaki, K.N. Trohidou, M.A. Roldán, M. Varela, D.C. Stanley, M. Sinko, M.J. Pechan, D. J. Keavney, M. Laver, K.L. Krycka, J.A. Borchers; S. Suriñach, M.D. Baró, J. Nogués (Invited)



Tuning the magnetic properties of Co thin films by oxygen ion implantation, Autum Meeting of the Japanese Society of Applied Physics, organized by Hokkaido University. Sapporo (Japan), 17-20/09/2014, J.F. López-Barberá, E. Menéndez, H. Modarresi, M. Haidar, B.J. Kirby, J. Akerman, J.A. Borchers, A. Vantomme, K. Temst, J. Nogués (Invited)

Size-dependent magnetism in FeO/Fe3O4 core/shell nanoparticles, Energy Materials Nanotechnology Open Access Week, organized by OAHOST. Chengdu (China), 22-25/09/2014, A.G. Roca, M. Estrader, A. López-Ortega, G. Salazar-Álvarez, S. Estradé, E. Winkler, I.V. Golosovsky, M. Vasilakaki, K.N. Trohidou, J.S. Ardisson, W. Macedo, F. Peiró, S. Suriñach, R.D. Zysler, M.D. Baró, J. Nogués (Invited)

Plasmonics phase tuning of magneto-optics in ferromagnetic nanostructures, NanoPortugal. Porto (Portugal), 12-14/02/2014, N. Maccaferri, A. Berger, S. Bonetti, V. Bonanni, M. Kataja, S. van Dijken, J. Nogués, J. Akerman, Z. Pirzadeh, A. Dmitriev, P. Vavassori (Oral presentation)



Fabrication and magneto-optical properties of nickel nanoparticles, **Physics Days**, organized by Tampere University of Technology. Tampere (Findland), 11-13/03/2014, M. Kataja, Q.H. Qin, S. van Dijken, P. Vavassori, N. Maccaferri, V. Bonanni, S. Bonetti, J. Nogués, J. Akerman, A. Dmitriev (Oral presentation)

Atomic Resolution Analysis of Bi-magnetic Core/Shell Oxide Nanoparticles, Materials Research Society Spring Meeting, organized by Materials Research Society. San Francisco (USA), 21-25/04/2014, M. A. Roldán, A. López-Ortega, M.Estrader, J. Nogués, J. Salafranca, S.J. Pennycook, M. Varela (Oral presentation)

Atomic Resolutionmonitoring of structural phase transition in Bi-magnetic Core/Shell Oxide Nanoparticles, Microscopy and Mircoanalysis, organized by International Union of Microbeam Analysis Societies. Hartford (USA), 03-07/08/2014, M. A. Roldán, J. Salafranca, R. Ishikawa, R. Mishra, A. López-Ortega, M.Estrader, G. Salazar-Álvarez, J. Nogués, J. Salafranca, S.J. Pennycook, M. Varela (Oral presentation)

Mesoscopic modeling of the exchange bias behaviour of bi-magnetic nanoparticle assemblies, International Conference on Magnetism and Magnetic Materials, organized by IEE Magnetics Society. Honolulu (USA), 03-07/11/2014, K.N. Trohidou, G. Margaris, M. Vasilakaki, J. Nogués, D. Fiorani, D. Peddis, C. Binns (Oral presentation)

3D mapping of oxidation states in heterostructured nanomaterials, Materials Research Society Meeting (MRS), organized by Materials Research Society. Boston (USA), 30/11/2014 - 05/12/2014, P. Torruella, R. Arenal, Z. Saghi, L. Yedra, A. Eljarrat, F. de la Pena, M. Estrader, G. Salazar-Álvarez, A. López-Ortega, J. Nogués, P.A. Midgley, F. Peiró, S. Estradé (Oral presentation)

Beyond room temperatura exchaneg bais stabilisation in core-shell Co-CoO nanoparticles dispersed in a NiO matrix, Reunión del Grupo de Física del Estado Solido, organized by Universidad de Castilla La Mancha. Ciudad Real (Spain), 22-24/01/2014, D.P. Marques, J.A. de Toro, P. Muñiz, J.P. Andrés, R. López-Anton, P.S. Normile, J.A. González, J. Nogués, J.M. Riveiro (Poster)

Nanocrystalline CuNi alloys: improvement of mechanical properties and termal stability, American Physical Society Meeting. Denver (USA), 03-07/03/2014, J. Nogués, A. Varea, E. Pellicer, K.M. Sivaraman, S. Pane, B.J. Nelson, S. Suriñach, M.D. Baró, J. Sort (Poster)

Green electrochemical template synthesis of CoPt nanoparticles with tunable size, compositoion and magnetism from microemulsions using ionic liquids,

NanoSpain, organized by Red Española de Nanotecnología. Madrid (Spain), 11-14/03/2014, A. Serra, E. Gómez, J.F. López-Barberá, J. Nogués, E. Valles (Poster)

Interdependnece between training and magnetisation reversal in granular Co-CoO Exchange bias systems, International Conference on Ion Beam Modification of Materials. Leuven (Belgium), 14-19/09/2014, E. Menéndez, T. Dias, A. Vantomme, K. Temst, J. Geshev, J.F. López-Barberá, J. Nogués, R. Steitz, B.J. Kirby, J.A. Borchers, L. Pereira (Poster)

Magnetic properties of plasma-nitrided austenitic stainless steel single crystals, International Conference on Ion Beam Modification of Materials. Leuven (Belgium), 14-19/09/2014, E. Menéndez, C. Templier, J.F. López-Barberá, K. Temst, A. Vantomme, J. Sort, J. Nogués (Poster)

Unconventional size dependence of the magnetic properties of antiferromagnetic-core/ferromagnetic-shell nanoparticles, International Conference on Magnetism and Magnetic Materials, organized by IEE Magnetics Society. Honolulu (USA), 03-07/11/2014, M. Vasilakaki, K.N. Trohidou, J. Nogués (Poster)



AWARDS

- Fellow of the American Physical Society
- First-prize winner of the Science as Art competition of the MRS-Spring Meeting
- Outstanding reviewer of the American Physical Society, 2014
- Outstanding reviewer of the Journal of Magnetism and Magnetic Materials, 2014

NanoBioelectronics and Biosensors Group

Main Research Lines -

- Nanoparticles study and application in innovative sensing technologies
- Development of novel nanostructured, nanochannel flexible platforms based on nanoimprinting and inkjet printing technologies
- Study of graphene related materials and their integration into biosensing platforms
- Development of novel paper-based platforms with improved architecture, microfluidics and enhanced detection capabilities
- Design and application of lab-on-a-chip devices for biosensing, drug screening and other applications



GROUP MEMBERS

Abdellatif Alt Lahcen, Visiting Doctoral Student Irene Álvarez, Technician
Wicem Argoubi, Visiting Doctoral Student
Joan Ariño, Bachelor Student
Alessandra Baiocco, Visiting Doctoral Student
Luis Miguel Baptista-Pires, FPI Doctoral Student
Michaela Cadkova, Visiting Doctoral Student
Fabio Roberto Caetano, Visiting Doctoral Student
Andrzej Chalupniak, Doctoral Student

Alejandro Chamorro, Doctoral Student
Natalia Chamorro, Master Student
Dun-Wei Cheng, Visiting Doctoral Student
Mari Ángeles Crespo, Undergraduate Student
Everson Thiago Da Silva, Visiting Doctoral Student
Alfredo de la Escosura, Senior Researcher
Loubna El Harrad, Visiting Doctoral Student
Marisol Espinoza, FPU Doctoral Student
Livia Florio, Visiting Doctoral Student



GROUP LEADER



ICREA Prof Arben Merkoçi

ICREA Professor and head of Nanobioelectronics & Biosensors Group at ICN2 (Institut Català de Nanociència i Nanotecnologia). He obtained his PhD at the University of Tirana working on ion selective electrodes. Since 1992 he has been doing research as postdoctoral fellow and research professor at Polytechnic Univ. of Budapest, Univ. of Ioanina, Univ. degli Studi di Padua, Univ. Politècnica de Catalunya, Univ.

David Forns, Undergraduate Student Houda Gaigi, Visiting Doctoral Student

Hamed Gol Mohammadi Ghane, Visiting Doctoral Student

Alfredo Maria Gravagnuolo, Visiting Doctoral Student

Dumitru - Daniel Herea, Visiting Postdoctoral Researcher

Jedrzej Rafal Malec, Undergraduate Student
Abdelmoneim Mars, Visiting Doctoral Student
Patricia Martín, Undergraduate Student
Carme Martínez, Doctoral Student
Carmen Mayorga, Postdoctoral Researcher
Arben Merkoçi, ICREA Research Professor and Group

Sandrine Miserere, Postdoctoral Researcher Helena Montón, Doctoral Student

Leader

Eden Morales, Postdoctoral Researcher Tina Naghdi, Visiting Doctoral Student Giulia Pecchielan, Visiting Doctoral Student Hongzhen Peng, Visiting Doctoral Student Flavio Pino, Doctoral Student Anna Puig, Project Manager and Group Administrator Daniel Quesada, Doctoral Student Amal Rabti, Visiting Doctoral Student Charlene Santos, Visiting Doctoral Student Jarinya Sittiwong, Visiting Doctoral Student Ichrak Slama, Visiting Doctoral Student Joan Antoni Soler, Undergraduate Student Albert Vila, Undergraduate Student Héctor Yáñez, Undergraduate Student Alejandro Zamora, Doctoral Student Erhan Zor, Visiting Doctoral Student



Autònoma de Barcelona and New Mexico State Univ. His research is focused on the integration of biological molecules and other species with micro- and nanostructures with interest for the design of novel (bio)sensors. Prof Merkoçi has been awarded the IAAM Medal 2011 and Nano Award-2013 for outstanding research in the field of nanoscience and nanotechnology by the International Association of Advanced Materials. He has published more than 200 articles and supervised around 20 PhD theses.



NEW PROJECTS & MILESTONES

During 2014 the group started becoming involved in new competitive and challenging projects at national and international levels. In the framework of the FP7 SMS project we started to develop, in collaboration with EU partners, innovative electrochemical and optical detection platforms for contaminants detection in sea water while with two national projects in collaboration with other national research centres and companies we will be involved in nanobiosensors development for smart paper applications. Last year two of our PhD students Marisol Espinosa and Miquel Cadevall defended their PhD theses.



PUBLICATIONS

A simple on-plastic/paper inkjet-printed solid-state Ag/AgCl pseudo-reference electrode, Everson T. S. G. da Silva; Sandrine Miserere; Lauro T. Kubota; Arben Merkoçi, *Analytical Chemistry* (21): vol. 86, 10531-10534 (2014). IF: 5.825

Alzheimer Disease Biomarker Detection Through Electrocatalytic Water Oxidation Induced by Iridium Oxide Nanoparticles, Rivas L., de la Escosura-Muniz A., Pons J., Merkoçi A., *Electroanalysis* (6): vol. 26, 1287- 4 (2014). IF: 2.502

An inkjet-printed field-effect transistor for label-free biosensing, Medina-Sánchez M., Martínez-Domingo C., Ramon E., Merkoçi A., *Advanced Functional Materials* (40): vol. 20, 6291-6302 (2014). IF: 10.439

An integrated phenol 'sensoremoval' microfluidic nanostructured platform, Mayorga-Martínez C.C., Hlavata L., Miserere S., López-Marzo A., Labuda J., Pons J., Merkoçi A., *Biosensors and Bioelectronics*: vol. 55, 355-359 (2014). IF: 6.451

Electrocatalytic tuning of biosensing response through electrostatic or hydrophobic enzyme – graphene oxide interactions, Luis Baptista-Pires, B. Pérez-López, Carmen C. Mayorga-Martínez, Eden Morales-Narváez, Neus Domingo, María José Esplandiu, Francesc Alzina, C.M. Sotomayor Torres, A. Merkoçi, *Biosensors and Bioelectronics*: vol. 61, 655-662 (2014). IF: 6.451

Extremely fast and high Pb2+ removal capacity using a nanostructured hybrid material, Adaris López-Marzo, Josefina Pons and Arben Merkoçi, *Journal of Materials Chemistry* A: vol. 2, 8766-8772 (2014). IF: 6.626

Graphene/Silicon Heterojunction Schottky Diode for Vapors Sensing Using Impedance Spectroscopy, Ali Fattah, Saeid Khatami, Carmen C. Mayorga-Martínez, Mariana Medina-Sánchez, Luis Baptista-Pires and Arben Merkoçi, *Small* (20): vol. 10, 4193-4199 (2014). IF: 7.514

Improving sensitivity of gold nanoparticles-based lateral flow assays by using wax-printed pillars as delay barriers of microfluidics, Lourdes Rivas, Mariana Medina, Alfredo de la Escosura-Muñiz and Arben Merkoçi, *Lab Chip*: vol. 14, 4406-4414 (2014). IF: 5.748

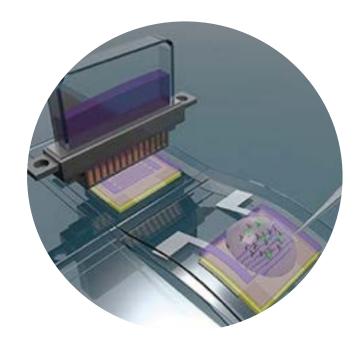
Iridium oxide nanoparticle induced dual catalytic/inhibition based detection of phenol and pesticide compounds, Mayorga-Martínez C.C., Pino F., Kurbanoglu S., Rivas L., Ozkan S.A., Merkoçi A., *Journal of Materials Chemistry B* (16): vol. 2, 2233-2239 (2014). IF: 6.626

Micromotor-enhanced microarray technology for protein detection, Morales-Narváez E., Guix M., Medina-Sánchez M., Mayorga-Martinez C.C., Merkoçi A., *Small* (13): vol. 10, 2542-2548 (2014). IF: 7.514

Nano/Micromotors in (Bio)chemical science applications, Guix M., Mayorga-Martínez C.C., Merkoçi A., *Chemical Reviews* (12): vol. 114, 6285-6322 (2014). IF: 45.661

On-chip magneto-immunoassay for Alzheimer's biomarker electrochemical detection by using quantum dots as labels, Medina-Sánchez M., Miserere S., Morales-Narváez E., Merkoci A., *Biosensors and Bioelectronics*: vol. 54, 279-284 (2014). IF: 6.451

Supramolecular interaction of dopamine with β-cyclodextrin: An experimental and theoretical electrochemical study, Palomar-Pardave M., Corona-Avendano S., Romero-Romo M., Alarcón-Ángeles G., Merkoci A., Ramírez-Silva M.T., Journal of Electroanalytical Chemistry, 717-718, 103-109 (2014). IF: 2.871





PROJECTS

SGR (2009 SGR 076), funded by **AGAUR**, 10/09/2009-30/04/2014, Arben Merkoçi

SGR (2014 SGR 260), funded by **AGAUR**, 01/01/2014-31/12/2016, Arben Merkoçi

Accions de promoció de doctorats industrials (2014 PRODI 00012), funded by **AGAUR**, 30/09/2014, Arben Merkoçi

Nanosystems for early Diagnosis of Neurodegenerative Diseases, NADINE (246513), funded by **EC**, 01/09/2010 - 31/08/2015, Arben Merkoci

Development of Electrochemical Peptide Nanosensors for protein and antibody detection., PEPTIDE NANOSENSORS (294901), funded by EC, 01/05/2012 - 30/04/2015, Arben Merkoçi

Point-of-care diagnostics for rapid and cheap pathogen detection of companion animals, POC4PETS (315653), funded by **EC**, 01/09/2012 - 31/08/2014, Arben Merkoçi

Sensing toxicants in Marine waters makes Sense using biosensors, SMS (613844), funded by **EC**, 01/12/2013 - 31/08/2017, Arben Merkoçi

ICREA Workshop on Graphene Nanobiosensors, funded by **ICREA**, 01/08/2014 - 31/12/2015, Stephan ROCHE / Arben Merkoçi

Nanomateriales con alta capacidad de reconocimiento modulable electrónicamente, tipo on-off,para su aplicación en biosensores electroquímicos con características excepcionales, NANOHEROES (MAT2011-25870), funded by MINECO, 01/01/2012 - 31/12/2014, Arben Merkoçi

SMART PRINTED PAPER: Printed Electronics para nuevas funcionalidades en papel (RTC-2014-2619-7), funded by **MINECO**, 01/02/2014 -31/12/2016, Arben Merkoçi

Desarrollo de un sistema de detección de endotoxina de alta sensibilidad y libre de interferencias basado en nanomateriales y fenómenos nuevos, ENDOSENSE (BIO2013-49464-EXP), funded by **MINECO**, 01/09/2014 - 31/08/2016, Arben Merkoçi



CONTRIBUTIONS

Nanobiosensing devices using plastic and paper-based platforms, 2nd International Conference on Analytical Chemistry, organized by Valahia University of Targoviste, Targoviste, Rumania, 17-21/09/2014, Arben Merkoçi (Invited)

Nanomaterials-based biosensing platforms, 2nd International Conference on Applied Biotechnology, organized by University of Tirana, Tirana, Albania, 22/09/2014, Arben Merkoçi (Invited)

Antithyroid drug detection using an enzyme cascade blocking in a nanoparticle-based labon-a-chip, XIX Trobada Transfronterera sobre Sensors i Biosensors, organized by ICN2, Bellaterra, Spain, 25-26/09/2014, Sevinc Kurbanoglu, Carmen C. Mayorga-Martínez, Mariana Medina, Lourdes Rivas, Sibel A. Ozkan, Arben Merkoçi (Invited)

Enhancement of in-chip quantum dots labelled protein electrochemical analysis through the use of an in-situ bismuth modified detector, XIX Trobada Transfronterera sobre Sensors i Biosensors, organized by ICN2, Bellaterra, Spain, 25-26/09/2014, Mariana Medina-Sánchez, Sandrine Miserere, Miquel Cadevall, and Arben Merkoçi (Invited)

Gold Nanoparticles Hydrogen Evolution Reaction by Electrochemical Impedance Spectroscopy for (Bio)sensing applications, XIX Trobada Transfronterera sobre Sensors i Biosensors, organized by ICN2, Bellaterra, Spain, 25-26/09/2014, Carmen C. Mayorga-Martínez, Alejandro Chamorro-García, Arben Merkoçi (Invited)

Graphene oxide-related forms for biosensing applications, XIX Trobada Transfronterera sobre Sensors i Biosensors, organized by ICN2, Bellaterra, Spain, 25-26/09/2014, L. Baptista-Pires, B. Pérez-López, Carmen C. Mayorga-Martínez, Eden Morales-Narváez, Neus Domingo, María José Esplandiu, Francesc Alzina, C. M. Sotomayor Torres and A. Merkoçi (Invited)

Graphene/Silicon heterojunction schottky diode for vapors sensing using impedance spectroscopy, XIX Trobada Transfronterera sobre Sensors i Biosensors, organized by ICN2, Bellaterra, Spain, 25-26/09/2014, Ali Fattah, Carmen C. Mayorga-Martínez, Mariana Medina-Sánchez, Luis Baptista-Pires, Saeid Khatami and Arben Merkoçi (Invited)

Label-free impedimetric aptasensor for Ochratoxin-A using iridium oxide nanoparticles, XIX Trobada Transfronterera sobre Sensors i Biosensors, organized by ICN2, Bellaterra, Spain, 25-26/09/2014, Lourdes Rivas, Carmen C. Mayorga-Martínez, Alejandro Zamora, Daniel Quesada, Alfredo de la Escosura-Muñiz, Arben Merkoçi (Invited)

Magnetic plug-based platform modelling and application in a microfluidics/quantum dots based electrochemical biosensing system, XIX Trobada Transfronterera sobre Sensors i Biosensors, organized by ICN2, Bellaterra, Spain, 25-26/09/2014, Sandrine Miserere, Mariana Medina-Sánchez, Miquel Cadevall, and Arben Merkoçi (Invited)

Nanoparticle-induced dual catalytic/inhibition-based detection of phenol and pesticide compounds, XIX Trobada Transfronterera sobre Sensors i Biosensors, organized by ICN2, Bellaterra, Spain, 25-26/09/2014, Carmen C. Mayorga-Martínez, Flavio Pino, Sevinc Kurbanoglu, Lourdes Rivas, Sibel A. Ozkan, Arben Merkoçi (Invited)

Porous magnetic microspheres as efficient capturing/pre-concentrating platforms for detection of Alzheimer disease biomarkers using electrocatalytic gold nanoparticle tags, XIX Trobada Transfronterera sobre Sensors i Biosensors, organized by ICN2, Bellaterra, Spain, 25-26/09/2014, Alfredo de la Escosura-Muñiz, Z. Plichta, D. Horák, Arben Merkoçi (Invited)

Quantum dots for biomedical and biosensing applications, XIX Trobada Transfronterera sobre Sensors i Biosensors, organized by ICN2, Bellaterra, Spain, 25-26/09/2014, Helena Montón, Eden Morales-Narváez, Claudio Parolo, Carme Nogués, A. Merkoçi (Invited)

Rapid and sensitive detection of Escherichia coli O157:H7 in minced beef and water using electrocatalytic gold nanoparticles, XIX Trobada Transfronterera sobre Sensors i Biosensors, organized by ICN2, Bellaterra, Spain, 25-26/09/2014, A.H.A.Z. Hassan, Alfredo de la Escosura-Muñiz, Arben Merkoçi (Invited)

Micro/Nanomaterials and microarray technology, XIX Trobada Transfronterera sobre Sensors i Biosensors, organized by ICN2, Bellaterra, Spain, 25-26/09/2014, Eden Morales-Narváez, Arben Merkoçi (Invited)

Simple Lab-on-a-chip devices for biomarkers and pollutants detection, XIX Trobada Transfronterera sobre Sensors i Biosensors, organized by ICN2, Bellaterra, Spain, 25-26/09/2014, Andrzej Chałupniak, Eden Morales, Sandrine Miserere, Arben Merkoçi (Invited)

Graphene in Biosensing Platforms, XXX Trobades Científiques de la Mediterrània, organized by Societat Catalana de Física, Mahón, Spain, 15-17/10/2014, Eden Morales-Narváez, Arben Merkoçi (Invited)

Nanochannel array devices for sensitive label-free immunodetection of cancer biomarkers, **24th Biosensors World Congress**, organized by Elsevier, Melbourne, Australia, 27-30/05/2014, Marisol Espinoza-Castañeda, Alejandro Chamorro, Carmen de Torres, Arben Merkoçi, Alfredo de la Escosura-Muñiz (Oral presentation)

Integration of micro/nanomaterials into microarray technology: boosting biosensing platform, **24th Biosensors World Congress**, organized by Elsevier, Melbourne, Australia, 27-30/05/2014, Eden Morales-Narváez, Arben Merkoçi (Oral presentation)

Nanomaterials-based biosensors, **Cell Models Systems Summer School**, Rome, Italy, 18-19/06/2014, Eden Morales, Arben Merkoçi (Oral presentation)

Biosensing using graphene, Graphene & 2D Materials, Singapore-Spain Workshop, organized by National University of Singapore, Singapore, 19-20/06/2014, Arben Merkoçi (Oral presentation)

On-chip magneto-immunoassay for Alzheimer's biomarker electrochemical detection using QDs as labels, **WORKSHOP WAM NANO**, organized by University of Copenhagen, Copenhaguen, Denmark, 22-24/06/2014, Sandrine Miserere, Arben Merkoçi (Oral presentation)

Nanobiosensing and actuating in lab-on-a-chip and paper-based lateral flow platforms, **New frontiers of nanomaterial technologies for applications in biology and medicine**, organized by University of Tirana, Tirana, Albania, 10-11/07/2014, Arben Merkoçi (Oral presentation)

Graphene-based sensing and biosensing platforms, The International Graphene Innovation Conference (GrapChina, 2014), organized by Graphene CGIA, Ningbo, China, 01-03/09/2014, Arben Merkoçi (Oral presentation)

Bioanalytical nanosystems. Building nanoblocks (Part I & II), **3rd Bioanalytical Nanotechnology School**, organized by Bioanalytical Nanotechnology School, Manila, Philippines, 29/01/2014-01/02/2014, Arben Merkoçi (Poster)

Biosensing using nanomaterials, 34th Summer School of Chemistry in Brazil, organized by University of Sao Carlos, Sao Carlos, Brazil, 17-21/02/2014, Arben Merkoçi (Poster)

Point-of-care diagnostics using simple nanomaterials-based platforms, **Universitat Pompeu Fabra**, organized by Universitat Pompeu Fabra, Barcelona, Spain, 07/03/2014, Arben Merkoçi (Poster)

Recent trends and applications of nanomaterialbased biosensing systems, **Advances in Biodetection and Biosensors**, organized by SelectBio, Berlin, Germany, 10-11/03/2014, Arben Merkoci (Poster) Carbon-based electrodes in nanomaterialsinvolved biosensing systems, International Symposium on Diamond Electrochemistry, organized by Keio University, Yokohama, Japan, 18-19/03/2014, Arben Merkoçi (Poster)

