

A watercolor illustration of the ICMAB-CSIC building, a modern structure with a curved facade and a rooftop terrace. The building is rendered in warm orange and yellow tones, with a prominent blue glass section. In the foreground, there are green trees and a red flower bed. The sky is a mix of blue and white, suggesting a bright day. The overall style is artistic and painterly.

ANNUAL REPORT

2017

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FOREWORD OF THE DIRECTOR

Welcome to
THE INSTITUTE OF MATERIALS SCIENCE OF BARCELONA (ICMAB)

Annual Report 2017

Xavier Obradors,
Director ICMAB-CSIC



This is the second year of our recognition as Severo Ochoa "Center of Excellence" label based on our Research Program "Smart FUNctional MATerials for social grand challenges" (FUNMAT). This Research Program established scientific and technological priorities which should address three social "