Nanomaterials-based platforms for biosensing applications, **Nagoya University**, organized by Nagoya University, Nagoya, Japan, 20/03/2014, Arben Merkoçi (Poster)

Nanomaterials-based biosensing systems for diagnostics and environment monitoring applications, **Department of Chemical Sciences, University of Naples**, organized by University of Naples, Napoli, Italy, 28/04/2014, Arben Merkoçi (Poster)

Quantum dots for biomedical and biosensing applications, Integrated approaches for biomolecular detection: nanostructures, biosensors and lab-on-a-chip devices, organized by COST Action TD 1003, Catania, Italy, 28-30/04/2014, Helena Montón, Carme Nogués, Eden Morales-Narváez, Claudio Parolo, Arben Merkoçi (Poster)

Nanomaterials as signalling and actuation tools in biosensing, EHPS2014 - Electrospinning for High-Performance Sensing, organized by Institute of Atmospheric Pollution Research, Rome, Italy, 29-30/04/2014, Arben Merkoçi (Poster)

Antithyroid drug detection using an enzyme cascade blocking in a nanoparticle-based labon-a-chip system, **24th Biosensors World Congress**, organized by Elsevier, Melbourne, Australia, 27-30/05/2014, Sevinc Kurbanoglu, Carmen C. Mayorga-Martínez, Mariana Medina, Lourdes Rivas, Sibel A. Ozkan, Arben Merkoçi (Poster)

Electrochemical Impedance Spectroscopy (bio)sensing through hydrogen evolution reaction induced by gold nanoparticles, **24th Biosensors World Congress**, organized by Elsevier, Melbourne, Australia, 27-30/05/2014, Alejandro Chamorro, Carmen C. Mayorga-Martínez and Arben Merkoçi (Poster)

Enhancement of in-chip quantum dots labelled protein electrochemical analysis through the use of an in-situ bismuth modified detector, **24th Biosensors World Congress**, organized by Elsevier, Melbourne, Australia, 27-30/05/2014, Mariana Medina-Sánchez, Sandrine Miserere, Miquel Cadevall, and Arben Merkoçi (Poster)

Highly sensitive and rapid determination of Escherichia coli O157:H7 in minced beef and water using electrocatalytic gold nanoparticle tags, **24th Biosensors World Congress**, organized by Elsevier, Melbourne, Australia, 27-30/05/2014, Abdel-Rahim Hussein Abdel-Azzem Hassan, Alfredo de la Escosura-Muñiz, Arben Merkoçi (Poster)

Magnetic plug-based platform modelling and application in a microfluidics/quantum dots based electrochemical biosensing system, **24th Biosensors World Congress**, organized by Elsevier, Melbourne, Australia, 27-30/05/2014, Sandrine Miserere, Mariana Medina-Sánchez, Miguel Cadevall, and Arben Merkoçi (Poster)

Label-free impedimetric aptasensor for ochratoxin-A using iridium oxide nanoparticles, **24th Biosensors World Congress**, organized by Elsevier, Melbourne, Australia, 27-30/05/2014, Lourdes Rivas, Carmen C. Mayorga-Martinez, Alejandro Zamora, Daniel Quesada, Alfredo de la Escosura-Muñiz, Arben Merkoçi (Poster)

Nanoparticle-induced dual catalytic/inhibition-based detection of phenol and pesticide compounds, **24th Biosensors World Congress**, organized by Elsevier, Melbourne, Australia, 27-30/05/2014, Carmen C. Mayorga-Martínez, Flavio Pino, Sevinc Kurbanoglu, Lourdes Rivas, Sibel A. Ozkan, Arben Merkoçi (Poster)

Novel porous magnetic microspheres as enhanced capturing platforms for the detection of Alzheimer disease biomarkers in human samples using electrocatalytic gold nanoparticle tags, **24th Biosensors World Congress**, organized by Elsevier, Melbourne, Australia, 27-30/05/2014, Alfredo de la Escosura-Muñiz, Zdeněk Plichta, Daniel Horák, Arben Merkoçi (Poster)



BOOKS

Application of Nanomaterials for DNA Sensing, Alfredo de la Escosura-Muñiz, Arben

Merkoçi, Springer, 2014

Graphene and Carbon Nanotubebased Electrochemical Biosensors for Environmental Monitoring, Georgina Alarcón-Ángeles, Giaan Arturo Álvarez Romero, Arben Merkoçi, John Wiley & Sons, Inc., 2014

Graphene: Insights of its Application in Electrochemical Biosensors for Environmental Monitoring, Giaan Arturo Álvarez Romero, Georgina Alarcón-Ángeles, Arben Merkoçi, John Wiley & Sons, Inc., 2014

Medical Nanobiosensors, Eden Morales-Narváez, Arben Merkoçi, Springer New York, 2014



COURSES

Module: Nanochemistry, in Master in Nanotechnology and Materials Science, **Universitat Autònoma de Barcelona, Barcelona, Spain**, 13/01/2014, Dr Alfredo de la Escosura-Muñiz

Module: Nanochemistry, in Master in Nanotechnology and Materials Science, **Universitat Autònoma de Barcelona, Barcelona, Spain**, 15/01/2014, Dr Eden Morales

Module: Nanochemistry, in Master in Nanotechnology and Materials Science, **Universitat Autònoma de Barcelona, Barcelona, Spain**, 17/01/2014, Prof Arben Merkoçi



THESES

Doctorand: Marisol Espinoza

Title: Study and Development of New Biosensors Based on Nanoparticles and

Nanochannels.

Defense Date: 21/07/2014

Directors: Prof Arben Merkoçi / Dr Alfredo de

la Escosura

Doctorand: Miquel Cadevall

Title: Bismuth-based (nano)materials and

pleatforms for (bio) sensing. Defense Date: 14/11/2014

Directors: Prof Arben Merkoçi / Prof Josep Ros



OTHER HIGHLIGHTS

European Patents filed

European Patent (EP) application. ICN PAT 12/13. Method of forming an electronic device on a flexible substrate, With Ref. EP14382240 and priority date 20/06/2014

PCT Extensions filed

ICNPAT 07/13. Sensitive qualitative bioassay using graphene oxide as analyte revealing agent

More information:

http://www.nanobiosensors.org/

NanoBiosensors and Bioanalytical **Applications Group**

Main Research Lines

- Plasmonic and nanoplasmonic biosensor
- Silicon photonic biosensor
- Nanomechanical biosensor
- Bioanalytical applications



GROUP MEMBERS

Maria del Mar Álvarez, CSIC Postdoctoral Researcher Iulia Arghir, CSIC Visiting Doctoral Student (KU Leuven, Belgium) Carlos Caro, CSIC Postdoctoral Researcher Blanca Chocarro, FPI Doctoral Student Ihonattan Cordoba, CSIC Visiting Doctoral Student (Campinas University, Brazil) Stefania Dante, CSIC FPU Doctoral Student Rebeca Diéguez, Group Project Manager Santos Domínguez, CSIC Doctoral Student

Firehun Tsige Dullo, CSIC Visiting Doctoral Student

Daphné Duval, CIBER Postdoctoral Researcher M.ª Carmen Estévez, CIBER Postdoctoral Researcher David Fariña, CIBER Technician Adrián Fernández, Postdoctoral Researcher Silvia Gómez, CIBER Technician Ana Belén González, CSIC Postdoctoral Researcher Daniel Grajales, CSIC Visiting Doctoral Student (CONACYT, Mexico) Joel Hernández, CSIC Visiting Doctoral Student Sonia Herranz, CSIC Postdoctoral Researcher Laura Lechuga, CSIC Research Professor, Group Leader



GROUP LEADER

(University of Tromso, Norway)



CSIC Research Professor Laura M. Lechuga

Prof Laura M. Lechuga received her PhD in Chemistry from the University Complutense of Madrid (Spain) in 1992. She is Full Professor of the Spanish National Research Council (CSIC); since 2012 she has been Adjunct Professor at the Dept. of Physics&Technology, at the Arctic University (Norway) and since 2013 she has been a Distinguished Visiting Professor at the Dept. of Microwaves and Photonics, School of Electrical and Computer Sciences, University of Campinas (Brazil).

Prof Lechuga is the Head of the Nanobiosensors and Bioanalytical Applications Group at the Catalan Institute for Nanoscience and Nanotechnology (ICN2) in Barcelona (Spain). The principal focus of her research programme is the technological development of photonic (plasmonics and silicon-



Gerardo Arturo López, CSIC Visiting Doctoral Student (CONACYT, Mexico)

Adrián Losoya, CSIC Visiting Doctoral Student (ITESM, Mexico)

Jesús Manuel Maldonado, CSIC Visiting Doctoral Student (CONACYT, Mexico)

Salomon Elieser Márquez, CSIC Visiting Doctoral Student (CONACYT, Mexico)

Elizabeth Medina, CSIC Visiting Student

Sebastián Mendoza, CSIC Visiting Student (University of California Santa Cruz, USA)

Marinus A. Otte, CSIC Postdoctoral Researcher

Alba Paramio, CSIC Visiting Student (University of Girona, Spain)

Roger Ponce, CSIC Visiting Student

Patricia Ramírez, CSIC Visiting Student (Universitat de Vic, Spain)

Mildred Samantha Razo, CSIC Visiting Student (Instituto Tecnológico Superior de Poza Rica, Mexico)

César Sánchez, Doctoral Student

Borja Sepúlveda, CSIC Tenured Scientist

Anna Serra, CSIC Visiting Student (University of Vic, Spain)

María Soler, CSIC FPI Doctoral Student

Verónica Iraís Solís, CSIC Visiting Doctoral Student (CONACYT, Mexico)

based) and nanomechanical biosensors, their integration in portable lab-on-a-chip platforms and their application in clinical and environmental diagnostics.

She has published over 160 articles, book chapters and conference proceedings, has 8 families of awarded patents at European, US or international level, and has presented more than 200 invited research papers. She has been the driving force for the establishment of one spin-off company in 2004 (SENSIA, SL) and co-founder of a new spin-off in 2010 (BIOD, SL).

Prof Lechuga is associate editor of the *IEEE Photonics Journal*, associate editor of the *Journal Optics and Laser Technology* (Elsevier) and is on the Editorial Board of the journal of *Nanobiosensors in Disease Diagnosis* and of the *Journal of Sensors*. She has been nominated as Fellow of the Optical Society (OSA) in 2014, and she is a member of the International Society for Optical Engineering (SPIE), and member of the European Optical Society (EOS). She is a member of Permanent Steering Committees for the Advanced Study Course on Optical Chemical Sensors (ASCOS) and Europt(r)ode Conference Series.



NEW PROJECTS & MILESTONES

In the research line of **integrated silicon nanophotonic** biosensors, important milestones have been reached for the implementation of a sensitive, affordable, hand-held and portable point-of-care device. The ultrasensitive limit of detection of this technology at the pM-fM level is far beyond the state of the art and the Group has demonstrated the detection of a few numbers of infectious microorganisms directly in patients' samples. A technological transfer plan with a private company has been developing during 2014. Several new projects have been granted in 2014 related to this research line:

 COLONTEST: Diseño y puesta a punto de kits para el diagnóstico del cáncer de colon en sangre basados en plataformas multiplex. Financial management: Programa RETOS-COLABORACIÓN. Ministerio de Economía y Competitividad. (RTC-2014-1518-1) Participants: Protein Alternatives, SL; Azurebio, SL; ICN2; CSIC; IDIBAPS.

Duration: 01/09/2014-01/09/2017

 RAIS: Scalable, point-of-care and label-free microarray platform for rapid detection of Sepsis. Financial management: UE. H2020-ICT-2014-1-644956 Duration: 01/01/2015-01/01/2018

The utility of our nanophotonic biosensing techniques for real bioanalytical applications has been successfully demonstrated. The Group is focusing on point-of-care detection of diseases as for example Malaria (collaboration with FIND diagnostics Foundation) or Tuberculosis (POCKET EU project); early detection of several types of cancer such as colorectal cancer (COLONTEST national project); early

detection of liver complications (CIBER internal project); monitoring of celiac or allergic patients directly in their body fluids, among others (most of them in collaboration with private companies).

In the environmental field, the Group is focusing on the early detection of toxic pollutants such as pesticides, antibiotics or alga toxins (BRAAVOO EU project).

The Group has successfully developed in 2014 the fundamental research line in Molecular Biology using our nanobiosensing technology for the deciphering of alterations in cellular pathways, including alternative splicing of RNA, and epigenetics modifications (DNA metylation or microRNA release).



PUBLICATIONS

Direct detection of protein biomarkers in human fluids using site-specific antibody immobilisation strategies, Soler M., Estévez M.-C., Álvarez M., Otte M.A., Sepúlveda B., Lechuga L.M., *Sensors* (2): vol. 14, 2239-2258 (2014). IF: 2.048

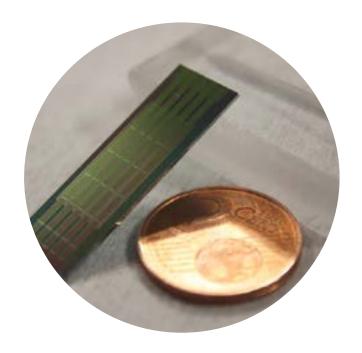
Molecular inversion probe-based SPR biosensing for specific, label-free and real-time detection of regional DNA methylation, Carrascosa L.G., Sina A.A.I., Palanisamy R., Sepúlveda B., Otte M.A., Rauf S., Shiddiky M.J.A., Trau M., *Chemical Communications* (27): vol. 50, 3585-3588 (2014). IF: 6.718

On-line surface plasmon resonance biosensing of vascular endothelial growth factor signaling in intact human hepatoma cell lines, Mauriz E., Carbajo-Pescador S., Ordonez R., García-Fernández M.C., Mauriz J.L., Lechuga L.M., González-Gallego J., *Analyst* (6): vol. 139, 1426-1435 (2014). IF: 3.906

Substrate Effect on the Refractive Index Sensitivity of Silver Nanoparticles, Erik Martinsson, Marinus A. Otte, Mohammad Mehdi Shahjamali, Borja Sepúlveda, Daniel Aili, Journal of Physical Chemistry C (42): vol. 118, 24680-24687 (2014). IF: 4.835

The effects of lipids and surfactants on TLR5-proteoliposome functionality for flagellin detection using surface plasmon resonance biosensing, Olguin Y., Carrascosa L.G., Lechuga L.M., Young M., *Talanta* vol. 126, 136-144 (2014). IF: 3.511

Trends and challenges of refractometric nanoplasmonic biosensors: A review, Estévez M.-C., Otte M.A., Sepúlveda B., Lechuga L.M., *Analytica Chimica Acta* vol. 806, 55-73 (2014). IF: 4.517





PROJECTS

Nanobiosensors and Bioanalytical Applications, funded by **AGAUR**, 01/01/2014 - 31/12/2016, Laura Lechuga

Advanced diagnostic tool for early identification of liver failure (LIVERPOC), funded by CIBER-BBN, 2012-2014, Laura Lechuga

Advanced diagnostic tool for early identification of liver diseases and infections in Intensive Care Units (HEPATOPOC), funded by CIBER-BBN, 2014-2015, Laura Lechuga

Development of a biosensing diagnostic tool for the fast identification of infection by Pneumocystis (PcP-Sens), funded by CIBER-BBN, 2014-2015, Laura Lechuga

Point of Care biosensor devices to detect biomarkers as evaluation end-points for therapeutic clinical trials in ocular surface inflammation (EYEPOC), funded by CIBER-BBN, 2014-2015, Laura Lechuga

Development of a low-cost point-of-care test for tuberculosis detection (POCKET), funded by **EC**, 01/11/2013 - 31/10/2016, Laura Lechuga

Biosensors, Reporters and Algal Autonomous Vessels for Ocean Operation (BRAAVOO), funded by **EC**, 01/12/2013 - 30/11/2016, Laura Lechuga

Modulación óptica de fase para biosensores interferométricos avanzados para aplicaciones "point-of-care", funded by **MECD**, 16/10/2010 - 15/10/2014, Laura Lechuga

Pistas celulares durotácticas para la detección in vivo de interacciones entre ligandos y receptores de membrana (iDuroSens), funded by **MINECO**, 20/12/2011 - 30/06/2014, Borja Sepúlveda

Innovación y desarrollo de sistemas portátiles de detección biológica óptica de alta eficiencia (INNBIOD), funded by **MINECO**, 30/06/2012 - 31/12/2014, Laura Lechuga

Integración Lab-on-a-chip de dispositivos biofotónicos para el estudio de alteraciones de la expresión génica en rutas celulares (EPISENS), funded by **MINECO**, 01/01/2013 - 31/12/2015, Laura Lechuga

Petición y Coordinación de proyectos colaborativos ICT y Health de H2020 (CoorEU), funded by **MINECO**, 01/11/2013 - 31/10/2015, Borja Sepúlveda

Nanoresonadores Magneto-Opto-Mecanicos (MORE), funded by **MINECO**, 01/09/2014 - 31/08/2015, Borja Sepúlveda

Proyecto COLONTEST: Diseño y puesta a punto de kits de diagnóstico del cáncer de colon en sangre basados en plataformas multiplex (COLONTEST), funded by MINECO, 01/09/2014 - 31/12/2017, Laura Lechuga



CONTRIBUTIONS

Nanophotonic lab-on-a-chip biosensors for point-of-care diagnostics: from concept to real applications, Conferencia Nacional de Nanotecnología, organized by Gobierno de Chile, Puerto Varas, Chile, 10-12/09/2014, Laura M. Lechuga (Invited)

Nanophotonic lab-on-a-chip biosensors for advanced nanodiagnostics, 19th Transfrontier Meeting of Sensors and Biosensors, Bellaterra, Barcelona (Spain), 25-26/09/2014, Laura M. Lechuga (Invited)

Point-of-care nanobiosensors for global health diagnostics: challenges and opportunities, **9th Ibero-American Congress on Sensors-IBERSENSOR**, organized by Universidad de Los Andes, Bogotá, Colombia, 15-18/10/2014, Laura M. Lechuga (Invited)

Dispositivos nanobiosensores para la detección precoz de enfermedades infecciosas y cancer, **45th Union World Conference on Lung Health**, Barcelona (Spain), 28-29/11/2014, A.B. González and L.M. Lechuga (Invited)

Nanophotonic lab-on-chip biosensors for point-of-care diagnostics, TNT 2014 Trends in Nanotechnology International Conference, Barcelona (Spain), 27-31/10/2014, L.M. Lechuga (Keynote speaker)

Nanophotonic biosensors for the next diagnostics generation, The Latin America Optics and Photonics (LAOP) Conference (OSA Conferences), Cancún (Mexico), 17-21/11/2014, L.M. Lechuga (Plenary Lecture)

Full integration of Photonic nanobiosensors in portable and multiplexed lab-on-a-chip platforms, EUROPT(R)ODE XII: 12th European Conference on Optical Chemical Sensors and Biosensors, Athens (Greece), 13-16/04/2014, Laura M. Lechuga (Oral presentation)

Experiències d'èxit en emprenedoria femenina, I Jornada Interuniversitària: Dones, Emprenedoria i Coneixement, organized by Generalitat de Catalunya, Barcelona (Spain), 28/05/2014, Laura M. Lechuga (Oral presentation)

Nanobiosensor devices for the direct and label-free deciphering of cellular pathways, Workshop Physics and Biological Systems 2014, Paris-Saclay (France), 24-27/06/2014, Laura M. Lechuga (Oral presentation)

Nanobiotechnology for advanced nanodiagnostics and nanotherapy, **Biotech Annual Congress 2014**, organized by Federación Española de Biotecnólogos, Barcelona (Spain), 09-11/07/2014, Laura M. Lechuga (Oral presentation)

Towards real point-of-care diagnostics using interferometric nanobiosensors, Advanced Photonics Conference 2014, organized by Optical Society of America Sensors (OSA), Barcelona (Spain), 27-31/07/2014, Laura M. Lechuga (Oral presentation)

Lab-on-a-chip nanophotonic biosensors for ultrasensitive diagnostics, Workshop on "Optical nano-fibers in Applications 2014", organized by International Scientific Seminars, sponsored by the Royal Society, Chicheley Hall, London, UK, 01-02/10/2014, Laura M. Lechuga (Oral presentation)

Nanoplasmonic biosensors for label-free deciphering of cellular pathways, The Latin America Optics and Photonics (LAOP) Confer, organized by OSA conferences, Cancun, Mexico, 17-21/11/2014, Laura M. Lechuga (Oral presentation)

Nanomedicina y salud: últimos avances en nanodiagnóstico y nanoterapia, III Congreso Nacional de la Sociedad Española de Cabeza y Cuello, organized by Sociedad Española de Cabeza y Cuello, Las Caldas, Spain, 27-28/11/2014, Laura M. Lechuga (Oral presentation)

Analysis of miRNA biomarkers related to thyroid cancer using a bimodal waveguide interferometric biosensor, **Europtrode XII, Athens**, organized by NCSR 'Demokritos', Greece, 13-16/04/2014, S. Dante, D. Duval, C.S. Huertas, and L.M. Lechuga (Poster)

Wavelength-Modulated Bimodal Interferometer for Highly Sensitive Biosensing Applications, Advanced Photonics 2014 (Optical Sensors meeting), organized by OSA, Barcelona (Spain), 2014, S. Dante, D. Duval, A.B. González-Guerrero, D. Fariña, C. Domínguez and L.M. Lechuga (Poster)

Biosensores SPR yTLR5-proteoliposomas como elementos de afinidad para la detección de flagelan bacteriana: efecto de lípidos y surfactantes sobre la funcionalidad del sistema, Conferencia Nacional de Nanotecnología, organized by Gobierno de Chile, Puerto Varas, Chile, 10-12/09/2014, Y. Olguín, L. Carrascosa, L.M. Lechuga, M. Young (Poster)

Fabrication of an Array of Microbridge Resonators with Integrated Microfluidic Channels for Biosensing Applications, IEEE Sensors 2014, Valencia (Spain), 02-05/11/2014, Salomon Márquez, Mar Álvarez, Carlos Domínguez, Laura Lechuga (Poster)

Nucleic Acids For Biosensing Applications, Nanobiomed 2014, Barcelona, Spain, 18-21/11/2014, Anna Aviñó, César Sánchez, Mar Oroval, Laura Carrascosa, Ramón Martínez-Máñez, Laura Lechuga, Ramon Eritja (Poster)

Fabricación de un Biosensor Nano-Optomecánico para el Estudio del Comportamiento Celular, IV Simposio Becarios CONACYT en Europa, Strasbourg, France, 05-07/11/2014, Verónica Iraís Solís, Laura M. Lechuga (Poster)



BOOKS

Optical waveguide biosensors, D. Duval and L. M. Lechuga, Editors: D. L. Andrews, Wiley-Blackwell, (2014)



COURSES

Dispositivos nanobiosensores "point-ofcare" para el diagnóstico ultrasensible en tiempo real, **Instituto Universitario de Oftalmobiología Aplicada (IOBA), Universidad de Valladolid**, Valladolid (Spain), 29/01/2014, L. Lechuga

Nanophotonic lab-on-a-chip biosensors for ultrasensitive and early diagnostics, Cambridge Graphene Centre (CGC), **University of Cambridge**, Cambridge, (United Kingdom) 09/02/2014, L. Lechuga

Nanophotonic lab-on-a-chip biosensors for advanced diagnostics, **Universitat Rovira i Virgili**, Tarragona (Spain), L. Lechuga

Nanophotonic biosensors as diagnostic tools for deciphering cellular pathways, Instituto de Biología Molecular y Celular (IBMC), **Universidad Miguel Hernández. Campus de Elche**, Elche (Spain), 28/02/2014, L. Lechuga

Photonic lab-on-a-chip nanobiosensors for deciphering cellular pathways, **Chalmers University of Technology**. Gothenburg, Gothenburg (Sweden), 04/04/2014, L. Lechuga

Nanophotonic Lab-on-a-chip biosensors as interactive diagnostics tools for deciphering cellular pathways, **BIONAND**, **Centro Andaluz de Nanomedicina y Biotecnología**, Málaga (Spain), 09/05/2014, L. Lechuga

Part 1. General Introduction.
Biofunctionalisation. Nanoplasmonics
biosensors, **Department of Microwaves and Optics. School of Electrical and Computer Science. University of Campinas**, Campinas
(Brazil), 18/08/2014, L. Lechuga

Part 2. Photonic biosensors based on integrated optics. Integration in lab-on-a-chip platforms, **Department of Microwaves and Optics. School of Electrical and Computer Science**. University of Campinas, Campinas (Brazil), 25/08/2014, L. Lechuga

The future of diagnostics: point-of-care mobile devices, **SAMSUNG Research Institute**, Campinas (Brazil), 26/08/2014, L. Lechuga

Photonic lab-on-a-chip nanobiosensors for ultrasensitive diagnostics, **School of Electrical and Computer Science. University of Campinas**, Campinas (Brazil), 27/08/2014, L. Lechuga

Photonic lab-on-a-chip nanobiosensors for ultrasensitive diagnostics, **Instituto de Pesquisas Tecnológicas (IPT). University of Sao Paulo**, Sao Paulo (Brazil), 01/09/2014, L. Lechuga

Nanobiosensores lab-on-a-chip para el diagnóstico descentralizado, **Universidad de Valparaíso**, Valparaíso (Chile), 08/09/2014, L. Lechuga



THESES

Doctorand: Stefania Dante

Title: All-optical phase modulation for advanced interferometric point-of-care

biosensors

Defense Date: 11/12/2014

Director: Dra Laura Lechuga Gómez

Doctorand: Esteban David Fariña

Title: Desarrollo de un sistema biosensor opto-mecánico basado en cantilevers

Defense Date: 31/10/2014

Directors: Dra Laura M. Lechuga, Dra Mar

Álvarez and Dr José Ramón Senra



AWARDS

OSA Fellow. Prof Laura Lechuga was elected as Fellow of the Optical Society (OSA) in 2014 due to her significant research leadership and pioneering development of a novel and compact biomedical sensor based on advanced integrated photonic techniques and plasmonic devices, combining science with real-life applications and technology transfer.

More information:

http://nanob2a.cin2.es/

Nanostructured Functional Materials Group

Main Research Lines

- Future and emerging technologies
- Biomaterials
- Sustainability



GROUP MEMBERS

Christian Bellacanzone, Doctoral Student Marta Borges, CSIC Visiting Doctoral Student Sebastián Castilla, CSIC Visiting Student Beatriz García, Doctoral Student Pablo González, Technician Mireia Guardingo, CSIC Doctoral Student Alejandro Ricar Julià, CSIC Visiting Student Juan Mancebo, Postdoctoral Researcher David Martínez, CSIC Visiting Student Giuseppina Massaro, CSIC Visiting Doctoral Student David Montpeyó, Doctoral Student Miguel Ángel Moreno, CSIC Visiting Student Fabiana Nador, CSIC Visiting Postdoctoral Researcher

Fernando Novio, Beatriu de Pinós Postdoctoral Researcher Guadalupe Del Carmen Pizarro, CSIC Visiting Senior Researcher Claudio Roscini, CSIC Postdoctoral Researcher Daniel Ruiz, CSIC Research Scientist and Group Leader Josep Sedó, CSIC Project Manager Juliane Simmchen, CSIC Doctoral Student Rubén Solorzano, CSIC Visiting Student Salvio Suárez, CSIC Visiting Student Héctor Torres, CSIC Visiting Doctoral Student Núria Alexandra Vázquez, Doctoral Student Jon Vilasau, Postdoctoral Researcher Karolina Wnuk, CSIC FI Doctoral Student



GROUP LEADER



CSIC Research Scientist Dr Daniel Ruiz-Molina

Daniel Ruiz-Molina earned his PhD on polyradical dendrimers at the Institute of Materials Science of Barcelona (CSIC) with Prof Jaume Veciana. Afterwards he took a postdoctoral position at the UC San Diego working on single-molecule magnets and molecular switches for three years. Since 2001 he has held a permanent position at the CSIC and more recently at CIN2 - CSIC, where he is heading the Nanostructured Functional Materials group. His main research areas are fabrication of hybrid colloids and surfaces, biomimetic functional nanostructures and micro-/ nanoparticles for smart applications and encapsulation/ delivery systems.



NEW PROJECTS & MILESTONES

- Mussel-Inspired Hydrophobic Coatings for improved adhesion properties, waterrepellent and functional oil removal interphases
- Development of novel coordination polymer particles for Biomedicine, including drug delivery and MRI
- 3. Novel approaches for the fabrication of spin transition molecular nanoparticles with designed morphologies and smart responses in front of external stimuli
- 4. Novel micromotors with enhanced performances and durability

The objective of the Nanostructured Functional Materials group (NANOSFUN) is to obtain (bio) molecular nanostructures with tailored properties and smart responses to external stimuli, taking advantage of the flexibility and richness of (supra)molecular chemistry and self-assembly processes.



PUBLICATIONS

Bioinspired catechol-terminated self-assembled monolayers with enhanced adhesion properties, Guardingo M., Bellido E., Miralles-Lluma R., Faraudo J., Sedó J., Tatay S., Verdaguer A., Busqué F., Ruiz-Molina D., *Small* (8): vol. 10, 1594-1602 (2014). IF: 7.514

Carboxyl Group (-CO2H) Functionalized Coordination Polymer Nanoparticles as Efficient Platforms for Drug Delivery, F. Novio, P. González-Monje, J. Lorenzo, D. Ruiz-Molina, *Chemical European Journal*: vol. 20, 15443-15450 (2014). IF: 5.696

Controlling spin transition in onedimensional coordination polymers through polymorphism, Novio F., Campo J., Ruiz-Molina D., *Inorganic Chemistry* (16): vol. 53, 8742-8748 (2014). IF: 4.794



Effect of surfactants on the performance of tubular and spherical micromotors - a comparative study, Simmchen J., Magdanz V., Sánchez S., Chokmaviroj S., Ruiz-Molina D., Baeza A., Schmidt O.G., *RSC Advances* (39): vol. 4, 20334-20340 (2014). IF: 3.708

Hydrophobic coordination polymer nanoparticles and application for oil-water separation, Novio F., Ruiz-Molina D., *RSC Advances* (29): vol. 4, 15293-15296 (2014). IF: 3.708

Improving catalase-based propelled motor endurance by enzyme encapsulation, Simmchen J., Baeza A., Ruiz-Molina D., Vallet-Regi M., *Nanoscale* (15): vol. 6, 8907-8913 (2014). IF: 6.739

Mussel-inspired hydrophobic coatings for water repellent textiles and oil removal,

B. García, J. Saiz-Poseu, R. Gras-Charles, J. Hernando, R. Alibés, F. Novio, J. Sedó, F. Busqué, D. Ruiz-Molina, *ACS Applied Materials & Interfaces*: vol. 6, 17616-17625 (2014). IF: 5.9

Nanoscale coordination polymers with ligand-centred pH-responses and spin transition, D. Ruiz-Molina, F. Novio, F. Nador, *Chemical Communications*: vol. 50, 14570-14572 (2014). IF: 6.718

Synthesis of polydopamine at the femtoliter scale and confined fabrication of Ag nanoparticles on surfaces, M. Guardingo, M. J. Esplandiu and D. Ruiz-Molina, *Chemical Communications*: vol. 50, 12548-12551 (2014)



PROJECTS

Smart theranostic metal-organic nanostructures for cancer cure, funded by **AGAUR**, 01/04/2013 - 31/03/2016, Daniel Ruiz-Molina

Ordered hetero- and Nano-structures with Epitaxial Dielectrics for magnetic and electronics Applications (ONDA), funded by **EC**, 15/06/2010 - 14/06/2014

Dispositivos Moleculares, MOLDEV, funded by **MINECO**, 01/01/2013 - 31/12/2015, Daniel Ruiz-Molina

Desarrollo de nanoencapsulación funcionalizada de fragancias para aplicación en formulación de suavizantes, MICROFRAG, funded by **MINECO**, 28/02/2013 - 31/12/2014, Daniel Ruiz-Molina

Pinturas fotocrómicas en polvo para su uso en arquitectura de exteriores de alto valor añadido, ADAPTALITE, funded by **MINECO**, 01/09/2014 - 31/12/2017, Daniel Ruiz-Molina



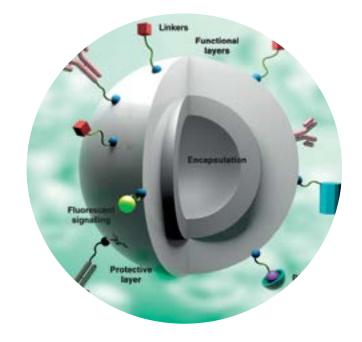


воокѕ

Amorphous Coordination Polymer Particles for Biomedicine, F. Novio, D. Ruiz-Molina, J. Lorenzo, In *Bio- and Bioinspired Nanomaterials*, (Eds. D. Ruiz-Molina, F. Novio and C. Roscini), Wiley-VCH, 2014

Bio- and Bioinspired Nanomaterials, D. Ruiz-Molina, F. Novio and C. Roscini, Wiley-VCH, 2014

Catechol-Based Biomimetic Functional Materials and their applications, J. Saiz-Poseu, D. Ruiz-Molina, J. Sedó, F. Busqué, In *Bio- and Bioinspired Nanomaterials*, (Eds. D. Ruiz-Molina, F. Novio and C. Roscini), Wiley-VCH, 2014





OTHER HIGHLIGHTS

1 SPIN-OFF created: Futurechromes SL.

A new spin-off company, Futurechromes, S.L., based on the patent Ref. CIN2PAT 01/12 - WO2013/132123 Coating with photochromic properties, method for producing said coating and use thereof applicable to optical articles and glazed surfaces developed by the Nanostructured Functional Materials Group was created in June 2014.

More information:

http://nanosfun.icn2.cat/

Nanostructured Materials for Photovoltaic Energy Group

Main Research Lines

- Organic, Hybrid, Dye-sensitized, Halide Perovskite and All-oxide Solar Cells: materials synthesis and characterisation and complete device fabrication
- Synthesis of metal oxides by low-cost, lowtemperature 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



GROUP MEMBERS

Irene Álvarez de Lasarte, Technician Andressa Antunes Bortoti, CSIC Visiting Doctoral Student

Julio Bastos, CSIC Visiting Postdoctoral Researcher Chloé Bonnet, CSIC Visiting Doctoral Student Andreia de Morais, CSIC Visiting Doctoral Student Francisco Anderson de Sousa Lima, CSIC Visiting Doctoral Student

Fernando Echeverría, CSIC Visiting Doctoral Student Enrique Fernández, CSIC Visiting Student

Marta Fonrodona, Project Manager

Mónica Lira, CSIC Tenured Track and Group Leader



GROUP LEADER



CSIC Tenured Scientist Dr Mónica Lira-Cantú

Mónica Lira-Cantú (Chemistry, 1992), obtained a Master and PhD degrees in Materials Science at the Materials Science Institute of Barcelona (ICMAB) / Universitat Autònoma de Barcelona (1995/1997) and completed her postdoctoral work under a contract with the company Schneider Electric/ICMAB (1998). From 1999 to 2001 she worked as permanent Senior Staff Chemist at ExxonMobil Research & Engineering (formerly Mobil Technology Co) in New Jersey (USA) initiating a laboratory on energy-related applications. Currently, she is Group Leader of the Nanostructured Materials for Photovoltaic Energy Group (nanostructuredmaterials.icn2.cat) of the Catalan Institute of Nanoscience and Nanotechnology, ICN2.



NEW PROJECTS & MILESTONES

The Nanostructured Materials for Photovoltaic Energy Group focuses on different objectives, all related to the **development of highly efficient**, **highly stable and low-cost solution processable photovoltaic and optoelectronic devices**:

The synthesis of nanostructured materials, especially those involving transition metal oxides (TMOs) and graphene, applying low-cost and solution processing methods is a major goal for the group. TMOs have many possible applications as main active materials or barrier layers, but are also applied as materials for external light management. The application of low-temperature

Amador Pérez-Tomás, Postdoctoral researcher

María Inmaculada Suárez, Project Manager

Javier Suárez, CSIC Visiting Student Cicero Venancio, CSIC Visiting Doctoral Student

Marc Vidal, CSIC Visiting Student

synthesis methods (sol-gel, hydrothermal, SILAR, among many others) permits tuning and control of the properties of the final device.

The stability and long life of optoelectronic devices, especially organic solar cells, is a major limitation for these technologies to reach the marketplace. A consortium of more than 260 members, among them 60



She received different awards/fellowships as a visiting scientist to the following laboratories: University of Oslo, Norway (2003), Riso National Laboratory, Denmark (2004/2005) and the Center for Advanced Science and Innovation, Japan (2006). She obtained a permanent position in 2007 at the Spanish National Research Council (CSIC, Spain) and started the laboratory on Photovoltaic Energy at CIN2 in 2007. Since then she has directed more than 20 researchers (including Postdocs, PhD students and undergraduate students). She has been the PI of several projects (including national, industrial and European), and she is the principal coordinator of a COST Action Proposal (approved in 2013) related to the study of the stability of Organic solar cells (OPVs).

Her research interests are the synthesis and application of nanostructured materials for stable next-generation thin film solar cells: Perovskite solar cells, Dye-sensitized, Hybrid and Organic Solar Cells. Mónica Lira-Cantú has more than 70 published papers, 7 patents and 8 book chapters, h index = 25

internationally-recognized research laboratories and 17 industries from 31 countries, have joined an EU COST Action project related to the stability of organic solar cells. The project is led by ICN2 trough Group Leader Mónica Lira-Cantú, coordinator of the consortium. The goal is to take advantage of the multiple characterisation techniques available from the different partners to elucidate the degradation mechanism of these devices and propose disruptive solutions towards highly stable Organic solar cells.

The review article "Vertically-aligned nanostructures of ZnO for excitonic solar cells: a review" by Irene González-Valls and Mónica Lira-Cantú, has been in the top 10 most cited articles of the journal Energy & Environmental Science (impact factor 15.49) since 2009.



PUBLICATIONS

Solution processable titanium dioxide precursor and nanoparticulated ink:
Application in Dye-Sensitized Solar Cells,
Bosch-Jiménez P., Yu Y., Lira-Cantú M., Domingo

C., Ayllon J.A., *Journal of Colloid and Interface*Science: vol. 416, 112-118 (2014). IF: 3.552

Worldwide outdoor round robin study of organic photovoltaic devices and modules,

Madsen M.V., Gevorgyan S.A., Pacios R., Ajuria I., Etxebarria I., Kettle J., Bristow N.D., Neophytou M., Choulis S.A., Stolz Roman L., Yohannes T., Cester A., Cheng P., Zhan X., Wu J., Xie Z., Tu W.-C., He J.-H., Fell C.J., Anderson K., Hermenau M., Bartesaghi D., Jan Anton Koster L., Machui F., González-Valls I., Lira-Cantú M., Khlyabich P.P., Thompson B.C., Gupta R., Shanmugam K., Kulkarni G.U., Galagan Y., Urbina A., Abad I., Roesch R., Hoppe H., Morvillo P., Bobeico E., Panaitescu E., Menon L., Luo Q., Wu Z., Ma C., Hambarian A., Melikyan V., Hambsch M., Burn P.L., Meredith P., Rath T., Dunst S., Trimmel G., Bardizza G., Mullejans H., Goryachev A.E., Misra R.K., Katz E.A., Takagi K., Magaino S., Saito H., Aoki D., Sommeling P.M., Kroon J.M., Vangerven T., Manca J., Kesters J., Maes W., Bobkova O.D., Trukhanov V.A., Paraschuk D.Y., Castro F.A., Blakesley J., Tuladhar S.M., Alexander Rohr J., Nelson J., Xia J., Parlak E.A., Tumay T.A., Egelhaaf H.-J., Tanenbaum D.M., Mae Ferguson G., Carpenter R., Chen H., Zimmermann B., Hirsch L., Wantz G., Sun Z., Singh P., Bapat C., Offermans T., Krebs F.C., Solar Energy Materials and Solar Cells: vol. 130, 281-290 (2014). IF: 5.03



PROJECTS

Nanostructured Materials for Photovoltaic Energy, funded by **AGAUR**, 01/01/2014-31/12/2016, Mónica Lira-Cantú

Produção De Células Solares De Terceira Geração Baseadas Em Zno E Sno2 Sintetizados Por Eletrodeposição, Moagem Mecânica E Sol-gel Proteico, funded by **Brasilian government** (FUNCAP), 01/01/2014-31/12/2016, Mónica Lira-Cantú / Igor Vasconcelos

Stable Next-Generation Photovoltaics: Unravelling Degradation Mechanisms of Organic Solar Cells by Complementary Characterisation Techniques, StableNextSol, funded by **EC**, 01/06/2014-31/05/2018, Mónica Lira-Cantú

Células Solares Nanoestructuradas Fabricadas a partir de disoluciones: Nuevos Nanomateriales basados en Óxidos de Metales de Transición y Grafeno, NanoSOL-DEV, funded by **MINECO**, 01/01/2014-31/12/2016, Mónica Lira-Cantú

Xarxa de Referència en Materials Avançats per a l'Energia - XaRMAE, funded by XaRMAE, 01/01/2009-31/12/2014, Mónica Lira-Cantú



CONTRIBUTIONS

Low-Temperature Solution Processed Layered V2O5 Hydrate as Hole-Transport Layer in Stable Organic Solar Cells, 2nd International Conference on the Evaluation & Standardisation of Organic Solar Cells (ICES2014), organized by RATO, Hokkaido, Japan, 06-08/02/2014, Nanostructured Materials for Photovoltaic Energy, Mónica Lira-Cantú (Invited)

Low-Temperature Solution Processed Layered V2O5 Hydrate as Hole-Transport Layer in Stable Organic Solar Cells, 23rd International Materials Research Congress (IMRC 2014), organized by SPIE, Cancún, México, 18/08/2014, Nanostructured Materials for Photovoltaic Energy, Gerardo Teran-Escobar, Jonas Pampel and Mónica Lira-Cantú (Invited)

Low-Temperature Solution Processed Layered V2O5 Hydrate as Hole-Transport Layer in Stable Organic Solar Cells, **SPIE Meeting**, organized by SPIE, San Diego, USA, 20/08/2014, Nanostructured Materials for Photovoltaic Energy, Gerardo Teran-Escobar, Jonas Pampel and Mónica Lira-Cantú (Invited)

Unraveling Degradation Mechanisms of Organic Solar Cells, 7th Workshop entitled: "Creating the Organic & Printed Electronics Industry in Greece", organized by MRS, Thesaloniki, Greece, 18-19/12/2014, Nanostructured Materials for Photovoltaic Energy, Mónica Lira-Cantú (Invited)

Nanostructured Oxide Semiconductors for Thin Film Photovoltaics, Nanoselect, organized by Consolider, St Feliu de Guíxols, Spain, 06/07/2014, Nanostructured Materials for Photovoltaic Energy, Gerardo Teran-Escobar, Jonas Pampel and Mónica Lira-Cantú (Oral presentation)

Stable Next-Generation Photovoltaics: Unraveling degradation mechanisms of Organic Solar Cells by complementary characterisation techniques (StableNextSol), MNPS 8th Annual Progress Conference (APC), organized by COST, Heraklion, Greece, 10/09/2014, Nanostructured Materials for Photovoltaic Energy, Mónica Lira-Cantú (Oral presentation)

Novel Energy-Oriented Materials Group

Main Research Lines -

- Hybrid electrode materials for supercapacitors and hybrid energy storage devices
- Cathode materials with fractal granularity for Li-ion batteries based on LiFePO4
- Nanofluids. Thermal nanofluids for heat transfer in solar conversion. Molten salts
- Electroactive nanofluids for energy storage in flow cells. Redox flow batteries based on quinones
- Graphene synthesis, hybridisation and applications in energy storage



GROUP MEMBERS

Omar Ayyad, Postdoctoral Researcher
Zahilia Caban, Doctoral Student
Deepak Prakash Dubal, CSIC Beatriu de Pinós
Postdoctoral Researcher
Andrea Fedorková, Visiting Postdoctoral Researcher
Ramón García, CSIC Visiting Student
Daniel Gómez, Assistant
Pedro Gómez, CSIC Full Professor and Group Leader
Girish Gund, CSIC Postdoctoral Researcher

Rita Humana, CSIC Visiting Doctoral Student
Tomas Kazda, CSIC Visiting Doctoral Student
Mara Olivares, CSIC Visiting Postdoctoral Researcher
Daniel Rueda, CSIC Visiting Student
Amel Slamani, CSIC Visiting Doctoral Student
Jullieth Gabriela Suarez, CSIC Doctoral Student
Franciele Wolfart, CSIC Visiting Doctoral Student



GROUP LEADER



CSIC Research Prof Dr Pedro Gómez-Romero

Prof Pedro Gómez-Romero (BSc and MSc Universidad de Valencia, Spain. PhD in Chemistry, Georgetown University, USA, 1987, with Distinction). CSIC Researcher since 1990 (ICMAB, 1990-2007). Sabbatical as NATO Senior Research Fellow at the National Renewable Energy Laboratory (Golden, CO, USA, 1998-99). CSIC Full Research Professor (2006-) and Group Leader of NEO-Energy lab at CIN2 (CSIC) (2007-2013) now part of ICN2. Fellow of the Royal Society of Chemistry.



NEW PROJECTS & MILESTONES

2014 witnessed the consolidation of the new research topics in the group. Among them, we developed redox flow batteries based on quinones, new molten salt formulations for heat transfer and storage and the low-cost synthesis of high-quality graphene that we had begun in 2013

Hybrid materials as improved electrodes for electrochemical supercapacitors. The boundaries between batteries and capacitors

are now quickly blurring. Nanostructure control is of great importance in the design of high-performance energy storing devices. Thus, we are developing materials with a high specific surface, and ultradispersed molecular materials, for applications in electrochemical supercapacitors that have greater power density than that of batteries. Examples of this type of electrodes prepared for the first time in our laboratory include activated carbons or graphene with polyoxometalates or oxide nanoparticles. (NANOCARHIBE MAT2012 National Project).



Directs projects on hybrid organic-inorganic nanostructures, nanocomposite materials for energy storage and conversion (lithium batteries, supercapacitors, PEM FCs, solar-thermal energy, nanofluids, graphene). Vicedirector of MATGAS (2010-2014).

Author of 10² (ten to the two) scientific publications in refereed international journals. Scientific editor of the book "Functional Hybrid Materials" P. Gómez-Romero, C. Sánchez (Eds.) (Wiley-VCH 2004) and author of two award-winning popular science books (*Metaevolución. La Tierra en el espejo*, Celeste, 2001 and *Un planeta en busca de energía*, Síntesis, 2007).

Micro-supercapacitors based on Si Nanowires and MnO2-coated Si Nanowires.

Also related with supercapacitors we collaborate with an international consortium led by CEA (France) on the development of nanowire electrodes for energy storage (NEST EU Project). One of our main contributions to this project has been the coating of these Nanowire electrodes with MnO2 nanoflakes. This approach has led to microsupercapacitors with excellent performance which are one of the main milestones of this European Project

Eco-friendly high-performance electrodes for rechargeable lithium batteries. It

includes our work on the optimisation of micro- and nanostructures of electroactive inorganic materials such as LiFePO4 with fractal granularity used in electrodes for lithium batteries. Here, we are aiming for low-cost, safe batteries, prepared under the mildest conditions with faster recharging rates (SOMABAT EU Project).

Nanofluids. The development of nanofluids, including electroactive nanofluids and heat-transfer nanofluids for 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 load-levelling of renewable energies, Electric Vehicles or high temperature (concentration) solar power electricity generation.

Graphene. The new kid in the Nanocarbon town is the subject of our interest too. We work on large-scale methods for the preparation of high-quality graphene and its use in the synthesis of nanohybrid materials.



PUBLICATIONS

Alcohol mediated growth of a-MnO2 thin films from KMnO4 precursor for high performance supercapacitors, N.

R. Chodankar, G. S. Gund, D. P. Dubal, C. D. Lokhande, *RSC Advances*: vol. 4, 601503-601513 (2014). IF: 3.708

Development of hybrid materials based on sponge-supported reduced graphene oxide and transition metal hydroxides for hybrid energy storage devices, D. P. Dubal, R. Holze, P. Gómez-Romero, *Scientific reports*: vol. 4 (2014). IF: 5.078

High performance of symmetric microsupercapacitors based on silicon nanowires using N-methyl-N-propylpyrrolidinium bis(trifluoromethylsulfonyl)imide as electrolyte, Aradilla D., Gentile P., Bidan G., Ruiz V., Gómez-Romero P., Schubert T.J.S., Sahin H., Frackowiak E., Sadki S., *Nano Energy*: vol. 9, 273-281 (2014). IF: 10.211

Hybrid energy storage: High-voltage aqueous supercapacitors based on activated carbon-phosphotungstate hybrid materials, Suárez-Guevara J., Ruiz V., Gómez-Romero P., Journal of Materials Chemistry A (4): vol. 2, 1014-1021 (2014)

Nanoflower-like CuO/Cu(OH)2 hybrid thin films: Synthesis and electrochemical supercapacitive properties, S. K. Shinde; D. P. Dubal, G. S. Ghodake, D. Y. Kim, V. J. Fulari, Journal of Electroanalytical Chemistry: vol. 732, 80-85 (2014). IF: 2.871

Novel hybrid micro-supercapacitor based on conducting polymer coated silicon nanowires for electrochemical energy storage, Aradilla D.; Bidan G.; Gentile P.; Weathers P.; Thissandier F.; Ruiz V.; Gómez-Romero P.; Schubert T.J.S.; Sahin H.; Sadki S., *RSC Advances* (50): vol. 4, 26462-26467 (2014). IF: 3.708

Screen Printed Asymmetric Supercapacitors based on LiCoO2 and Graphene Oxide, A.

B. Dighe, D. P. Dubal, R. Holz, *Zeitschrift für anorganische und allgemeine Chemie*: vol. 640 (2014). IF: 1.25

Stable graphene-polyoxometalate nanomaterials for application in hybrid supercapacitors, Suárez-Guevara J., Ruiz V., Gómez-Romero P., *Physical Chemistry Chemical Physics* (38): vol. 16, 20411-20414 (2014), IF: 4.198

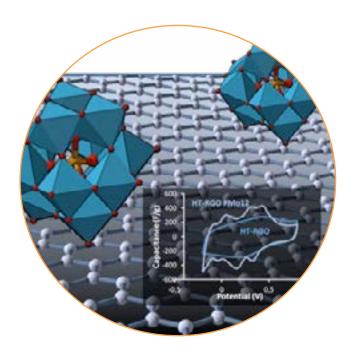


PROJECTS

High energy and high-power supercapacitorbattery hybrid energy storage devices based on graphene-enhanced (MnO2/G) electrode materials, funded by **AGAUR**, 15/04/2014 -14/04/2016, Pedro Gómez-Romero

Nanowires for Energy Storage (NEST), funded by **EC**, 01/11/2012 - 30/10/2015, Pedro Gómez-Romero

Materiales Nanoestructurados de Carbono e Hibridos para Almacenamiento de Energía, (NANOCARHIBES), funded by **MINECO**, 01/01/2013 - 31/12/2015, Pedro Gómez-Romero





CONTRIBUTIONS

Materials for electrochemical storage II: supercapacitors, MAT4Energy. Materials for Sustainable Energy Applications: Conversion, Storage and Eficiency, organized by LMGP. Grenoble (France), 16-18/06/2014, Pedro Gómez-Romero (Invited)

Synthesis of graphene hybrid nanocomposites for energy and environmental applications, International Graphene Innovation Conference, organized by GraphChina. Ningbo (China), 01-03/09/2014, Pedro Gómez-Romero (Invited)

Hybrid energy storage. Merging Battery and Supercapacitor Chemistries, **5th EUCHEMS Chemistry Congress**, organized by Turkish Chemical Society. Istambul (Turkey), 31/08/2014-04/09/2014, Pedro Gómez-Romero (Keynote)

Energy Nanomaterials, **Trends in Nanotechnology (TNT) Severo Ochoa Session**, organized by ICN2. Barcelona, Spain, 29-oct, 2014, Pedro Gómez-Romero (Keynote)

Investigating Energy, Plenary Opening Conference (60 min). MAT4Energy. Materials for Sustainable Energy Applications: Conversion, Storage and Eficiency, organized by LMGP. Grenoble (France), 16-18/06/2014, Pedro Gómez-Romero (Opening)

Hybrid Energy Storage: merging battery and supercapacitor chemistries, **Power our Future 2014**, organized by CIC energigune. Vitoria (Spain), 01-04/04/2014, Pedro Gómez-Romero (Oral)

Hybrid Energy Storage. Merging the Chemistries of Batteries and Supercapacitors Nanotech, **MEET**. Hammamet (Tunisia), 24-26/04/2014, Pedro Gómez-Romero (Oral)

Hybrid Materials for Energy Storage, XIII Congreso Nacional de Materiales, organized by UB, CPT, sociemat. Barcelona (Spain), 18-20/06/2014, Pedro Gómez-Romero (Oral)

All there is inside a pencil. The graphene revolution and other nanostories, **TEDx Conference**. Peralada (Spain), 27/06/2014, Pedro Gómez-Romero (Oral)

Heterogeneous hydrothermal redox reactions: Understanding nanostructure formation and shape evolution through nanomalleability,

4th International Solvothermal and Hydrothermal Association Conference ISHA 2014, organized by Université de Bordeaux. Bordeaux (France), 26-29/10/2014, D. Muñoz-Rojas, O. Ayyad, J. Oró-Solé, P. Gómez-Romero (Oral)

Silicon-based 3D hierarchical nanostructures for μ-supercapacitors implementation, NMEC-2, second International workshop on nano Materials for Energy conversion. Ho Chi Minh City (Vietnam), 17-20/11/2014, Gérard Bidan (Invited), David Aradilla, Pascal Gentile, Pedro Gómez-Romero, Jan Wimberg, Boyan Iliev Wolfgang Müller-Sebert, Fang Gao, Elżbieta Frackowiak, Saïd Sadki (Oral)

From Nanometers to Terawatts. Pending Breakthroughs in Materials for Energy, 2nd International Symposium on Energy Challenges and Mechanics (ECM2). Aberdeen (UK), 19-21/08/2014, Pedro Gómez-Romero (Principal lecture)

Microassemblies of LiFePO4 nanoparticles for use as cathodes in Lithium ion batteries, XIII Congreso Nacional de Materiales, organized by UB, CPT, sociemat. Barcelona, Spain, 18-20/06/2014, Z. Caban-Huertas, O. Ayyad and P. Gómez-Romero (Poster)



COURSES

Chemistry for Specific Materials, in Màster Universitari en Química Industrial i Introducció a la Recerca Química, **Universitat Autònoma de Barcelona, Barcelona (Spain)**, Prof Pedro Gómez-Romero



THESES

Doctorand: **Julieth Suarez-Guevara** Title: Materiales híbridos basados en

nanocarbones y polioxometalatos para aplicación como electrodos en supercondensadores con mecanismo dual de almacenamiento de energía Defense Date: 20/11/2014

Directors: Prof Pedro Gómez Romero and Dra

Vanesa Ruiz

Oxide Nanoelectronics 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

Umesh Kumar Bhaskar, Postdoctoral Researcher Gustau Catalán, ICREA Research Professor and Group Leader

Rohíni Kumara Cordero, Doctoral Student Neus Domingo, Ramón y Cajal Postdoctoral Researcher Jason Fleischman, Visiting Student

Víctor Pablo Galván Chacón, Doctoral Student

Yavuz Kurtulus, Visiting Student Xavier Martí, Postdoctoral Researcher lackeline Narváez, Doctoral Student Amador Pérez, Postdoctoral Researcher Spyridon Sovatzoglou, Technician James Arturo Zapata, Technician



GROUP LEADER



ICREA Prof Gustau Catalán

Prof Gustau Catalán earned his BSc in Physics at the Universitat de Barcelona (1997), and his PhD in Physics at Queen's University of Belfast (2001). He then took research positions at the Mediterranean Institute for Advanced Studies (2002-2004), the University of Groningen (2004-2005) and the University of Cambridge (2005-2009). In 2009 he joined CIN2 as an ICREA Research Professor and Group Leader of the Oxide Nanoelectronics (ON) Laboratory, and three years later he transferred his research to ICN. Both Institutions recently joined their efforts and became ICN2, where he continues to lead the Group. In 2012, he earned an ERC Starting Grant to set up in Barcelona the world's first dedicated laboratory of nanoflexoelectricity.





NEW PROJECTS & MILESTONES

Most of this year's effort was focused on completing the big investments (equipment purchase, hiring of personnel) for the ERC project. The human team is now complete and the equipment is up and running, so now that the big admin tasks are over we expect more scientific progress.

On the research front, the outstanding contributor has been Xavi Martí, who has produced a string of high-profile articles about spintronics with antiferromagnetic materials. This year has also finally seen the publication of our investigation on the origin of giant flexoelectricity in relaxors. We have also produced eye-catching results in layered iridium oxides (Sr₂IrO₄); but this work was not published until 2015, so we will talk about it in next year's annual report.



PUBLICATIONS

Anisotropic magnetoresistance in an antiferromagnetic semiconductor, I.Fina, X. Martí, D. Yi, J. Liu, J.H. Chu, C. Rayan-Serrao, S. Suresha, J. Železný, T. Jungwirth, J. Fontcuberta, and R. Ramesh, *Nature Communications*: vol. 5, 4671 (2014). IF: 10.742

Electrocatalytic tuning of biosensing response through electrostatic or hydrophobic enzyme – graphene oxide interactions, Luis Baptista-Pires, B. Pérez-López, Carmen C. Mayorga-Martínez, Eden Morales-Narváez, Neus Domingo, María José Esplandiu, Francesc Alzina, C.M. Sotomayor Torres, A. Merkoçi, *Biosensors and Bioelectronics*: vol. 61, 665-662 (2014). IF: 6.451

Improved performance of 4H-SiC PiN diodes using a novel combined high-temperature oxidation and annealing process, Fisher C.A., Jennings M.R., Sharma Y.K., Hamilton D.P., Gammon P.M., Pérez-Tomás A., Thomas S.M., Burrows S.E., Mawby P.A., *IEEE Transactions on Semiconductor Manufacturing*, 3, 27, 6857419, 443-451 (2014). IF: 0,977

On the Schottky barrier height-lowering effect of Ti₃SiC₂ in ohmic contacts to p-type 4H-SiC, C. A. Fisher, M. R. Jennings, Y. K. Sharma, A. Sánchez, D. Walker, P. M. Gammon, A. Pérez-Tomás, S. M. Thomas, S. E. Burrows and P. A. Mawby, *International Journal of Fundamental Physical Sciences* (3): vol. 4, 95-100 (2014). IF: 0

Origin of the enhanced flexoelectricity of relaxor ferroelectrics, Narváez J., Catalán G., *Applied Physics Letters*, 16, 104, 162903 (2014). IF: 3.515

Room temperature negative capacitance in a ferroelectric-dielectric superlattice heterostructure, Weiwei Gao; Asif Khan; Xavi Martí; Chris Nelson; Claudy Serrao; Jayakanth Ravichandran; Ramamoorthy Ramesh; Sayeef Salahuddin, *Nano Letters* (10): vol. 14, 5814-5819 (2014). IF: 12.94

Spectroscopy methods for molecular nanomagnets, Baker, M.L.; Blundell, S.J.; Domingo, N.; Hill, S., *Structure and Bonding*: vol. 164, 231-292 (2014). IF: 1.836

Spintronic Functionality of BiFeO₃ Domain Walls, J.H. Lee, I. Fina, X. Martí, Y.H. Kim, D. Hesse, and M. Alexe, *Advanced Materials* (41): vol. 26, 7078-7082 (2014). IF: 15.409

Tailoring the interfacial magnetic anisotropy in multiferroic field-effect devices, Preziosi D., Fina I., Pippel E., Hesse D., Marti X., Bern F., Ziese M., Alexe M., *Physical Review B - Condensed Matter and Materials Physics*, 12, 90, 125155 (2014). IF: 3.664



PROJECTS

SGR, funded by **AGAUR**, 01/01/2014 - 31/12/2016, Gustau Catalán

Flexoelectricity, funded by **EC**, 01/01/2013 - 31/12/2017, Gustau Catalán

Magnetism of nanostructures on surfaces: from isolated nanoparticles to magnetic domain walls, funded by **MINECO**, 01/12/2010-30/11/2015, Gustau Catalán

Estrestrónica de óxidos, OSTRES, funded by MINECO, 01/01/2014-31/12/2016, Gustau Catalán



CONTRIBUTIONS

Flexoelectricity, **Research Seminar**, organized by Peking University, Beijing, China, 2014, Gustau Catalán (Invited)

On the true size of flexoelectricity, **Conference on Advanced Topics in Ferroelectrics**, Jiang Tang, China, 2014, Gustau Catalán (Invited)

Pressure-induced effects at the nanoscale, organized by Max Planck Institute, Stuttgart, Germany, 2014, Neus Domingo (Invited)

Giant piezoresistance in oxide thin films, **3rd** International Workshop on Complex Oxides, organized by Vanderbilt University, Cyprus, 19-23/05/2014, Gustau Catalán (Invited)

Interplay between flexoeletricity and nanodomains, CIMTEC conference on Advanced Ceramics, Montecatini Terme, organized by CIMTEC, Montecatini Terme, Italy, 08-13/06/2014, Gustau Catalán (Invited)

Nanoscopically confined metal-insulator transitions in oxides, European Materials Research Society (E-MRS) Fall Meeting, organized by European Materials Research Society, Warsaw, Poland, 15-18/09/2014, Gustau Catalán (Invited)

Contribution of polar nanorregions to the giant flexoelectricity of relaxor ferroelectrics, **Spring Meeting of the American Physics Society** (APS), organized by APS, Denver, USA, 03-07/03/2014, J. Narváez (Oral)

Scanning piezoresistance: a new experimental tool (or what happens when you put an elephant on stilettos, **Multifrequency AFM**, organized by CSIC, Madrid, Spain, 16-18/06/2014, Neus Domingo (Oral)

Uniaxial Strain Control of Metal Insulator Transitions in Sr_2IrO_4 thin films, **Fuerzas y Tunel**, organized by Donostia International Physics Center, San Sebastián, Spain, 27-29/08/2014, Neus Domingo (Oral)

Scanning probe piezoresistance: a new experimental tool, **Trends in Nanotechnology (TNT2014)**, Barcelona, Spain, 27-31/10/2014, Neus Domingo (Oral)



BOOKS

Physics of Ferroic and Multiferroic Domain Walls (book chapter for the book *Mesoscopic Phenomena in Multifunctional Materials*), Catalán G., Springer Series in Materials Science, 2014

Phononic and Photonic Nanostructures Group

Main Research Lines -

- Nanophononics and Nanophotonics
- Nanofabrication
- Nanometrology
- Oxide-based Nanostructures



GROUP MEMBERS

Francesc Alzina, Senior Researcher Noèlia Arias, Group Administrator and Project Manager Eglantina Benavente, Visiting Profesor Monica Emperatriz Bernal, Visiting Doctoral Student Sweta Bhansali, FI Doctoral Student Emigdio Chávez, Postdoctoral Researcher Claudia Delgado Simao, Postdoctoral Researcher Sindy Devis, Visiting Doctoral Student Alexandros El Sachat, Doctoral Student Ariadna Fernández, Doctoral Student Achille Leo Francone, Postdoctoral Researcher Yamila García, Postdoctoral Researcher Jordi Gomis, Juan de la Cierva Postdoctoral Researcher

Guillermo González, Visiting Profesor Bartlomiej Graczykowski, Postdoctoral Researcher Erwan Guillotel, Group Administrator and Project Manager

Martin Kreuzer, DFG Postdoctoral Researcher luan Ignacio Medina, Doctoral Student and Laboratory Engineer

Daniel Navarro, Beatriu de Pinós Postdoctoral

Juan Sebastián Reparaz, Postdoctoral Researcher Marianna Sledzinska, Laboratory Engineer Clivia Sotomayor, ICREA Research Professor and Group Leader

Markus Wagner, Marie Curie Postdoctoral Researcher



GROUP LEADER



ICREA Prof Dr Clivia M. Sotomayor Torres

ICREA Research Professor Dr Clivia M. Sotomayor Torres was awarded her PhD in Physics in 1984 by Manchester University (UK). She then held tenured academic appointments at St. Andrews and Glasgow Universities in the UK and became a C4 professor at Wuppertal University (Germany) in 1996. She was a research professor at University College Cork, Tyndall National Institute (Ireland) from 2004 to 2008. Since May 2007 she has been ICREA Research Professor based at the Catalan Institute of Nanotechnology (ICN), now ICN2.



NEW PROJECTS & MILESTONES

The Group completed two of its ongoing projects: EUPHONON (Building a European NanoPhononics Community) and NANO-TEG (Nanostructured ThermoElectric Systems for Green Transport & Energy Efficient Applications).

Seven projects are still ongoing: MERGING (Membrane-based phonon engineering for energy harvesting), PLAST4FUTURE (Injection-moulding production technology for multi-functional nano-structured

plastic components enabled by Nano Imprint Lithography), TAPHOR (Tailoring Acoustic Phonon Dispersion Relations), and QUANTIHEAT (Quantitative scanning probe microscopy techniques for heat transfer management in nanomaterials and nanodevices), nanoTHERM (Spanish CONSOLIDER on Tailoring electronic and phononic properties of nanomaterials: Towards ideal Thermoelectricity), NANO-RF (Carbon-based smart systems for wireless applications), and NANOTHERM (Innovative Nano and Micro Technologies for Advanced Thermo and Mechanical Interfaces).



She has received awards from the Royal Society of Edinburgh, the Nuffield Foundation and an Amelia Earhart Fellowship from ZONTA International (USA). She is author of over 450 scientific publications and has edited six books (Researcher ID; E-8418-2010, Hirsch index 38, over 6000 citations). She leads a strong team working on phonon engineering and is actively engaged in European-level research. She serves on Scientific Advisory Committees in Nanoscience and Nanotechnology in France and she is a jury member of the FWO Research Foundation Flanders Odysseus Programme. She is a Member of the Board of Stakeholders of Photonics21 and a Visiting Professor at the Royal Institute of Technology, KTH, in Sweden.

Recently the group designed a silicon 1D Optomechanical crystal built up so that it allows stable localisation of both phonons and photons. In 2014 the results were reported in *Nature Communications* (vol. 5, 4452 (2014) and later highlighted in Nature Photonics (vol. 8, 746 (2014).



PUBLICATIONS

A novel contactless technique for thermal field mapping and thermal conductivity determination: Two-Laser Raman Thermometry, Reparaz J.S., Chávez-Ángel E., Wagner M.R., Graczykowski B., Gomis-Bresco J., Alzina F., Sotomayor Torres C.M., *Review of Scientific Instruments* (3): vol. 85 (2014). IF: 1.584

A one-dimensional optomechanical crystal with a complete phononic band gap,

Gomis-Bresco J., Navarro-Urrios D., Oudich M., El-Jallal S., Griol A., Puerto D., Chávez E., Pennec Y., Djafari-Rouhani B., Alzina F., Martínez A., Sotomayor Torres C. M., *Nature Communications*: vol. 5 (2014). IF: 10.742

A physics-based scoring function for protein structural decoys: Dynamic testing on targets of CASP-ROLL, Ruiz-Blanco Y.B.; Marrero-Ponce Y.; Garcia Y.; Puris A.; Bello R.; Green J.; Sotomayor Torres C. M., *Chemical Physics Letters*: vol. 610-611, 135-140 (2014). IF: 1.991

A Study of the Kinetics and Mechanism of Rapid Self-assembly in Block Copolymer Thin Films during "Solvo-microwave" Annealing, Mokarian-TabariP., Cummins C., Rasappa S., Simao C. C. D., Sotomayor Torres C. M., Holmes J. D., Morris M. A., *Langmuir* (35): vol. 30, 10728 (2014). IF: 4.384

Acoustic phonon propagation in ultrathin Si membranes under biaxial stress field, Graczykowski B., Gomis-Bresco J., Alzina F., Reparaz J. S., Shchepetov A., Prunnila M., Ahopelto J., Sotomayor Torres C. M., New Journal of Physics: vol. 16 (2014). IF: 3.671

Dynamical back-action at 5.5 GHz in a corrugated optomechanical beam, Navarro-Urrios D., Gomis-Bresco J., El-Jallal S., Oudich M., Pitanti A., Capuj N., Tredicucci A., Alzina F., Griol A., Pennec Y., Djafari-Rouhani B., Martínez A., Sotomayor Torres C. M., *AIP Advances*: vol. 4 (2014). IF: 1.59

Electrocatalytic tuning of biosensing response through electrostatic or hydrophobic enzyme – graphene oxide interactions, Baptista-Pires L., Pérez-López B., Mayorga-Martinez C. C., Morales-Narváez E., Domingo N., Esplandiu M. J., Alzina F., Sotomayor Torres C. M., Merkoçi A., *Biosensors and Bioelectronics*: vol. 61, 665-662 (2014). IF: 6.451

Embedded inkjet-printed silver grids for ITO-free organic solar cells with high fill factor, Burgués-Ceballos I., Kehagias N., Sotomayor Torres C. M., Campoy-Quiles M., Lacharmoise P. D., Solar Energy Materials and Solar Cells: vol. 127, 50-57 (2014). IF: 5.03

Formation of Titanium Nanostructures on Block Copolymer Templates with Varying Molecular Weights, Kreuzer M., Simao C., Díaz A., Sotomayor Torres C. M., *Macromolecules* (24): vol. 47, 8699 (2014). IF: 5.927

High-quality single-crystal Ge nanomembranes for opto-electronic integrated circuitry, Shah V. A., Rhead S. D., Halpin J. E., Trushkevych O., Chávez-Ángel E., Shchepetov A., Kachkanov V., Wilson N. R., Myronov M., Reparaz J. S., Edwards R. S., Wagner M. R., Alzina F., Dolbnya I. P., Patchett D. H., Allred P. S., Prest M. J., Gammon P. M., Prunnila M., Whall T. E., Parker E. H. C., Sotomayor Torres C. M., Leadley D.R., *Journal of Applied Physics* (14): vol. 115 (2014). IF: 2.185

Hypersonic phonon propagation in onedimensional surface phononic crystal, Graczykowski B., Sledzinska M., Kehagias N., Alzina F., Reparaz J. S., Sotomayor Torres C. M., Applied Physics Letters (12): vol. 104 (2014). IF: 3.515 Li-doped ZnO nanorods with single-crystal quality-non-classical crystallisation and self-assembly into mesoporous materials,

Lizandara-Pueyo C., Dilger S., Wagner M. R., Gerigk M., Hoffmann A., Polarz S., *CrystEngComm* (8): vol. 16, 1525-1531 (2014). IF: 3.858

Modification of Akhieser mechanism in Si nanomembranes and thermal conductivity dependence of the Q-factor of high frequency nanoresonators, Chávez-Ángel E., Zárate R. A., Gomis-Bresco J., Alzina F., Sotomayor Torres C. M., Semiconductor Science and Technology (12): vol. 29 (2014). IF: 2.206

Nanoarchitecture effects on persistent room temperature photoconductivity and thermal conductivity in ceramic semiconductors: Mesoporous, yolk-shell, and hollow ZnO spheres, Dilger S., Wessig M., Wagner M. R., Reparaz J. S., Sotomayor Torres C. M., Qijun L., Dekorsy T., Polarz S., *Crystal Growth and Design* (9): vol. 14, 4593-4601 (2014). IF: 4.558

Nanostructured p-type Cr/V2O5 thin films with boosted thermoelectric properties,

Loureiro J., Santos R., Nogueira A., Wyczisk F., Divay L., Reparaz S., Alzina F., Sotomayor Torres C. M., Cuffe J., Montemor M. F., Martins R., Ferreira I., *Journal of Materials Chemistry A* (18): vol. 2, 6456-6462 (2014)

Optical and mechanical mode tuning in an optomechanical crystal with light-induced thermal effects, Navarro-Urrios D., Gomis-Bresco J., Capuj N. E., Alzina F., Griol A., Puerto D., Martínez A., Sotomayor Torres C. M., Journal of Applied Physics: vol. 116, 093506 (2014). IF: 2.185

Optomechanic interaction in a corrugated phoxonic nanobeam cavity, Oudich M., El-Jallal S., Pennec Y., Djafari-Rouhani B., Gomis-Bresco J., Navarro-Urrios D., Sotomayor Torres C. M., Martínez A., Makhoute A., *Physical Review B - Condensed Matter and Materials Physics*: vol. 89, 245122 (2014). IF: 3.664



Order quantification of hexagonal periodic arrays fabricated by in situ solvent-assisted nanoimprint lithography of block copolymers, Simao C., Khunsin W., Kehagias N., Salaun M., Zelsmann M., Morris M. A., Sotomayor Torres C. M., *Nanotechnology* (17): vol. 25 (2014). IF: 3.672 (cover-featured article)

Ordered 2D colloidal photonic crystals on gold substrates by surfactant-assisted fast-rate dip coating, Armstrong E., Khunsin W., Osiak M., Blomker M., Sotomayor Torres C. M., O'Dwyer C., *Small* (10): 10, 1895-1901 (2014). IF: 7.514

Reduction of the thermal conductivity in free-standing silicon nano-membranes investigated by non-invasive Raman thermometry, Chávez-Ángel E., Reparaz J. S., Gomis-Bresco J., Wagner M. R., Cuffe J., Graczykowski B., Shchepetov A., Jiang H., Prunnila M., Ahopelto J., Alzina F., Sotomayor Torres C. M., APL *Materials* (1): vol. 2 (2014)

Synthetic Routes for the Preparation of Ordered Vanadium Oxide Inverted Opal Electrodes for Li-Ion Batteries, Armstrong E., Khunsin W., Sotomayor Torres C. M., Osiaka M., O'Dwyera C. *ECS Transactions* (58): vol. 25, 7-14. (2014) Tensile strain mapping in flat germanium membranes, Rhead S. D., Halpin J. E., Shah V. A., Myronov M., Patchett D. H., Allred P. S., Kachkanov V., Dolbnya I. P., Reparaz J. S., Wilson N. R., Sotomayor Torres C. M., Leadley D. R., *Applied Physics Letters* (17): vol. 104 (2014). IF: 3.515

Transparent aluminium zinc oxide thin films with enhanced thermoelectric properties, Loureiro J., Neves N., Barros R., Mateus T., Santos R., Filonovich S., Reparaz S., Sotomayor Torres C. M., Wyczisk F., Divay L., Martins R., Ferreira I., *Journal of Materials Chemistry A* (18): vol. 2, 6649-6655 (2014)



PROJECTS

SGR, funded by **AGAUR**, 18/07/2009-30/04/2014, Clivia Sotomayor Torres

Thermal properties of SrTiO3: Nanotechnology for thermoelectric generation, funded by **AGAUR**, 02/01/2013-01/01/2015, Clivia Sotomayor Torres

SGR, funded by **AGAUR**, 01/01/2014-31/12/2016, Clivia Sotomayor Torres

Nanostructured ThermoElectric Systems for Green Transport & Energy Efficient Applications (NANOTEG), funded by **EC**, 01/07/2011-28/02/2015, Clivia Sotomayor Torres

Carbon-based smart systems for wireless applications (NANO-RF), funded by **EC**, 01/09/2012-31/08/2015, Clivia Sotomayor Torres

Innovative Nano and Micro Technologies for Advanced Thermo and Mechanical Interfaces (NANOTHERM), funded by **EC**, 01/09/2012-31/08/2015, Clivia Sotomayor Torres (Coordinator)

Injection-moulding production technology for multi-functional nano-structured plastic components enabled by Nano Imprint Lithography (PLAST4FUTURE), funded by EC, 01/01/2013-31/12/2015, Clivia Sotomayor Torres

Membrane-based phonon engineering for energy harvesting (MERGING), funded by **EC**, 01/01/2013-31/12/2015, Clivia Sotomayor Torres (Coordinator)

Building a European NanoPhononics Community (EUPHONON), funded by **EC**, 01/11/2013-31/10/2014, Clivia Sotomayor Torres

QUANTItative scanning probe microscopy techniques for HEAT transfer management in nanomaterials and nanodevices (QUANTIHEAT), funded by **EC**, 01/12/2013-30/11/2017, Clivia Sotomayor Torres

Heat Propagation and Thermal Conductivity in Nanomaterials for Nanoscale Energy Management (HeatProNano), funded by **EC**, 01/03/2014-29/02/2016, Clivia Sotomayor Torres

Tailoring Electronic and Phononic Properties of Nanomaterials: Towards Improved Thermoelectricity (nanoTHERM), nanoTHERM, funded by **MINECO**, 27/12/2010-26/12/2015, Clivia Sotomayor Torres (Coordinator)

Diseño de las Relaciones de Dispersión de Fonónes Acústicos (TAPHOR), funded by **MINECO**, 01/01/2013-31/12/2015, Clivia Sotomayor Torres



CONTRIBUTIONS

Developments in nanoscience and nanotechnology, **U de Chile, Fac. Sciences, CEDENNA, UTEM**. Santiago (Chile), 07-09/01/2014, C. M. Sotomayor Torres (Invited)

Dimensional and defectivity metrology in NIL and NIL-related nanofabrication technologies, NIL Industrial Day. Linz (Austria), 13-15/03/2014, J. Gomis-Bresco, C. Simao, N. Kehagias, and C. M. Sotomayor Torres (Invited)

Thermal transport in suspended Si membranes, Linneus Seminar to the Dept of Physics, Chemistry and Biology. Linkoeping (Sweden) 15/05/2014, 2014, C. M. Sotomayor Torres (Invited)

Photonics in Europe: Trends and roadmap, **Optopub**. Kista (Sweden), 22/05/2014, C. M. Sotomayor Torres (Invited)

Optomechanics, **Cleo**. San Jose (USA), 08-13/06/2014, J. Gomis-Bresco, et al. (Invited)

Optomechanics, **ICTON 2014**. Graz (Austria), 06-10/jul/2014, J. Gomis-Bresco, C. M. Sotomayor Torres (Invited)

Phonon Transport and Scattering in Rough and Porous Silicon Nanowires, **2014 ECS and SMEQ Joint International Meeting**. Cancun (Mexico), 05-10/10/2014, C. M. Sotomayor Torres, C. O'Dwyre (Invited)

Phonons in free-standing Si membranes, International School on Quantum Electronics,

Third Mediterranean International Workshop on Photoacoustic and Photothermal phenomena. Erice (Italy), 05-12/10/2014, C. M. Sotomayor Torres (Invited)

A coherent phonon source driven by optical sources, **ADOPT Day 2014**. Stockholm (Sweden), 23/10/2014, C. M. Sotomayor Torres (Invited)

Silicon free-standing membranes: Fabrication, thermal transport and phonon confinement, **Department of Applied Electronics, Tokyo University of Science**. Tokyo (Japan), 30/10/2014, C. M. Sotomayor Torres (Invited)

Nanoimprint lithography as a directed selfassembly tool: approaches and nanometrology, 27th International Microprocesses and Nanotechnology Conference MNC. Fukuoka (Japan), 04-07/11/2014, C. Simao, C. M. Sotomayor Torres (Invited)

A novel contactless technique for thermal field mapping and thermal conductivity determination: Two-Laser Raman Thermometry, Nanospain. Madrid (Spain), 11-14/03/2014, J. S. Reparaz, E. Chávez-Ángel, M. R. Wagner, B. Graczykowski, J. Gomis-Bresco, F. Alzina, and C. M. Sotomayor Torres (Oral)

Dimensional and Defectivity Nanometrology of sub-20 nm line arrays prepared by directed self-assembly, Nanospain. Madrid (Spain), 11-14/03/2014, C. Simão, D. Tuchapsky, W. Khunsin, A. Amann, M. A. Morris and C. M. Sotomayor Torres (Oral)

A 1D phoXonic crystal, Nanospain. Madrid (Spain), 11-14/03/2014, J. Gomis-Bresco, D. Navarro-Urrios, M. Oudich, S. El-Jallal, A. Griol, D. Puerto, E. Chávez, Y. Pennec, B. Djafari-Rouhani, F. Alzina, A. Martínez, C. M. Sotomayor Torres (Oral)

One-dimensional surface phononic crystals, Nanospain. Madrid (Spain), 11-14/03/2014, B. Graczykowski, M. Sledzinska, N. Kehagias, F. Alzina, S. Reparaz, and C. M. Sotomayor Torres (Oral)

Metal incorporation in block copolymer templates, **Nanospain**. Madrid (Spain), 11-14/03/2014, M. Kreuzer, C. Delgado Simao, A. Diaz, and C. Sotomayor Torres (Oral)

Order and defectivity nanometrology by image processing and analysis of sub-20 nm BCPs features for lithographic applications, SPIE DSS. Baltimore (USA), 05-09/04/2014, C. Simao, D. Tuchapsky, W. Khunsin, A. Amann, M. A. Morris and C. M. Sotomayor Torres (Oral)

Dimensional and Defectivity Nanometrology of sub-20 nm line arrays prepared by directed self-assembly, **Industrial Technologies 2014**. Athens (Greece), 09-11/04/2014, C. Simao, D. Tuchapsky, W. Khunsin, A. Amann, M. A. Morris and C. M. Sotomayor Torres (Oral)

Theoretical thermal rectification in Si and Ge thin films, **E-MRS**. Lille (France), 27-29/05/2014, E. Chávez et al. (Oral)

Modelling of the phonon attenuation in Si-based nanostructures, **E-MRS**. Lille (France), 27-29/05/2014, E. Chávez et al. (Oral)

Optomechanics, **E-MRS**. Lille (France), 27-29/05/2014, J. Gomis-Bresco, et al. (Oral)

Imprint-based techniques for the fabrication of embedded silver grid electrodes for organic solar cells applications, **ISFOE 2014**. Thessaloniki (Greece), 07-10/07/2014, N. Kehagias (Oral)

Large Area Phononic Crystals Based on Free-Standing Silicon Membranes, 11th International Conference on Nanosciences & Nanotechnologies (NN14). Thessaloniki (Greece), 08-11/07/2014, M. Sledzinska, B. Graczykowski, F. Alzina, and C. M. Sotomayor Torres (Oral)

Theoretical thermal rectification in Si and Ge thin films, **MSE 2014**. Darmstadt (Germany), 23-25/09/2014, E. Chávez et al. (Oral)

Modification of the Akhieser mechanism in Si nanoresonators, **Eurotherm 103, Nano scale and Microscale Heat Transfer IV**. Lyon (France), 15-17/10/2014, C. M. Sotomayor Torres (Oral)

Dimensional and defectivity nanometrology of directed self-assembly patterns, SPIE Advanced Lithography. San Jose (USA), 23-27/02/2014, C. Simao, W. Khunsin, A. Amann, N. Kehagias, M. A. Morris, and C. M. Sotomayor Torres (Poster)

Theoretical thermal rectification in Si and Ge thin films, Nanospain. Madrid (Spain), 11-14/03/2014, E. Chávez-Ángel, F. Alzina, and C. M. Sotomayor Torres (Poster)

Subwavelength diffraction for quality control in nano fabrication processing, Nanospain. Madrid (Spain), 11-14/03/2014, J. Gomis-Bresco, C. Simao, M. Kreuzer, and C. M. Sotomayor Torres (Poster)

Etch-free method to prepare nanoporous metal layers using directed self-assembly, Nanospain. Madrid (Spain), 11-14/03/2014, M. Bernal Salamanca, C. Simao, M. Sledzinka and C. M. Sotomayor Torres (Poster)

Anti-wetting surfaces fabricated by Reverse Nanoimprint Lithography on Silicon and metalcoated substrates, **Nanospain**. Madrid (Spain), 11-14/03/2014, A. Fernández, J. Medina, C. Benkel, M. Gutteman, B. Bilenberg, T. Nielsen, C. M. Sotomayor Torres, and N. Kehagias (Poster)

Acoustic phonon dynamics in free-standing group IV semiconductor membranes studied by ultra-fast pump & probe spectroscopy,

Nanospain. Madrid (Spain), 11-14/03/2014,
M. R. Wagner, J. S. Reparaz, J. Gomis-Bresco, E. Chávez-Ángel, B. Graczykowski, F. Alzina, and C. M. Sotomayor Torres (Poster)

Nanoimprint-assisted directed self-assembly of low-molecular weight block copolymers for advanced lithographic applications, **SPIE DSS**. Baltimore (USA), 05-09/04/2014, C. Simao, Nikos Kehagias, M. Morris, C. M. Sotomayor Torres (Poster)

Towards 3D nano-injection moulding: Residual layer-free Reverse Nanoimprint Lithography on Silicon and metal-coated substrates, Polymer Replication on Nanoscale PRN 2014.
Copenhagen (Denmark), 12-13/05/2014, J. Medina, A. Fernández, C. Benkel, M. Gutteman, B. Bilenberg, T. Nielsen, C. M. Sotomayor Torres, and N. Kehagias (Poster)



BOOKS

Beyond CMOS Nanodevices 1 - Chap. 7 Thermal Energy Harvesting, M. Mouis, E. Chávez-Ángel, C. M. Sotomayor Torres, F. Alzina, M. V. Costache, A. G. Nassiopoulou, K. Valaki, E. Hourdakis, S. O. Valenzuela, B. Viala, D. Zakharov, A. Shchepetov, and J. Ahopelto, Wiley, 2014. ISBN: 978-1-84821-654-9

Beyond CMOS Nanodevices 1 - Chap. 12 Thermal Isolation through Nanostructuring, D. Leadley, V. Shah, J. Ahopelto, F. Alzina, E. Chávez-Ángle, J. Muhonen, M. Myronov, A. G. Nassiopoulou, H. Nguyen, E. Parker, J. Pekola, M. Prest, M. Prunnila, J. S. Reparaz, A. Shchepetov, C. M. Sotomayor Torres, K. Valalaki, and T. Whall, Wiley, 2014. ISBN: 978-1-84821-654-9

Defect analysis and alignment quantification of line arrays prepared by directed self-assembly of a block copolymer, Simao C., Tuchapsky D., Khunsin W., Amann A., Morris M.A., Sotomayor Torres C. M., Proceedings of SPIE, 9050, Metrology, inspection, and process control for microlithography XXVIII. Doi: 10.1117/12.2046075

Order and defectivity nanometrology by image processing and analysis of sub-20 nm BCPs features for lithographic applications, Simao C., Tuchapsky D., Khunsin W., Amann A., Morris M.A., Sotomayor Torres C. M., Proceedings of SPIE, 9110, Dimensional opetical metrology and inspection for practical applications III. Doi: 10.1117/12.2050182



THESES

Doctorand: **Emigdio Chávez Ángel**Title: Confined acoustic phonons in Si
nanomembranes: impact on thermal

properties

Defense date: 03/10/2014

Director: Prof Dr Clivia M. Sotomayor Torres



OTHER HIGHLIGHTS

European Patents filed

European patent (EP) application ICN PAT 02/13 Inspecting nanostructures With Ref. EP14156430 and priority date 24/02/2014 P2N Group.

PCT Extensions filed

ICN PAT 08/12 Methods and devices for analysing nanostructure array images With Ref. PCT/EP2014/075560 on 25/11/2014 P2N Group

More information:

http://www.icn.cat/~p2n/

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



GROUP MEMBERS

Frédéric Bonell, Marie Curie Postdoctoral Researcher Marius Vasile Costache, Ramón y Cajal Postdoctoral Researcher Jo Cuppens, Postdoctoral Researcher Ingmar Neumann, Postdoctoral Researcher Bart Raes, Postdoctoral Researcher luan Francisco Sierra, Juan de la Cierva Postdoctoral Researcher Sergio Valenzuela, ICREA Research Professor and Group Leader



GROUP LEADER



ICREA Prof Sergio Valenzuela

Prof Valenzuela obtained his PhD in Physics in 2001 at the University of Buenos Aires, Argentina, and went on to be a Postdoctoral Fellow and Research Associate at Harvard University, and a Research Scientist at the Massachusetts Institute of Technology (MIT). Since July 2008, Prof Valenzuela has been an ICREA Research Professor as well as Group Leader of ICN's, now ICN2's, Physics and Engineering of Nanoelectronic Devices Group. Since September 2008 he has also served as Associate Professor at the Physics department of the Universitat Autònoma de Barcelona (UAB).



NEW PROJECTS & MILESTONES

In 2014 the Physics and Engineering of Nanodevices Group continued with its progress on the ERC Starting Grant project to investigate the spin properties of materials with large spin-orbit interaction, in particular topological insulators. The project (SPINBOUND) was launched in February 2013 and, in January 2014, the first results were published in the journal *Physical Review Letters*. The work reported the role of electron-phonon coupling in the electronic properties of surface states of topological insulators, putting forward constraints that will be key for future devices based on these materials. In addition, the group started a

new project (Spintronics in 2-Dimensional Dirac Systems, S2DDS), and has been active in the investigation of spin transport properties in graphene (e.g. Nature Physics article) in collaboration with S. Roche's group. It also participated in Training Networks; hosting researcher Frédéric Bonell with a Marie Curie project (STIFNANO), which was awarded in 2013 to work on the electronic properties of ferromagnet / topological insulators heterostructures. From the point of view of infrastructure, a crucial milestone was achieved for the future activities of the group with the installation of a dual-chamber Molecular Beam Epitaxial (MBE) system, which will allow the growth of ultrahigh purity epitaxial thin films.



Prof Valenzuela's research is focused on the unique properties of materials in samples with nanoscale dimensions. Such studies are motivated both by their intrinsic scientific interest and by their potential importance for electronic applications, and they rely on innovative devices or innovative implementations of known devices. Recent research has encompassed spintronics, quantum computation with superconducting circuits, and nanoelectromechanical systems (NEMS).

Prof Valenzuela received the 2009 IUPAP Young Scientist Prize in Magnetism for his contributions to the field of spintronics, and was awarded an ERC Starting Grant in 2012. He has authored over 40 papers, three patents and four books or book chapters.



PUBLICATIONS

Determination of the magnetic penetration depth in a superconducting Pb film, Brisbois J., Raes B., Van De Vondel J., Moshchalkov V.V., Silhanek A.V., *Journal of Applied Physics*: vol. 10, 115 (2014). IF: 2.185

Fingerprints of inelastic transport at the surface of the topological insulator Bi 2 Se 3: Role of electron-phonon coupling, Costache M.V., Neumann I., Sierra J.F., Marinova V., Gospodinov M.M., Roche S., Valenzuela S.O., *Physical Review Letters*: vol. 8, 112 (2014). IF: 7.728

Graphene spintronics: Puzzling controversies and challenges for spin manipulation, Roche S., Valenzuela S.O., *Journal of Physics D: Applied Physics*: vol. 9, 47 (2014). IF: 2.521

Observing vortex motion on NbSe2 with STM, Timmermans M., Samuely T., Raes B., Van De Vondel J., Moshchalkov V.V., *Physica C: Superconductivity and its Applications*: vol. 503, 154-157 (2014). IF: 1.11

Pseudospin-driven spin relaxation mechanism in graphene, Van Tuan D., Ortmann F., Soriano D., Valenzuela S. O., Roche S., *Nature Physics* (2014). IF: 20.603



PROIECTS

Spin pumping and magnetisation dynamics in metallic nanostructures, funded by **AGAUR**, 01/01/2013-31/12/2014, Sergio Valenzuela

SGR, funded by **AGAUR**, 01/01/2014-31/12/2016, Sergio Valenzuela

Exploring the spin physics at the boundaries of materials with strong spin orbit interaction, SpinBound, funded by **EC**, 01/02/2013-31/01/2018, Sergio Valenzuela

Spintronics with Topological Insulator/ Ferromagnet Nanodevices, STIFnano, funded by EC, 01/04/2014-31/03/2016, Sergio Valenzuela

Spin transport and magnetisation dynamics in nanostructures, funded by **MINECO**, 01/01/2012-31/12/2016, Sergio Valenzuela

Espintrónica en Sistemas de Dirac en 2 Dimensiones, S2DDS, funded by **MINECO**, 01/01/2014-31/12/2016, Sergio Valenzuela



BOOKS

Thermal Energy Harvesting (Chap. 7). M. Mouis, E. Chávez-Ángel, C. Sotomayor Torres, F. Alzina, M. V. Costache, A. G. Nassiopoulou, K. Valaki, E. Hourdakis, S. O. Valenzuela, B. Viala, D. Zakharov, A. Shchepetov, and J. Ahopelto, Wiley, 2014



THESES

Doctorand: Ingmar Neumann

Title: Spin Transport and Thermoelectric

Effects in Graphene.

Defense Date: 21/05/2014

Director: Prof Sergio O. Valenzuela

More information:

http://www.icn.cat/~pend/PEN.html

Supramolecular NanoChemistry and Materials Group

Main Research Lines -

- Nanoporous Metal-Organic Frameworks and related nanoparticles
- Frontier nanochemistry-based methodologies towards new multifunctional nanocarriers
- New products based on Micro- and Nanoencapsulation Technologies



GROUP MEMBERS

Celia Aranda, Visiting Student lavier Ariñez, FPU Doctoral Student Civan Avci, Doctoral Student Abraham Ayala, Visiting Doctoral Student Ivan Patricio Burneo, Visiting Doctoral Student Antonia Maria Cano, Postdoctoral Researcher Carlos Carbonell, Laboratory Engineer Arnau Carné, Doctoral Student Jorge Cruz, Visiting Postdoctoral Researcher Jordi Espín, FPI Doctoral Student María Emilia Evangelio, Beatriu de Pinós Postdoctoral Researcher Sonia García, Postdoctoral Researcher Luís Carlos Garzón, Doctoral Student Marta González, Group Project Manager Inhar Imaz, Ramón y Cajal Postdoctoral Researcher Jaya Ramulu Kolleboyina, Postdoctoral Researcher

David Martínez, Visiting Student Rubén Mas, Visiting Postdoctoral Researcher Daniel Maspoch, ICREA Research Professor and Group Leader Nereida Mejías, Technician Elsa Rivoire, Technician Sabina Rodríguez, Postdoctoral Researcher David Rodríguez, Visiting Doctoral Student Àngels Ruyra, Doctoral Student Vahid Safarifard, Visiting Doctoral Student Kyriakos Stylianou, Marie Curie Postdoctoral Researcher Min Ying Tsang, Visiting Doctoral Student Claudia Vignatti, Doctoral Student Christian Vila, Visiting Student Zhuopeng Wang, Visiting Postdoctoral Researcher Heng Xu, Doctoral Student



GROUP LEADER



ICREA Prof Daniel Maspoch

Born in l'Escala (Girona) in 1976. He graduated in chemistry at the Universitat de Girona and obtained his PhD in materials science at the Universitat Autònoma de Barcelona & Institut de Ciència de Materials de Barcelona. He then moved to Northwestern University, where he worked as a postdoctoral fellow in the group of professor Chad A. Mirkin. He moved back to the Institut Català de Nanotecnologia (ICN), now ICN2, thanks



NEW PROJECTS & MILESTONES

In 2014, NANO^{UP} Group completed two of its on-going projects ("NanoBioMOFs, Nanoscale Metal-Organic Frameworks for Biomedical Applications", a Marie-Curie project supported by the European Commission under the 7th FP, and "MOFINP Starting Grant: Multifunctional Hybrid Nanoparticle Pairs made from Metal-Organic Frameworks and Inorganic Nanoparticles", a Complementary Action

supported by MINECO). The group also began the project "InanoMOF: Multifunctional micro- and nanostructures assembled from nanoscale metal-organic frameworks and inorganic nanoparticles", for which a prestigious ERC Consolidator Grant was awarded to Prof Daniel Maspoch.

The Group has also continued its development of customised micro- and nanoencapsulation technologies for companies, working in parallel with 7 different companies.



to a Ramón y Cajal contract, and he founded the Supramolecular NanoChemistry & Materials Group. Since September 2011, he has been ICREA Research Professor and Group Leader at the ICN2, and in 2014 he was awarded European Research Council (ERC) Consolidator Grant.

Prof Maspoch has authored 70 scientific publications, 5 book chapters and 7 patents, and has established 14 contracts with private companies, including 3 successful transfers of in-house technology for immediate application to consumer products.



PUBLICATIONS

Localized, stepwise template growth of functional nanowires from an amino acid-supported framework in a microfluidic chip, Puigmartí-Luis J., Rubio-Martínez M., Imaz I., Cvetkovic B.Z., Abad L., Pérez Del Pino A., Maspoch D., Amabilino D.B., ACS Nano (1): vol. 8, 818-826 (2014). IF: 12.033

Metal-organic frameworks: From molecules/metal ions to crystals to superstructures, Carné-Sánchez A., Imaz I., Stylianou K.C., Maspoch D., *Chemistry - A European Journal* (18): vol. 20, 5192-5201 (2014). IF: 5.696

Selective CO₂ capture in metal-organic frameworks with azine-functionalized pores generated by mechanosynthesis, Masoomi M.Y., Stylianou K.C., Morsali A., Retailleau P., Maspoch D., *Crystal Growth and Design* (5): vol. 14, 2092-2096 (2014). IF: 4.558

Sponge-like molecular cage for purification of fullerenes, García-Simón C., Garcia-Borràs M., Gómez L., Parella T., Osuna S., Juanhuix J., Imaz I., Maspoch D., Costas M., and Ribas X., *Nature Communications*: vol. 5 (2014). IF: 10.742

Targeting and stimulation of the zebrafish (*Danio rerio*) innate immune system with LPS/dsRNA-loaded nanoliposomes, Ruyra A., Cano-Sarabia M., García-Valtanen P., Yero D., Gibert I., Mackenzie S.A., Estepa A., Maspoch D., Roher N., *Vaccine* (31): vol. 32, 3955-3962 (2014). IF: 3.485

The influence of the enantiomeric ratio of an organic ligand on the structure and chirality of Metal-Organic Frameworks, Burneo I., Stylianou K. C, Imaz I., Maspoch D., *Chemical Communications* (89): vol. 50, 13829-13832 (2014). IF: 6.718



PROJECTS

SGR, **AGAUR**, 01/01/2014-31/12/2016, Daniel Maspoch

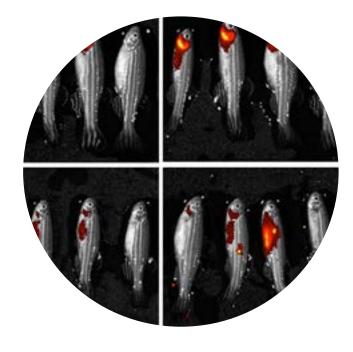
Multifunctional micro- and nano-structures assembled from nanoscale metal-organic frameworks and inorganic nanoparticles (InanoMOF), funded by **EC**, 01/04/2014-31/03/2019, Daniel Maspoch

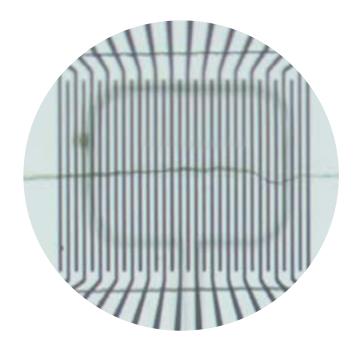
Micro- and nano-encapsulated biocides: the next generation of disinfectants with short + long2Life antimicrobial activity, BIOCIDE2LIFE?, funded by CERCA, 2012-2014, Daniel Maspoch

Desarrollo de una nueva generación de productos biocidas con efecto inmediato, remanente y capacidad para reducir la transferencia de microorganismos (DESPRO-CIDE), funded by **MINECO**, 15/07/2012-31/12/2015, Daniel Maspoch

Starting Grant: Multifunctional Hybrid Nanoparticle Pairs made from Metal-Organic Frameworks and Inorganic Nanoparticles (Bio2nanoMOF), funded by **MINECO**, 01/01/2013-30/06/2014, Daniel Maspoch

Diseño y Síntesis de Metal-Organic Frameworks Nanoscópicos para Aplicaciones Biomédicas Avanzadas (MOFs@bio), funded by **MINECO**, 01/01/2013-31/12/2015, Daniel Maspoch







CONTRIBUTIONS

A new type of nanomaterials, Nanoscale Metal-Organic Frameworks, organized by Universitat de Barcelona. Barcelona (Spain), 22/04/2014, Daniel Maspoch, (Invited)

Biocide2Life, Catalan Technology: an overview on Prova't Projects, **First CERCA Conference**. Barcelona (Spain), 28/04/2014, Daniel Maspoch (Invited)

Nanoscale Metal-Organic Frameworks, Instituto de Nanociencia de Aragón (INA). Zaragoza (Spain), 14/05/2014, Daniel Maspoch (Invited)

Nanotechnology & Supramolecular Chemistry: hand in hand, Symposium of Supramolecular Chemistry in Science. Girona (Spain), 16/09/2014, Daniel Maspoch (Invited)

Nanoscale Metal-Organic Frameworks (nanoMOFs), Institut Ciència de Materials de Barcelona (ICMAB-CSIC). Barcelona (Spain), 22/09/2014, Daniel Maspoch (Invited)

Nanoscale MOFs: Synthesis, Toxicity and New Properties, 4th International Conference on Metal-Organic Frameworks & Open-Framework Compounds. Kobe (Japan), 29/09/2014-01/10/2014, Daniel Maspoch (Invited)

Encapsulation of Insulin Peptides in Liposomes for Preventing Type 1 Diabetes in NOD Mice, Controlled Release Society Annual Meeting and Exposition. Chicago (USA), 13-16/07/2014, Mary Cano (Poster)

Massive Production of nanoMOFs by Spray-Drying, 1st International Symposium on Nanoparticles/Nanomaterials and Applications (isn2a2014), organized by Universidade NOVA de Lisboa. Caparica (Portugal), 20-22/01/2014, I. Imaz, A. Carné, M. Cano, D. Maspoch (Talk)

Femtolitre Chemistry assisted by Microfluidic Pen Lithography (MPL), 1st International Symposium on Nanoparticles/ Nanomaterials and Applications (isn2a2014), organized by Universidade NOVA de Lisboa. Caparica (Portugal), 20-22/01/2014, K. Stylianou, D. Maspoch (Talk)

Lipidic-Coated Bacteriophages for Controlling Salmonella Colonisation, EMBO conference: Viruses of microbes structure and function, from molecules to communities. Zurich (Switzerland), 14-18/07/2014, Joan Colom (Talk)

Nanoscale MOFs for Contrast Agent Applications, Young MOF Symposium 2014. Kyoto (Japan), 26/09/2014, Inhar Imaz (Talk)

Liposome-based Immunotherapy for Type 1 Diabetes, Reunión annual del grupo de islotes de la sociedad Española de Diabetes (SED). Madrid (Spain), 16/10/2014, Imma Pujol (Talk)



BOOKS

Nanoscale metal-organic frameworks, in Metal-Organic Frameworks Materials. Encyclopedia of Inorganic and Biorganic Chemistry 2014, K. Stylianou, I. Imaz, D. Maspoch, Wiley, 2014



COURSES

UT Austin/UAB Nanotechnology Innovation Course, in Curso de grado, **Universitat Autònoma de Barcelona, Barcelona (Spain)**, 14/06/2014, Mary Cano

Chemistry for Specific materials/metal-organic frameworks, in Màster Universitari en Quimica Industrial i Introduccio a la Recerca Quimica., **Universitat Autònoma de Barcelona, Barcelona (Spain)**, 28/10/2013, Inhar Imaz

Nanotecnología y Sociedad, in Grado de Nanotecnología, **Universitat Autònoma de Barcelona, Barcelona (Spain)**, 18/11/2014, Mary Cano



THESES

Doctorand: Marta Rubio

Title: Coordination Polymer Nanofibers made of Amino Acids and Peptides and their Use as Templates to Synthesize Inorganic Nanoparticle

Superstructures

Defense date: 28/05/2014

Directors: Dr Inhar Imaz and Prof Daniel

Maspoch

Doctorand: Arnau Carne

Title: A New Synthetic Method for Nanoscale Metal-organic Frameworks and their

Application as Contrast Agents for Magnetic

Resonance Imaging

Defense date: 10/10/2014

Directors: Prof Daniel Maspoch and Dr Inhar

Imaz

Doctorand: Carles Carbonell

Title: Surface Structuration of Metal-Organic Frameworks Using Tip-Based Lithographies

Defense date: 09/12/2014

Directors: Prof Daniel Maspoch and Dr Inhar

Imaz



OTHER HIGHLIGHTS

European Patents filed

European Patent (EP) application, ICN PAT 09/13, Novel compositions comprising lipidic-coated bacteriophages, With Ref. EP14382057.9 and priority date 20/02/2014

European Patent (EP) application, ICN PAT 03/13, Biocidal composition with dual inmediate and remnant activity, With Ref. EP14382498 and priority date 05/12/2014

European Patent (EP) application, ICN PAT 10/13, Liposome-based immunotherapy, With Ref. EP14151629.4 and priority date 17/01/2014

Patents entered into national phases

ICN PAT 01/11, Method for the preparation of metal organic frameworks entered regional phases in USA on 04/04/2014 and in Europe on 29/04/2014

More information:

http://www.nanoup.org/

Theoretical and Computational Nanoscience Group

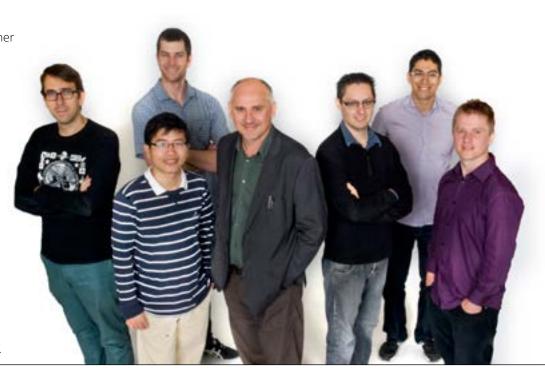
Main Research Lines -

- Leading-edge theoretical research on quantum transport phenomena in Graphene
- Spin dynamics in Dirac Matter (graphene, topological insulators)
- Thermal properties and Thermoelectricity in twodimensional Materials
- Predictive Modelling and Multiscale numerical simulation of complex nanomaterials and quantum nanodevices



GROUP MEMBERS

José Eduardo Barrios,
Visiting Postdoctoral Researcher
Aron Cummings,
Postdoctoral Researcher
Van Tuan Dinh,
Postdoctoral Researcher
Nicolas Leconte,
Postdoctoral Researcher
Stephan Roche,
ICREA Research Professor
and Group Leader
David Soriano,
Postdoctoral Researcher





GROUP LEADER



ICREA Prof Stephan Roche

Prof Stephan Roche is a theoretician with more than twenty years of experience in the study of transport theory of low-dimensional systems, including graphene, carbon nanotubes, semiconducting nanowires, organic materials and topological insulators. He has published more than 100 papers in journals such as *Review of Modern Physics*, *Nature Physics*, *Nano Lett.* and *Phys. Rev. Lett.* (40 papers) and he is the co-author



NEW PROJECTS & MILESTONES

1) A successful computational implementation of the Hall Kubo conductivity to study high-magnetic field transport regimes in disordered graphene.

Graphene displays an anomalous Quantum Hall Effect (QHE) due to the peculiar nature of low-energy electronic excitations, but the nature and role of disorder is extremely difficult to include in the theory and simulation. Roche's group has successfully developed an unrivalled method to study OHE in disordered graphene. A first demonstration of its scientific validity was given in PRL 110,086602 (2013) in a case study, while a successful application to the European PRACE high-performance infrastructure has provided massive computing resources and has allowed the stimulation or models of realistic disordered graphene containing several hundred millions of carbon atoms, giving the group an international leadership in this research area. Remarkable results showing unprecedented features in the OHE and driven by the presence of defect-induced resonances have been recently obtained, and should lead to a revised analysis of prior literature and current state of the art.

2) A comprehensive understanding of fundamental limits of polycrystalline graphene-based materials and devices.

While single-crystal graphene is the best choice for highest device performances (such as graphene field effect transistors), the most promising approach for mass-producing wafer-scale graphene is chemical vapour

deposition (CVD), which results in a material that is polycrystalline. Roche's group has performed the first charge transport study in realistic models of polycrystalline graphene. An important scaling law which dictates the variation of the elastic mean free path (and related mobility) to the average grain sizes of the polycrystalline sample and the quality of grain boundaries was found and the quantitative description of grain boundary resistivity in polycrystalline samples was reported in Advanced Materials in 2014. Such results provide strategic guidance to engineers for predicting device performances based on morphology characterisation, thus providing a clear milestone for the understanding of transport properties in CVDgrown graphene-based devices, the material of choice for large-scale integration and applications in nanoelectronics, transparent electrodes or sensors

3) The discovery of a new mechanism of spin relaxation unique to graphene.

Roche's group has discovered a completely new mechanism for spin relaxation in weakly-disordered graphene, in sharp contrast with the conventional use of semiclassical approaches such as Elliott-Yafet and Dyakonov-Perel. The mechanism discovered is driven by quantum dephasing effects and spin-pseudospin entanglement and should lead to a thorough revision of the field, potentially gathering massive scientific and technological impact by creating novel ways of controlling electron spin dynamics. The paper was published in *Nature Physics* in 2014.

of the recently published book on "Introduction to Graphene-Based Nanomaterials: From Electronic Structure to Quantum Transport" (Cambridge University Press 2014). He received the Authorisation to conduct PhD projects in 2004 at the University Joseph-Fourier (Grenoble, France), and since then he has supervised 5 PhD students and more than a dozen postdoctoral researchers in France, Germany and Spain. S. Roche has been awarded the prestigious Friedrich Wilhelm Bessel prize by the Alexander Von-Humboldt Foundation (Germany), and finally, since 2011, he has been actively involved in the Graphene Flagship project, currently as a co-leader of the Graphene spintronics workpackage.

PUBLICATIONS

Anisotropic behavior of quantum transport in graphene superlattices: Coexistence of ballistic conduction with Anderson insulating regime, Pedersen J.G., Cummings A.W., Roche S., Theoretical and Computational Nanoscience, Physical Review B - Condensed Matter and Materials Physics (16): vol. 89 (2014). IF: 3.664

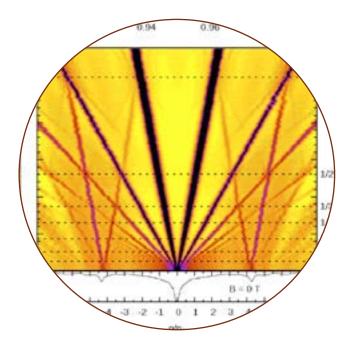
Anomalous dissipation mechanism and Hall quantisation limit in polycrystalline graphene grown by chemical vapor deposition, Lafont F., Ribeiro-Palau R., Han Z., Cresti A., Delvallee A., Cummings A.W., Roche S., Bouchiat V., Ducourtieux S., Schopfer F., Poirier W., Theoretical and Computational Nanoscience, Physical Review B - Condensed Matter and Materials Physics (11): vol. 90 (2014). IF: 3.664

Anomalous exchange interaction between intrinsic spins in conducting graphene systems, Santos H., Soriano D., Palacios J.J., Theoretical and Computational Nanoscience, Physical Review B - Condensed Matter and Materials Physics (19): vol. 89 (2014). IF: 3.664

Charge transport in polycrystalline graphene: Challenges and opportunities, Cummings A.W., Duong D.L., Nguyen V.L., Van Tuan D., Kotakoski J., Barrios Vargas J.E., Lee Y.H., Roche S., *Theoretical and Computational Nanoscience, Advanced Materials* (30): vol. 26, 5079-5094 (2014). IF: 15.409

Fingerprints of inelastic transport at the surface of the topological insulator Bi 2 Se 3: Role of electron-phonon coupling, Costache M.V. Neumann L. Sierra J.E. Marin

Costache M.V., Neumann I., Sierra J.F., Marinova V., Gospodinov M.M., Roche S., Valenzuela S.O., *Theoretical and Computational Nanoscience, Physical Review Letters* (8): vol. 112 (2014). IF: 7.728



Graphene spintronics: Puzzling controversies and challenges for spin manipulation, Roche S., Valenzuela S.O., Theoretical and Computational Nanoscience, Journal of Physics D: Applied Physics (9): vol. 47 (2014). IF: 2.521

Impact of graphene polycrystallinity on the performance of graphene field-effect transistors, David Jiménez, Aron W. Cummings, Ferney Chaves, Dinh Van Tuan, Jani Kotakoski, Stephan Roche, *Theoretical and Computational Nanoscience, Applied Physics Letters* (4): vol. 104 (2014). IF: 3.515

Multiple quantum phases in graphene with enhanced spin-orbit coupling: from the quantum spin Hall regime to the spin Hall effect and a robust metallic state, Cresti A., Van Tuan D., Soriano D., Cummings A.W., Roche S., *Phys Rev Lett.* 2014; 113(24): 246603. IF: 7.728

Physical model of the contact resistivity of metal-graphene junctions, Chaves F.A., Jimenez D., Cummings A.W., Roche S., Theoretical and Computational Nanoscience, Journal of Applied Physics (16): vol. 115 (2014). IF: 2.185

Pseudospin-driven spin relaxation mechanism in graphene, Van Tuan D., Ortmann F., Soriano D., Valenzuela S. O., Roche S., Theoretical and Computational Nanoscience, Nature Physics (2014). IF: 20,603

Quantum Hall Effect in Polycrystalline Graphene: The Role of Grain Boundaries,

Aron W. Cummings; Alessandro Cresti; Stephan Roche, *Theoretical and Computational Nanoscience, Physical Review B - Condensed Matter and Materials Physics*: vol. 90 (2014). IF: 3.664

Quantum transport in chemically functionalized graphene at high magnetic field: defect-induced critical states and breakdown of electron-hole symmetry,

Nicolas Leconte; Frank Ortmann; Alessandro Cresti; Jean-Christophe Charlier; Stephan Roche, Theoretical and Computational Nanoscience, 2D Materials (2): vol. 1 (2014)

Transport fingerprints at graphene superlattice Dirac points induced by a boron nitride substrate, Martínez-Gordillo R., Roche S., Ortmann F., Pruneda M., Theoretical and Computational Nanoscience, Physical Review B - Condensed Matter and Materials Physics (16): vol. 89 (2014). IF: 3.664

Tunneling magnetoresistance phenomenon utilizing graphene magnet electrode,

Hashimoto T., Kamikawa S., Soriano D., Pedersen J. G., Roche S., Haruyama J., *Appl. Phys. Lett.* 105, 183111 (2014). IF: 3.515



PROIECTS

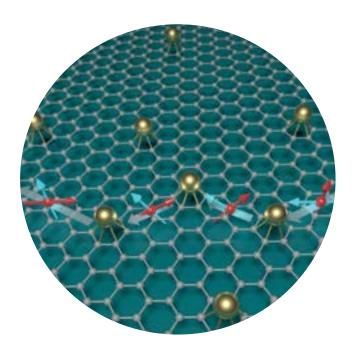
SGR, funded by **AGAUR**, 01/01/2014 - 31/12/2016, Stephan Roche

Graphene-Based Revolutions in ICT And Beyond, GRAPHENE, funded by **EC**, 01/10/2013 - 31/03/2016, Stephan Roche

ICREA Workshop on Graphene Nanobiosensors, funded by **ICREA**, 01/08/2014 - 31/12/2015, Stephan Roche, Arben Merkoçi

Simulación Multi-escala de transporte cuántico en grafeno y aislantes topológicos, MQT-GRAPHTI, funded by **MINECO**, 01/01/2013 -31/12/2015, Stephan Roche

Multiscale simulation of charge transport properties in polycrystalline graphene, funded by **SAMSUNG** (Company), 01/03/2014 - 28/02/2015, Stephan Roche





Surprises in GRAPHENE spintronics,

International Winterschool on Electronic Properties of Novel Materials, organized by Institut für Festkörperphysik. Kirchberg (Austria), 12/03/2014, Stephan Roche (Invited)

Multiscale simulation of two-dimensional materials-based devices, Singapore-Spain workshop on Two-dimensional Materials, organized by National University of Singapore. Singapore (Singapore), 18/06/2014, Stephan Roche (Invited)

Introduction to quantum transport properties and spin dynamics in graphene, Graphene and Related Materials (GRM-2014) Summer School, organized by Izmir Institute of Technology. Urla-Izmir (Turkey), 09/07/2014, Stephan Roche (Invited)

Understanding Charge Transport in Graphenebased Materials: From Concepts to Applications, **GRAPHCHINA 2014**, organized by Graphene CGIA. Ningbo (China), 01/09/2014, Stephan Roche (Invited)

Order N Computational Methods for Exploring Charge, Phonon and Spin Transport in Condensed Matter: Benchmarking Materials and Assessing Novel Applications, 6th International Conference of the Institute for Biocomputation and Physics of Complex Systems (BIFI), organized by Universidad de Zaragoza. Zaragoza (Spain), 22/01/2014,

Predictive Modelling for Fostering Graphene and Two dimensional Materials Applications, **Trends in Nanotechnology JAPAN - NANOTECH 2014**, organized by NIMS, MANA. Tokyo (Japan), 29/01/2014, Stephan Roche (Keynote)

Stephan Roche (Keynote)

Quantum Transport in Graphene-based nanostructures, **Graphene School 2014**, organized by CNRS. Cargèse (Corsica) (France), 15/04/2014, Stephan Roche (Keynote) Spintronics in Graphene, **Graphene week 2014**, organized by Graphene Flagship. Gothenburg (Sweden), 24/06/2014, Stephan Roche (Oral)

Ad-atoms induced Spin-orbit coupling effect on Graphene: From Quantum Spin Hall effect to Spin Relaxation, CMD25-JMC14, organized by Université Paris-Descartes, CNRS. Paris (France), 26/08/2014, Stephan Roche (Oral)



воокѕ

Introduction to Graphene-Based Nanomaterials: From Electronic Structure to Quantum Transport, Luis E.F. Foa Torres, Stephan Roche and Jean-Christophe Charlier, Cambridge University Press, 2014



THESES

Doctorand: Dinh Van Tuan

Title: Charge and Spin Transport in Disordered

Graphene-Based Materials Defense date: 30/09/2014 Director: Prof Stephan Roche

More information:

http://www.icrea.cat/Web/ScientificStaff/Stephan-Roche-523

Theory and Simulation Group

Main Research Lines -

- Development of theoretical methods, numerical algorithms and simulation tools
- Codes: SIESTA & TRANSIESTA
- First Principles simulations at the nanoscale
- Novel physical properties in 2D materials



GROUP MEMBERS

Paula Abufager, Visiting Postdoctoral Researcher José Miguel A. Pruneda, CSIC Tenured Scientist Desanka Boskovic, Doctoral Student Francisco Javier Hidalgo, Visiting Postdoctoral Researcher Georg Huhs, Visiting Doctoral Student Nicolás Lorente, CSIC Research Scientist Rafael Martínez, Doctoral Student

Annapaola Migani, CSIC Ramon y Cajal Researcher Pablo Ordejón, Director and Group Leader Lorenzo Riches, Doctoral Student Maitreyi Robledo, Visiting Doctoral Student Roberto Robles, Postdoctoral Researcher Rubén Ruperez, Visiting Student losé Ángel Silva, FPI Doctoral Student



GROUP LEADER



CSIC Research Prof. Pablo Ordejón

Prof Ordejón earned his BSc in Physics (1987) and PhD in Science (1992) at the Universidad Autónoma de Madrid (Spain). 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 CIN2 (now ICN2), where he is currently CSIC Research Profesor. Since July 2012, he has served as Director of ICN2, where he also leads the Theory and Simulation Research Group.



NEW PROJECTS & MILESTONES

During 2014 the group has continued the study of the interface of molecules, clusters, and nanostructures with metals. Such studies are of great interest in fields such as supramolecular chemistry, catalysis, molecular electronics, and data storage. In particular, we have shown how chemical doping offers a promising mechanism to locally manipulate charge and spin of individual molecules

with unprecedented spatial resolution. We have also studied the formation of chiral supramolecular pentamers. These pentamers are able to self-assemble to form large ordered arrays, covering big areas of a gold surface using motifs with five-fold symmetry.

The group has also focused on new 2D materials. Firstly, pristine monolayers of MoS2 were studied and a new tight-binding model to describe its electronic properties proposed. Secondly, a number of hybrid heterostructures have been analysed.



He has published more than 190 scientific articles, which have received over 17,000 citations (h = 47). Since 2009 he has served as Co-Editor of *EPL* (formerly *Euro Physics Letters*) and since 2004, as Regional Editor of *physica status solidi*. He was in charge of the Condensed Matter Physics area of the Physics Panel of the Spanish National Scientific Evaluation Agency (ANEP), from 2003 to 2006, and 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.

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, among many others, electronic transport in nanoscale devices and electronic processes at surfaces. He maintains frequent collaborations with industrial laboratories on the simulation of materials processes at the atomic level.

Vertical stacks of graphene and BN revealed a wealth of surprising physical properties, with the appearance of new superlattice Dirac points that affect the electronic transport properties. These were studied with large-scale DFT calculations, but also with a simplified tight-binding model which was later applied to the study of transport properties within the Kubo formalism developed by Prof Stephan Roche. Finally, coplanar heterostructures of different 2D materials were examined, in search for novel interfacial effects due to polarity discontinuities, similar to those observed at the interfaces of complex oxides.



PUBLICATIONS

Classical limit of a quantal nano-magnet in an anisotropic environment, Gauyacq, IP; Lorente, N, Surface Science: vol. 630, 325-330 (2014). IF: 1.87

Coverage dependence of the level alignment for methanol on TiO2(110), Migani A., Mowbray D.J., Computational and Theoretical Chemistry: vol. 1040-1041, 259-265 (2014). IF: 1.368

Difficulties in the ab initio description of electron transport through spin filters,

Kepenekian M., Gauyacq J.-P., Lorente N., Journal of Physics Condensed Matter (10): vol. 26 (2014). IF: 2.223

Electron transport signature of H2 dissociation on atomic gold wires, Zanchet A., Roncero O., Dorta-Urra A., Aguado A., Martínez J.I., Flores F., Lorente N., Physical Review B - Condensed Matter and Materials Physics (4): vol. 90 (2014). IF: 3.664

Electronic properties of single-layer and multi-layer transition metal dichalcogenides MX2 (M=Mo, W and X=S, Se), R. Roldán; J.A. Silva-Guillén; M. Pilar- López-Sancho; F. Guinea; E. Cappelluti; P. Ordejón, Annalen der Physsik: vol. 526, 347-357 (2014). IF: 1.483

Excitation of bond-alternating spin-1/2 Heisenberg chains by tunnelling electrons, Gauyacq I.-P., Lorente N., Journal of Physics

Condensed Matter (39): vol. 26 (2014). IF: 2.223

Momentum dependence of spin-orbit interaction effects in single-Layer and multilayer transition metal dichalcogenides,

R. Roldán; M. Pilar López-Sancho; F. Guinea; J.A. Silva-Guillén; E.Cappelluti; P. Ordejón., 2D Materials: vol. 1 (2014). IF: Pending

Orbital Redistribution in Molecular Nanostructures Mediated by Metal-Organic

Bonds, Zechao Yang; Martina Corso; Roberto Robles; Christian Lotze; Roland Fitzner; Elena Mena-Osteritz; Peter Bäuerle; Katharina I. Franke; José I. Pascual, ACS Nano: vol. 8 (2014). IF: 12.033

Oxygen vacancies in self-assemblies of ceria nanoparticles, Mahasin Alam Sk; Sergey M. Kozlov; Kok Hwa Lim; Annapaola Migani; Konstantin M. Neymanbf, Journal of Materials Chemistry A: vol. 2, 18329-18338 (2014). IF: Pending

Piezoelectric monolayers as nonlinear energy harvesters, López-Suárez M.; Pruneda M.; Abadal G.; Rurali R., Nanotechnology (17): vol. 25 (2014). IF: 3.672

Quasiparticle level alignment for photocatalytic interfaces, Migani A., Mowbray D.J., Zhao J., Petek H., Rubio A., Journal of Chemical Theory and Computation (5): vol. 10, 2103-2113 (2014). IF: 5.31

Spin transport in dangling-bond wires on doped H-passivated Si(100), Mikaël Kepenekian; Roberto Robles; Riccardo Rurali;

Nicolás Lorente, Nanotechnology: vol. 25 (2014). IF: 3.672

Theoretical study on the influence of Mg2+ and Al3+ octahedral cations on the vibrational spectra of the hydroxy groups of dioctahedral 2:1 phyllosilicate models,

Hernandez-Haro N., Ortega-Castro J., Pruneda M., Sainz-Díaz C.I., Hernandez-Laguna A., Journal of Molecular Modeling (9): vol. 20 (2014). IF: 1.867

Transport fingerprints at graphene superlattice Dirac points induced by a boron nitride substrate, Martínez-Gordillo R., Roche S., Ortmann F., Pruneda M., *Physical Review B - Condensed Matter and Materials Physics* (16): vol. 89 (2014). IF: 3.664



PROJECTS

Atomic Scale and Single Molecule Logic Gate Technologies, ATMOL, funded by **EC**, 01/01/2012-31/12/2014, Nicolás Lorente

Simulaciones Atomísticas de Primeros Principios: Metodología y Aplicaciones en Nanociencia, SIESTA-CIN2, funded by **MINECO**, 01/01/2013-31/12/2015, Pablo Ordejón



CONTRIBUTIONS

Spin Correlations of supported nano-objects, MANA International Symposium, organized by NIMS, Epochal Tsukuba, Japan, 05/03/2014, Nicolás Lorente (Invited)

Spin correlations as revealed by the STM, **Aalto University Physics Boat Workshop**, organized by Aalto University, Espoo, Finland, 03/06/2014, Nicolás Lorente (Invited)

Piezoelectric effects in hybrid C/BN nanosheets, **Graphene and 2D Materials workshop**, organized by National University of Singapore, Singapore, 19-20/06/2014, M. Pruneda (Invited)

Spontaneous magnetic switching due to decoherence, Donostia International Physics Center, DIPC Workshop: A tribute to Heinrich Rohrer, organized by DIPC, San Sebastián, Spain, 11/09/2014, Nicolás Lorente (Invited)

STM studies of adsorbed magnetic atomic and molecular systems, **Spinmol 2014**, organized by Universität Bern, Bern, Switzerland, 26-30/10/2014, Nicolás Lorente (Invited)

Transport Fingerprints at Graphene Superlattice Dirac Points Induced by Boron-Nitride Substrate, **Graphene 2014**, organized by UCL, ICN2, Toulouse, France, 06-09/05/2014, R. Martínez-Gordillo, S. Roche, F. Ortmann and M. Pruneda (Oral presentation)

Electronic structure calculations on MX 2 dichalcogenide/Graphene hybrid structures, **GraphESP2014**, organized by Graphene Flagship, Lanzarote, Spain, 18-24/02/2014, J. A. Silva-Guillén, E. Cappelluti, R. Roldán, F. Guinea, P. Ordejón (Poster)

Minimal tight-binding model for transition metal dichalcogenides, **Graphene 2014**, organized by UCL, ICN2, Toulouse, France, 06-09/05/2014, J. A. Silva-Guillén, E. Cappelluti, R. Roldán, F. Guinea, P. Ordejón (Poster)



COURSES

CECAM School "Efficient DFT calculations with atomic orbitals: A hands-on tutorial of the SIESTA and TRANSIESTA codes", **Tel Aviv University, Tel Aviv (Israel)**, 08-11/09/2014, P. Ordejón

Simulación de sistemas nanométricos, 4th year Grado de Nanociencia, **Universitat Autònoma de Barcelona (UAB), Bellaterra (Spain)**, February-June 2014, J.M.A. Pruneda (Coordinator)



THESES

Doctorand: **Rafael Martínez Gordillo** Title: Atomistic simulations in hybrid C/BN structures

Defense date: 01/10/2014 Director: José Miguel A. Pruneda

Technical Development and Support

The research support divisions and core facilities constitute a centralized research support infrastructure, led by Dr Gustavo Ceballos, that allows research scientists shared access to sophisticated instruments, technologies and specialized services and expertise. It aims to offer, for the research groups within the ICN2 and neighbouring research institutions, a collaborative platform and a repository of expertise and know-how to develop new methods, materials, instruments and techniques. A highly qualified multidisciplinary team of experts supports activities within the research facilities providing expertise that may be lacking in research laboratories and fostering collaborations between investigators as well as inter-disciplinary research.



- > Electron Microscopy Division
- > Nanofabrication Division
- > Nanomaterials Growth Division
- > Nanoscience Instrument Development Division
- > Core Research Support Facilities

Electron Microscopy Division

Main Research Lines

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



DIVISION MEMBERS

Belén Ballesteros, Division Leader Francisco Javier Belarre, Technician Elzbieta Pach, Doctoral Student Marcos Rosado, PTA Technician





DIVISION LEADER



Dr Belén Ballesteros

Dr Belén Ballesteros earned her BSc in Chemistry with Honours at the Universitat Autònoma de Barcelona (UAB) in 2001 and obtained 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 University of Twente (Netherlands), University of Oslo (Norway), University of Saint Andrews (UK) and Universidad de



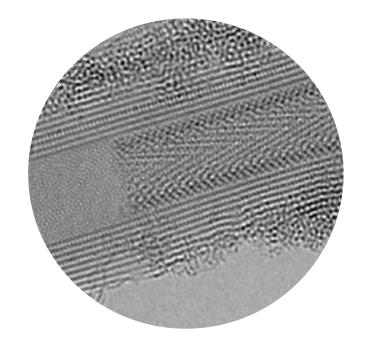
NEW PROJECTS & MILESTONES

During 2014 the Electron Microscopy Division strengthened its scientific-technical support, increasing the amount of internal and external users with respect to 2013.

Furthermore, the set of equipment at the sample preparation laboratory was completed by the transfer and installation of equipment from ICMAB (Ion milling system, diamond wire saw and automatic polishing system). The laboratory is now a joint project between this nearby institution and ICN2.

During 2014 the Division hosted a visiting postdoctoral researcher from University of Trieste (José Miguel González).

Researchwise the Electron Microscopy Division continued working on the study of functional carbon nanomaterials for biomedical applications in the framework of the ongoing project RADDEL. For instance, we studied MWCNTs functionalized with a Gd-chelate for MRI applications, graphene produced by dry milling with a hydrophobic drug and single-layered inorganic nanotubes formed inside MWCNTs. Also, the procedure for in-situ ice formation onto different substrates in the ESEM was optimized.



la Laguna (Spain). In July 2006 she began postdoctoral work at the University of Oxford, where she worked in Electron Microscopy Imaging and Nanoanalysis of carbon nanotubes, inorganic nanotubes and related materials. Since April 2009 she has led the Electron Microscopy Division at ICN2.

Dr Ballesteros has authored 47 articles and has around 600 citations.



PUBLICATIONS

Covalent Functionalisation of Multi-walled Carbon Nanotubes with a Gadolinium Chelate for Efficient T1-Weighted Magnetic Resonance Imaging, Marangon I., Ménard-Moyon C., Kolosnjaj-Tabi J., Béoutis M. L., Lartigue L., Alloyeau D., Pach E., Ballesteros B., Autret G., Ninjbadgar T., Brougham, D. F. Bianco A., Gazeau F., Advanced Functional Materials (2014). IF: 10.439

Fieldlike and antidamping spin-orbit torques in as-grown and annealed Ta/ CoFeB/MgO layers, Avci C.O., Garello K., Nistor C., Godey S., Ballesteros B., Mugarza A., Barla A., Valvidares M., Pellegrin E., Ghosh A., Miron I.M., Boulle O., Auffret S., Gaudin G., Gambardella P., Physical Review B - Condensed Matter and Materials Physics (21): vol. 89 (2014). IF: 3.664

Four molecular superconductors isolated as nanoparticles, De Caro D., Faulmann C., Valade L., Jacob K., Chtioui I., Foulal S., de Caro P., Bergez-Lacoste M., Fraxedas I., Ballesteros B., Brooks J.S., Steven E., Winter L.E., European Journal of Inorganic Chemistry (2014). IF: 2.965

Production of Water-Soluble Few-Layer Graphene Mesosheets by Dry Milling with Hydrophobic Drug, Rubio N., Serra-Maia R., Kafa H., Mei K. C., Pach E., Luckhurst W., Zloh M., Festy F., Richardson J. P., Naglik J. R., Ballesteros B., and Al-Jamal K. T., Langmuir: vol. 30, 14999-15008 (2014). IF: 4.384

Synthesis of PbI2 single-layered inorganic nanotubes encapsulated within carbon nanotubes, Cabana L., Ballesteros B., Batista E., Magen C., Arenal R., Oro-Sole J., Rurali R., Tobias G., Advanced Materials (13): vol. 26, 2016-2021 (2014). IF: 15.409

Ultraviolet pulsed laser irradiation of multi-walled carbon nanotubes in nitrogen atmosphere, Pérez Del Pino A., Gyorgy E., Cabana L., Ballesteros B., Tobias G., Journal of Applied Physics (9): vol. 115 (2014). IF: 2.185

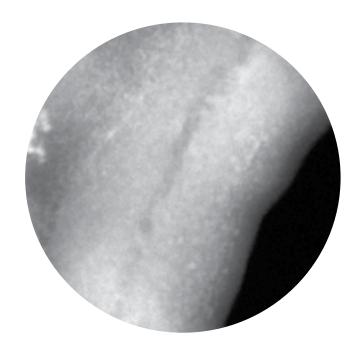


PROJECTS

Nanocapsules for targeted delivery of radioactivity, RADDEL, funded by Marie Curie **Actions**, 01/02/2012 - 31/01/2016, Dr Belén Ballesteros

Nanostructured materials for photovoltaic energy Group (SGR), funded by AGAUR, 01/01/2014 -31/12/2016, Dr Mónica Lira-Cantú

Solution Processable nanostructured solar cells: New nanomaterials based on transition metal oxides and graphene, funded by MINECO, 01/01/2014 - 31/12/2016, Dr Mónica Lira-Cantú



Nanofabrication Division

Main Research Lines

- Nanofabrication methods and techniques
- Flexible Nanofabrication platform for processing diverse materials and substrates
- High-quality services for internal and external users
- Process development and/or prototyping of novel nanostructures and devices
- Lithography techniques and materials



DIVISION MEMBERS

Nikos Kehagias, Division Leader Dina Augusta Simoes, Postdoctoral Researcher





NEW PROJECTS & MILESTONES

In 2012 ICN's Nanofabrication Division Leader Dr Kehagias, together with colleagues at the company PTMTEC Oy (Finland), developed a desk-top Rollto-Roll Ultraviolet Light-Assisted Nanoimprint Lithography Machine. This one-of-a-kind machine enables meter-per-meter production of nanoscale devices and components.

The Division completed a research collaboration with the technology centre CETEMMSA, aimed at replacing indium tin oxide (ITO), the dominant transparent conductor currently on the market. They developed alternative transparent electrodes based on nano-imprinted metallic grids to support inkjet-printed organic solar cells.



DIVISION LEADER



Dr Nikos Kehagias

Dr Nikos Kehagias earned a BSc in Physics from Aristotle University in Thessaloniki (Greece), in 2002; an MSc in Physics of Laser Communications, from Essex University (UK), in 2003; and a PhD from the National University of Ireland, Cork, in 2007, where he continued to work as a postdoctoral fellow until May 2008. At that point he joined ICN (now ICN2) as a member of the Phononic and Photonic Nanostructures Group. Since July 2010 he has led the Nanofabrication Division at ICN2. Dr Kehagias has co-authored more than 30 scientific journal articles, plus two book chapters in the field of Nanofabrication and Nanoimprint Lithography. He has pioneered the use of Reverse Ultraviolet Light-Assisted Nanoimprint Lithography (RUVNIL) as an alternative nanolithography technique.

It also began the new project "Moulding Production Technology for multifunctional structured plastic components enabled by nanoimprint lithography" (Plast4Future), part of the European Commission's Seventh Framework Programme (FP7).

Lastly, ICN's Nanofabrication Division began negotiations with a multinational company on a possible new research agreement on roll-toroll (R2R) nanofabrication.



SERVICES

ICN2's Nanofabrication Division offers diverse services to internal and external users for applications in Nanoelectronics, Nanophononics, Nanophotonics, Spintronics, Nanobioelectronics and Biosensors:

Lithography:

- Thermal and UV nanoimprinting Obducat 3 inch
- Hot embossing machine
- UV nanoimprinting module
- · SEM/Litho FEI/Raith
- Self-assembly growth set-up
- Roll to Roll UV-light-assisted nanoimprinting tool
- Reverse gravure coating
- CNI thermal nanoimprinting tool

Deposition:

- E-beam evaporator 1 (Au, Ag, Al, Cr, Ti, Pt, Al2O3) - AlA International
- ITO-Molecular beam epitaxy
- Sputter (Au) coater Edmunds
- · Spin coater Laurel

Characterisation:

- Atomic force microscope Veeco Instruments
- Optical microscope Nikon Eclipse LV100

· Gold-ball bonder - Delvotek

General:

- Plasma cleaner PVA Tepla PS210
- · Oven Memmert
- Hot plates
- Microwave annealing



PUBLICATIONS

Determination of heterogeneous electron transfer-rate constants at interdigitated nanoband electrodes fabricated by an optical mix-and-match process, Del Campo F.J., Abad L., Illa X., Prats-Alfonso E., Borrise X., Cirera J.M., Bai H.-Y., Tsai Y.-C., Sensors and Actuators, B: Chemical: vol. 194, 86-95 (2014). IF: 3.84

Embedded inkjet printed silver grids for ITO-free organic solar cells with high fill factor, Burgués-Ceballos I., Kehagias N., Sotomayor Torres C. M., Campoy-Quiles M., Lacharmoise P.D., Solar Energy Materials and Solar Cells: vol. 127, 50-57 (2014). IF: 5.03

Enabling electromechanical transduction in silicon nanowire mechanical resonators fabricated by focused ion beam implantation, Llobet J., Sansa M., Gerboles M., Mestres N., Arbiol J., Borrise X., Pérez-Murano F., Nanotechnology (13): vol. 25 (2014). IF: 3.672

Hypersonic phonon propagation in onedimensional surface phononic crystal,

Graczykowski B., Sledzinska M., Kehagias N., Alzina F., Reparaz J.S., Sotomayor Torres C. M., *Applied Physics Letters* (12): vol. 104 (2014). IF: 3.515

Order quantification of hexagonal periodic arrays fabricated by in situ solventassisted nanoimprint lithography of block copolymers, Simao C., Khunsin W., Kehagias N., Salaun M., Zelsmann M., Morris M.A., Sotomayor Torres C. M., Nanotechnology (17): vol. 25 (2014). IF: 3.672

Nanomaterials Growth Division

Main Research Lines

- Epitaxial thin film deposition and characterisation of different materials, mainly perovskite-structure related oxides. Interplay between strain and relaxation mechanisms, microstructure and functional properties of ultrathin films
- Present research is mainly devoted to thin epitaxial growth of mixed ionic-electronic conducting oxides and multilayers by PLD, their structure characterisation by RHEED and XRD, and hightemperature electronic transport properties. Oxide and Protonic Ionic conductivity in thin films
- Fundamental aspects of interfacial phenomena in the electrical characterisation of thin films of layered oxide materials and multilayers, for their use as components in intermediate temperature SOFCs
- Surface composition segregation and its effect on oxygen surface exchange kinetics and ageing phenomena



DIVISION MEMBERS

Núria Bagués Salguero, FPI-CSIC Doctoral Student José Manuel Caicedo, ICN2 Lab Engineer Araceli Gutiérrez, URIC Visiting Postdoctoral Researcher

Anna Magrasó, Abel-Nils Visiting Postdoctoral Researcher

Roberto Moreno, CSIC Visiting Doctoral Student laume Roqueta, CSIC Lab Engineer



DIVISION LEADER



CSIC Tenured Scientist Dr José Santiso

Dr José Santiso earned his BSc degree in Physics at the Universitat Autònoma de Barcelona (UAB), Spain, in 1988 and obtained his PhD from the University of Barcelona (UB) in 1993. After his doctoral studies, he worked as a Visiting Scientist at Cambridge University, UK from 1994 to 1996. After this stage he joined the Material Science Institute (ICMAB) as a research associate and became CSIC staff scientist in 2002. In 2007 he



NEW PROJECTS & MILESTONES

In 2014 the Nanomaterials Growth Division continued working on the following closelyrelated main objectives:

Thin film deposition of epitaxial oxide materials by means of pulsed Laser deposition technique. In this case our division produces films for a large number of groups within the ICN2, in close collaboration with these groups. In some cases the thin film deposition required the use of Reflection high energy electron diffraction

(RHEED). Our division carries out the preliminary structure characterisation concerning mostly X-Ray diffraction. (Some of the ICN2 group leaders who we collaborate with are: G. Catalan, J. Fraxedas, S. Valenzuela, C. Torres, and J. Nogués)

Investigation of the interplay between strain relaxation phenomena and functional properties in complex oxide films. Development of novel methods for the X-ray diffraction and diffuse scattering characterisation of microstructure features in epitaxial thin films. These included inplane diffraction, GISAXS analysis, as well as 3D reciprocal space mapping (this last type of analysis required the use of synchrotron radiation source: at BM25-ESRF and KMC2-Bessy). Most of the work is carried out in collaboration with Institut de Ciència de Materials de Barcelona (ICMAB).



Carlos Rubio, UAB Visiting MD Student José Santiso, CSIC Tenured Scientist and Division Leader José Manuel Vila, USC Visiting **Doctoral Student**

moved to CIN2 as leader of the Pulsed Laser Deposition and Nanoionics Group, Nanomaterials Growth Division, which recently turned into the ICN2 Nanomaterials Growth Division that he also leads. In 2012 he received the Somiya Award of the International Union of Materials Research Society (IUMRS) for his contribution to Solid State Ionics. Recently, in 2014, he obtained a grant from the Japan Society for Promotion of Science as a 3-month visitor at the International Institute for Carbon-neutral Research, I2CNER, (Univ. Kyushu).

The microstructure investigation is completed by HRTEM characterisation.

Study of fundamental aspects of ionic and electronic charge and mass transport in the electrical characterisation of thin films of layered oxide materials and multilayers, for their use as components in intermediate-temperature SOFCs. We are particularly interested in surface and interfacial oxygen exchange phenomena in order to obtain enhanced oxygen transport performance. Development of novel characterisation tools of the oxygen surface exchange kinetics: For this purpose we have developed a novel technique that uses the subtle chemical expansion measured by X-ray diffraction produced in transition metal oxide thin films when changing their oxygen stoichiometry to in-situ probe their redox kinetics at high temperature in time intervals as short as a few seconds. The setup also allows for electrical contacts which may be used either to simultaneously measure electrical conductivity relaxation or to apply an electric field for in-operando device electrochemical characterisation.

Investigation of the surface activity for oxygen reduction in transition metal oxide perovskite thin films. Development of novel methods for determining oxygen surface exchange rate by combination of electric conductivity relaxation and time-resolved X-ray diffraction experiments. We explore surface cation composition segregation mechanisms affecting the reactivity of the surfaces. This work is mostly carried out in collaboration with different international partners (Imperial College London, I2CNER at Kyushu Univ. and MIT).



PUBLICATIONS

Chemical Strain and Oxidation-Reduction Kinetics of Epitaxial Thin Films of Mixed **Ionic-Electronic Conducting Oxides Determined by X-Ray Diffraction**, R. Moreno, J. Zapata, J. Roqueta, N. Bagués and J. Santiso, *Journal of the Electrochemical Society* (11): vol. 161, F3046-F3051 (2014). IF: 2.859

Engineering the microstructure and magnetism of La2CoMnO6-δ thin films by tailoring oxygen stoichiometry, R. Galceran, C. Frontera, L. Balcells, J. Cisneros-Fernández, L. López-Mir, J. Roqueta, J. Santiso, N. Bagués, B. Bozzo, A. Pomar, F. Sandiumenge, B. Martínez, Applied Physics Letters: vol. 105 (2014). IF: 3.515

Growth kinetics engineered magnetoresistance response in La 2/3Sr1/3MnO3 thin films, Pomar A., Santiso J., Sandiumenge F., Oqueta J., Bozzo B., Frontera C., Balcells L., Martínez B., Konstantinovic Z., Applied Physics Letters (15): vol. 104 (2014). IF: 3.515

Interfaces and nanostructures of functional oxide octahedral framework structures, F. Sandiumenge; N. Bagués; I. Santiso, Frontiers in *Materials*: vol. 1 (2014)



PROIECTS

Nano-sized proton conductors for the next generation of environmentally-friendly fuel cells ABEL-NILS, 021-ABEL-AM-2013, funded by EEA, 01/07/2014-01/12/2015, Anna Magrasó

Low-Energy Ion Scattering measurements on atomically flat epitaxial layers of mixed ionic electronic conducting oxides for cathodes in SOFC/SOEC technology, funded by Japan Society for the Promotion of Science, 01/12/2014-01/02/2015, Jose Santiso, Tatsumi Ishihara



CONTRIBUTIONS

Oxygen Surface exchange kinetics in epitaxial thin films by time-resolved X-ray diffraction, MRS Spring meeting. Symposium L: Materials and Interfaces in Solid Oxide Fuel Cells. San Francisco (USA), 21/04/2014-25/04/2015, J. Santiso (Invited)

Chemical Strain and Oxidation-Reduction Kinetics of Epitaxial Thin Films of Mixed Ionic-Electronic Conducting Oxides Determined by X-Ray Diffraction, 225th ECS Spring Meeting 2014, Symp A3 Mechanical-Electrochemical Coupling in Energy-Related Materials and Devices. Orlando (USA), 11/05/2014-15/05/2014, J. Santiso, R. Moreno, J. Zapata, J. Roqueta, P. García, N. Bagués (Invited)

Chemical Strain Kinetics in epitaxial thin films measured by time-resolved X-ray diffraction, Oxide Thin Films for Advanced Energy and Information Applications. Materials Chemistry of Thin Film Oxides. Chicago (USA), 13/07/2014-16/07/2014, J. Santiso (Invited)

Band Diagrams for Electrochemical Devices, E-MRS - Symp C:Solid state ionics: thin films for energy and information applications. Lille (France), 26/05/2014-30/05/2014, J. Santiso, J. Roqueta (Oral)

Nanoscience Instrument **Development Division**

Main Research Lines

- Design, development and improvement of advanced precision Instrumentation
- Active collaboration for experimental research
- Scientific Computing, signal processing, data acquisition 3D-CAD design of precision devices



DIVISION MEMBERS

Gustavo Ceballos, Division Leader Marc Maymó, Laboratory Engineer





DIVISION LEADER



Dr Gustavo Ceballos

Dr Gustavo Ceballos earned his BSc in Chemistry at the Central University of 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 for postdoctoral studies, and from 2001 to 2002, worked at the Low-Temperature Scanning Tunnelling Microscopy (STM)



NEW PROJECTS & MILESTONES

The Division provides scientific and technical assistance in Applied Physics; Precision Instrumentation; Microengineering; Nanotechnology; Metrology, Scientific Computing; and 3D-design of precision devices, to address challenging instrumental projects in basic Nanoscience research as well as in applied technology.

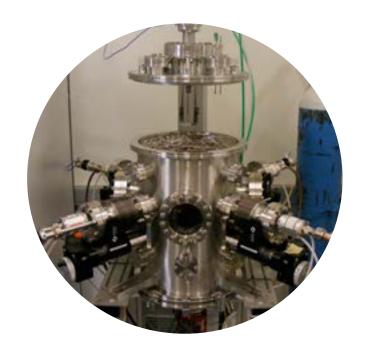


PUBLICATIONS

Atomic Monolayer, Deposition on the Surface of Nanotube Mechanical Resonators, A. Tavernarakis; J. Chaste; A. Eichler; G. Ceballos; M. C. Gordillo; J. Boronat; A. Bachtold, Physical Review Letters (19): vol: 112 (2014). IF: 7.728

Spin tuning of electron-doped metalphthalocyanine layers, Sebastian Stepanow, Alberto Lodi Rizzini, Cornelius Krull, Jerald Kavich, Julio C. Cezar, Flora Yakhou-Harris, Polina M. Sheverdyaeva, Paolo Moras, Carlo Carbone, Gustavo Ceballos, Aitor Mugarza, Pietro Gambardella, Journal of the American Chemical Society (14): vol. 136, 5451-5459 (2014). IF: 11.444

Spin-dependent electron scattering at graphene edges on Ni(111), Garcia-Lekue A., Balashov T., Olle M., Ceballos G., Arnau A., Gambardella P., Sanchez-Portal D., Mugarza A., Physical Review Letters (6): vol. 112 (2014). IF: 7.728



Group at the Fritz-Haber-Institut der Max-Planck-Gesellschaft, also in Berlin. From 2002 to 2006 he was Research Scientist at the XSTM and Low-Temperature STM of Nanostructures Division at the Laboratorio Nazionale TASC-INFM, Trieste, Italy. In 2006 he joined ICN (now ICN2) as a Senior Scientist, where he eventually created the Nanoscience Instrument Development Division and where he actively participates in the research of the Atomic Manipulation and Spectroscopy Group.

Throughout his career, when endeavouring to perform new experiments, Dr Ceballos has frequently had to modify existing instruments or experimental setups, or develop new ones.

Core Research Support Facilities



Gustavo Ceballos, Head of the Core Facilities Pablo García, Technician Juan Luis Marte, Technician Javier Saiz, Technician Guillaume Sauthier, Technician



The ICN2 Core Scientific Facilities provide an array of specialized equipment, technologies and services, efficiently operated by a highly qualified staff to enable scientists to achieve ambitious research goals in a cost-effective way. From routine, though essential support services to advanced technical and consulting services, these cores facilitate and enhance the important research conducted at the institute on a daily basis.



Facilities cover the following areas:

- Photoemission Spectroscopy for surface analysis (XPS/ARUPS)
- · Molecular Spectrometry (UV/Vis, FT-IR, Fluorescence)
- Physicochemical Instrumental Analysis (ICP-MS, LC-MS, TGA, DSC)
- Light Microscopy
- X-Ray Diffraction
- SQUID Magnetometry
- Bio-Lab

Management and Output



- > Management and Services
- > Scientific Output
- > Projects
- > Finances
- > Facilities and Equipment
- > Technology Transfer
- > Public Outreach

Management and Services



ICN2's Management and Services team performs a wide range of functions and provides numerous support services to the Institute's Research Groups. Its members are distributed across eights departments: Human Resources & Education, Finance, Projects, Information Technologies, General Services, Technology Transfer, Marketing and Communication, and **Strategy**. Additionally, the Strategy Department reports directly to the Director. Each department has been designed and scaled to provide services to the whole ICN2 community, including 15 Research Groups and 5 Technical Development and Support Divisions and Facilities.

HUMAN RESOURCES & EDUCATION

ICN2's HR policies are a key competitive advantage in recruiting international talent. During 2014, the Human Resources Department made all the necessary arrangements for an average workforce of 226.4 people having their activity at ICN2 (including full-time personnel, visiting researchers, interns and students).

FINANCE

All ICN2 financial management is supported by SAP, and the Finance team has been expanded to serve the 15 Research Groups and 5 Technical Development and Support Divisions and Facilities that configure ICN2.

PROJECTS

After the segregation off the Finance Department, the Projects Department has grown and has focused even further on providing a complete service to all ICN2 researchers, including those from CSIC. The Group Project Managers of some groups have been also involved in some of the Department's tasks in a more comprehensive and coordinated way. Also, institutional projects management acquired special relevance during 2014.

The number of submissions handled was the largest in the history of ICN2 and the number of active projects during 2014 was 114. The philosophy of the Department is based on direct contact with the researcher, who considers its Project Manager as a key-person in relation to any step related to project management.

INFORMATION TECHNOLOGIES

In 2014, the IT department continued the implementation of the infrastructure for ICN2's new headquarters (network, IP communications, firewalls, etc.). The Department provides support to all ICN2.

GENERAL SERVICES

During 2014, the General Services department satisfied the needs of Groups and equipment in the new headquarters. The Department takes care of infrastructure maintenance, the Risk Prevention plan and works to keep over 40 laboratories fully operational.

TECHNOLOGY TRANSFER

ICN2's Technology Transfer Department offers a specialised service to support technology transfer within ICN2. Some of the major goals achieved by the Department in 2014 are: 5 European patent (EP) applications, 2 PCT

extension filed and 1 patent entered into national phase, and a new spin-off company, Futurechromes, S.L., created in June 2014.

MARKETING AND COMMUNICATION

The Marketing and Communication Department supports the dissemination of the research activity and the impact of the work developed by the ICN2 community.

In addition to managing the public and media relations of the Institute, the Department developed a series of classroom activities and training sessions for school teachers. The Department also offered Illustration, Graphic Design and Web Design services to offer an appealing image and message in all major publications and public materials produced by ICN2 scientists and Departments. The museum exhibition on Nanotechnology inaugurated in 2012 and partly financed by FECYT, Dimension Nano, could be visited until December 2014 at the mNACTEC museum in Terrassa (Spain).

This Department is deeply involved in the implementation of the new ICN2 image and working on internal cohesion tasks.

STRATEGY

During 2014 the Strategy Department focused on developing the process and initial drafts of the 2015-2020 Strategic Plan, including full-day workshops involving all Group Leaders and Administration Managers. This was supported by the development of a wikimediabased intranet to facilitate collaborative and transparent management of the strategic plan, infrastructure investment and other issues. The Department plays a key role in developing joint actions with other research centres, such as the Barcelona Nanocluster (BNC-b), promoting commercialisation opportunities in CERCA centres to venture capital funds, seeking new local collaborations in order to develop proposals for RIS3CAT projects and actions (especially in the B30 area), and promoting internal continuous improvement processes.

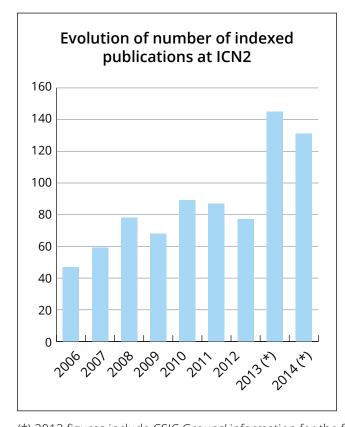
Scientific Output

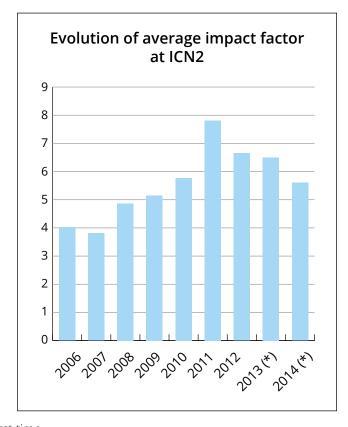
PUBLICATIONS

The scientific production of the ICN2 is remarkable. With 131 indexed publications in 2014, and an average impact factor of 5.61, the Institute achieves notable figures that are expected to increase in the years to come.

TOP 10 journals

Journal	IF	articles
Chemical Reviews	45.661	1
Nature Physics	20.603	1
Advanced Materials	15.409	3
Nano Letters	12.94	1
ACS Nano	12.033	5
Journal of the American Chemical Society	11.444	1
Nature Communications	10.742	3
Advanced Functional Materials	10.439	2
Nano Energy	10.211	1
Chemistry of Materials	8.535	1





(*) 2013 figures include CSIC Groups' information for the first time

ICN2 EVENTS

ICN2 researchers, with the support and collaboration of the administration departments, develop a leading role in Europe in the field of Nanoscience and Nanotechnology. It involves the organisation of international events attracting scientists from around the globe to Barcelona.

Some outstanding examples of events organized by ICN2 are:

TNT 2014 "Nanodevices for Societal Challenges"

- The Session gathered experts from around Europe in the areas of Biosensors, Theory, ICT and Energy. It was an opportunity to celebrate the Severo Ochoa accreditation in the context of a first-line international event.
- · Half-day Session.
- 4 Keynote Speakers, 4 ICN2 Group Leaders and the Director presented the ICN2 Severo Ochoa programme

International Summit on OPV Stability (ISOS-7) Summit

- StableNextSol, funded by the European Commission through a COST Action coordinated from ICN2 by Dr Mónica Lira-Cantú, is an interdisciplinary network of academic and industry researchers to study the degradation mechanisms occurring in state-of-the-art organic photovoltaic devices.
- 22 Presentations
- 2 round tables
- 100 participants

Aplicaciones Industriales de la Nanotecnología (AIN)

- · A yearly event co-organized with the Instituto de Nanociencia de Aragón (INA). With the support of LEITAT and the Chamber of Commerce, AIN brings together innovation, discussion and interaction at one unique event.
- 15 Speakers
- 100 participants







XXX Trobades Científiques de la Mediterrània

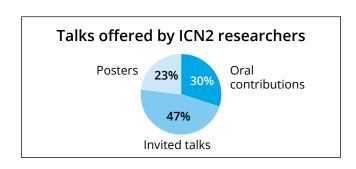
- · Stephan Roche, Group leader and ICREA researcher at ICN2 and European co-leader of Spintronics for the Graphene Flaghip, is among the event organizers. The meeting, held from October 15-17, offers a unique environment for collaboration
- 29 Presentations
- 1 round tables
- 60 participants

19th Transfrontier Meeting of Sensors and **Biosensors - TMSB**

- Researchers from the Euroregion between France and Spain (Catalonia, Languedoc-Roussillon, Midi-Pyrénées) and surroundings areas meet with the objective to share the latest achievements in the field of sensors and biosensors. The team led by ICREA Prof Arben Merkoçi organized the latest edition
- · 2 days Session
- · 2 Keynote Speakers, 20 presentations
- 60 participants

EVENTS IN WHICH ICN2 RESEARCHERS PARTICIPATED

In 2014 ICN2 researchers made 201 contributions at conferences related to Nanoscience and Nanotechnology. A breakdown of their contributions is shown beside.



ICN2 BOOTH IN TRADE SHOWS AND FAIRS

The Knowledge and Technology Transfer Department, together with the Strategy and the Marketing & Communication Departments, participates actively in the major international events about nanoscience and nanotechnology. The institutional booth travels with ICN2 representatives to events such as:

Nanospain

- Consolidated as a reference meeting of Nanoscience and Nanotechnology (N&N) in Spain
- ICN2 supported the event with a stand and several speakers
- 15 Keynote Speakers, 24 invited speakers
- · 200 participants

Graphene 2014

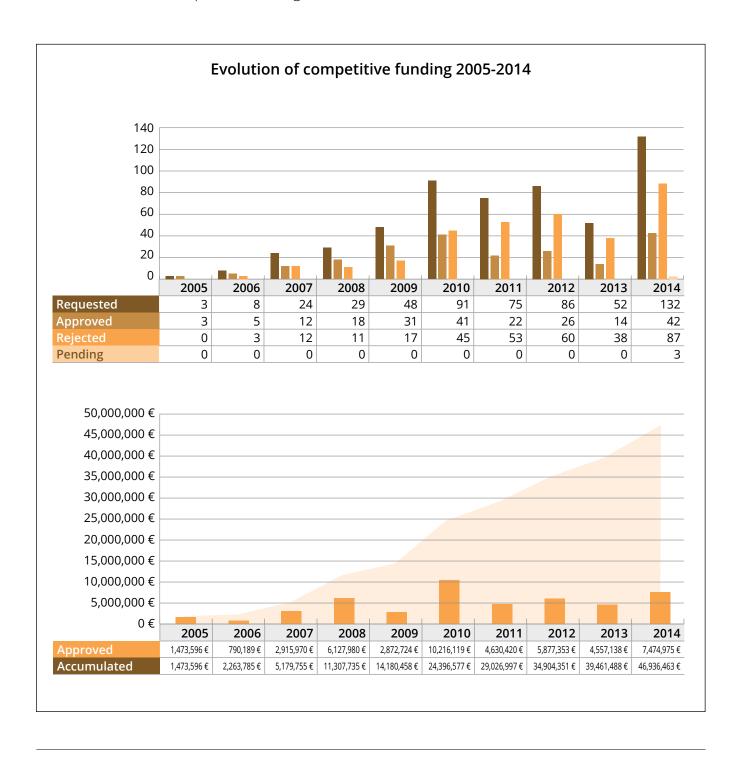
- Event in Toulouse, France, Dr Stephan Roche, Theoretical and Computational Nanosciences Group Leader is one of the members of the organising committee. ICN2 attended the event with an institutional booth
- 1,000 participants



Projects

Competitive research funding is vital for ICN2's financial viability and serves as an indicator of the quality and international competitiveness of the Institute's research. In 2014 competitive funding continued to stem in a high percentage from EU & International research projects.

The breakdown of competitive funding at ICN2 for 2014 is illustrated in the chart below:

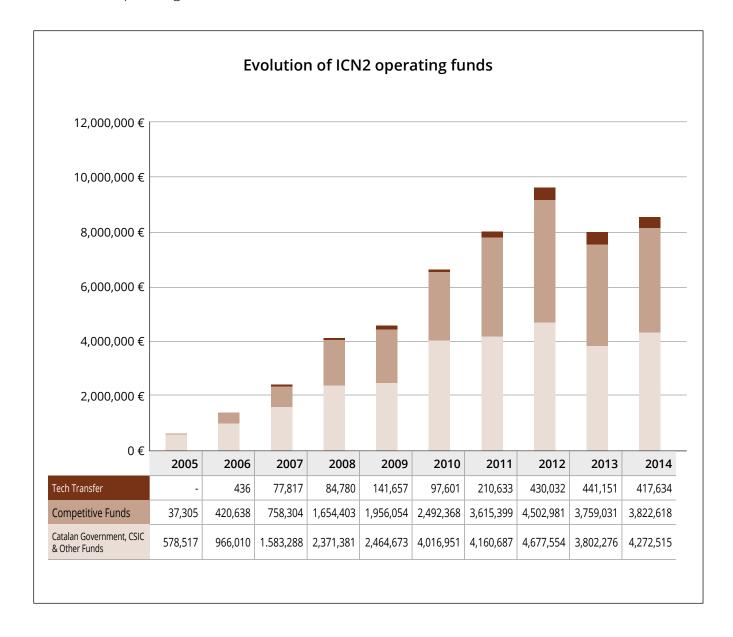


Finances

FINANCIAL ACCOUNTS 2014

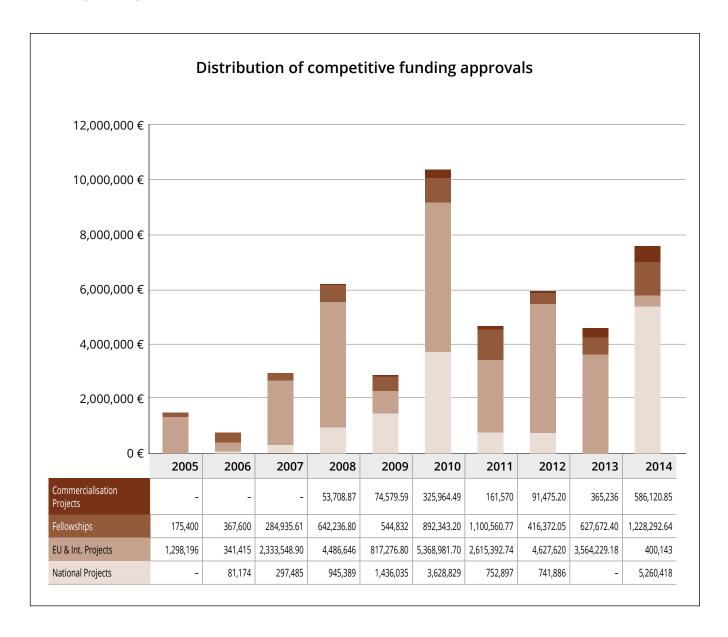
The Institute's operating budget comprises revenues from contributions by public administrations and agencies, from competitive grants, and from companies (via Technology Transfer). These revenues fund the operational activities of the Institute. The main items are Personnel Costs, General Operating Expenses and Depreciation (of equipment and facilities).

ICN2's total operating funds in 2014 were €8,512,497.



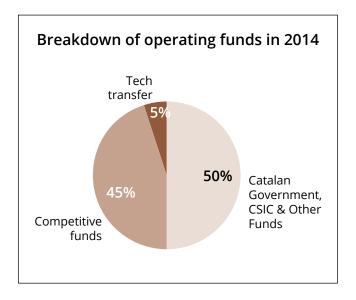
INTERNATIONAL COMPETITIVENESS

One of ICN2's principal objectives is to be highly competitive at the international level, both in the quality of the science it produces and the levels of competitive funding that it secures through national and international grants and fellowships and through commercialisation agreements with companies. To date, ICN2 has obtained competitive funding from numerous entities, including the European Commission; the Spanish Ministry of Economy and Competitiveness (MINECO), with special mention to the Severo Ochoa Excellence Award; ACC1Ó; and the Catalan Agency for the Administration of University and Research Grants (AGAUR).



INCOME

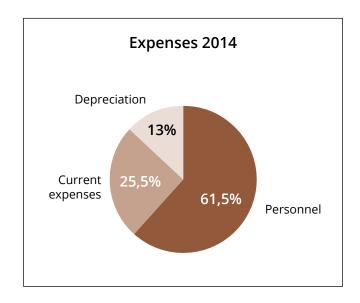
ICN2's total operating funds in 2014 were €8,512,497. In 2014 ICN2 obtained 50% of its operating funds from competitive grants (45%) and technology transfer projects (5%).



EXPENSES

In 2014 total expenditure at ICN2 was €8,677,564. Expenses, which comprise current expenses, personnel costs and depreciation, are classified as follows:

- · Project Expenses: These fund research and technology transfer.
- · Ordinary Expenses: These fund management structure and services.



Facilities and Equipment

In 2014 ICN2's total accumulated investment including scientific equipment, common services and general infrastructure was €17,859,554. Investment for the year 2014 was €1,100,066.

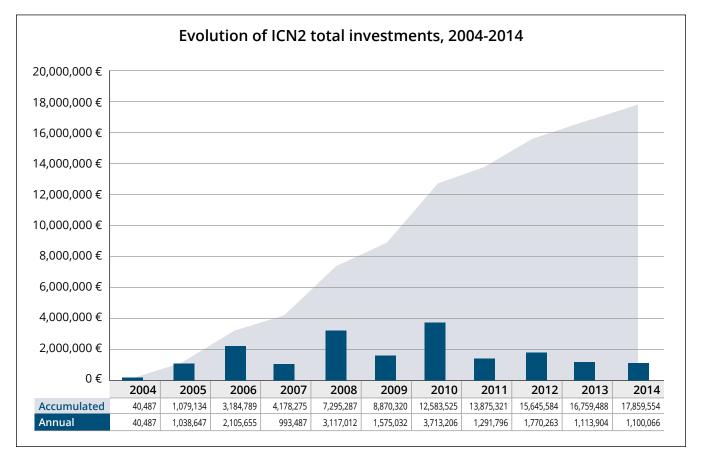
The main scientific, technical and IT equipment acquired in 2014 comprised:

- MBE Analysis Chamber and Electric Characterization Set-Up
- IT: Software Business One
- IT: Storage San
- IT: Computer and Network Infrastructure for ICN₂
- Gravimetric Analyzer Adsorption of Water and Organic Vapors
- Cryogen-Free Low Vibration Cryostat
- Cooling System Electric and Hydraulic

- Low Temperature Scanning Probe Microscope
- ICN2 Adaptation and Improvements in Building ICN2 and Boratories
- Holographic Microscope Digital Mems Analyzer
- System Multi Molecular Beam Epitaxy

Equipments funded with FEDER Funds:

- Fast Detector
- Optical Table
- · 4 Shaker RCT-Basic
- Multi Shaker
- Phmetro
- Electric Blanket 2CR-KE95
- XY Precision Stage
- Centrifuge Digicen 21



Technology Transfer

In 2014 ICN2 furthered its efforts to maximise the commercialisation of its research results through intellectual property and patents, commercial contracts, public sector collaborations, and other endeavours.

INTELLECTUAL PROPERTY AND SPIN-OFFS

5 European patent (EP) applications

- European patent (EP) application ICN PAT 02/13 Inspecting nanostructures. With Ref. EP14156430 and priority date 24/02/2014. P2N Group. Clivia Sotomayor Torres, Claudia Delgado Simao, Jordi Gomis, Timothy Kehoe.
- European Patent (EP) application ICN PAT 12/13 Method of forming an electronic device on a flexible substrate. With Ref. EP14382240 and priority date 20/06/2014. Nanobioelectronics and Biosensors Group. Arben Merkoçi, Carmen Mayorga, Luis Pires.
- European Patent (EP) application ICN PAT 09/13 Novel compositions comprising lipidic-coated bacteriophages. With Ref. EP14382057.9 and priority date 20/02/2014. Supramolecular NanoChemistry & Materials (NANOUP) Group. Daniel Maspoch, Mary Cano.
- European Patent (EP) application ICN PAT 03/13 Biocidal composition with dual inmediate and remnant activity. With Ref. EP14382498 and priority date 05/12/2014. Supramolecular NanoChemistry & Materials (NANOUP) Group. Gerard Martorell, Daniel Maspoch, Mary Cano, Vicente Ausina, Águeda Hernández.
- European Patent (EP) application ICN PAT 10/13 Liposome-based immunotherapy. With Ref. EP14151629.4 and priority date 17/01/2014. Supramolecular NanoChemistry & Materials (NANOUP) Group. Daniel Maspoch, Mary Cano, Irma Pujol, Marta Vives Pi, Joan Verdaguer.

1 patent entered into national phase

• Patent ICN PAT 01/11 Method for the preparation of metal organic frameworks has entered regional phases in USA on 04/04/2014 and in Europe on 29/04/2014.

2 international PCT extensions were filed

- ICN PAT 07/13 Sensitive qualitative bioassay using graphene oxide as analyte-revealing agent. With Ref. PCT/EP2014/072100 on 15/10/2014. Nanobioelectronics and Biosensors Group. Arben Merkoçi, Eden Morales.
- ICN PAT 08/12 Methods and devices for analysing nanostructure array images. With Ref. PCT/EP2014/075560 on 25/11/2014. P2N Group. Clivia Sotomayor Torres, Claudia Delgado Simao, Worawut Kunshin, Andreas Amman, Michael A. Morris, Dmitri Tuchapsky

1 Spin-off was created

• Futurechromes, S.L.. The new spin-off company based on the CSIC patent Ref. CIN2PAT 01/12 - WO2013/132123 (Coating with photochromic properties, method for producing said coating and use thereof applicable to optical articles and glazed surfaces), developed by the ICN2 Nanostructured Functional Materials Group, was created in June 2014.

OTHER HIGHLIGHTS

 Participation in main sector trade fairs: TNT in Barcelona, Graphene 2014 in Toulouse, 8th Aplicaciones Industriales de la Nanotecnología (AIN) in Barcelona.

Public Outreach

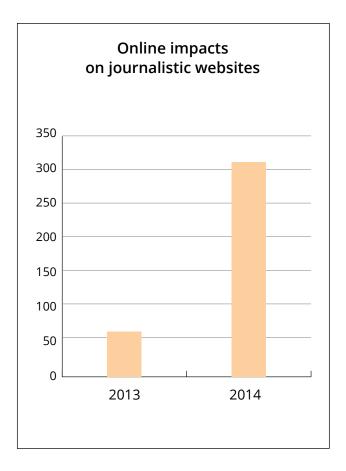
Beyond ICN2's principal mission to be a centre of scientific excellence and frontier research in Nanoscience and Nanotechnology, the Institute also has a social responsibility in Science Communication and Education. As a publicly-funded research institute, ICN2 is committed to serving, and engaging with the public at all levels.

Sparking the interest of young people in Nanoscience and Nanotechnology, and providing them with the tools they need to pursue careers in these fields, is paramount in ensuring ICN2's future success in the research arena. Furthermore, providing contents created for the general public about these areas is essential to guaranteeing that they can understand the implications of the Institute's research and its consequent developments.



HIGHLIGHTS 2014

Media relations: In 2014 ICN2 redoubled its efforts to reach the general public through the media. The following chart shows the number of Online Impacts on journalistic websites during the last two years.



Traditional media appearances of ICN2 in 2014

Magazines	2
Newspapers	36
Radio	2
TV	6

Dimensió Nano: ICN2, Recrea, La Mandarina de Newton and the museum mNACTEC created a multimedia exhibit dedicated to introducing Nanoscience and Nanotechnology to the public. Dimensió Nano was inaugurated at the Museum in June 2012 and was exhibited at mNACTEC until December 2014. Within the Severo Ochoa Programme the exhibit will be shown at new venues during the next few years.

ESCOLAB: Groups of secondary school children visited ICN2 labs to learn about Nanoscience and Nanotechnology and to ask researchers questions.

Joves i Ciència: High school students performed short research stays in the laboratories of ICN2 research groups during summer 2014.









Catalan Institute of Nanoscience and Nanotechnology (ICN2)

Campus de la UAB 08193 Bellaterra Barcelona, Spain Tel: +34 937 372 649

Email: info@icn2.cat Web: www.icn2.cat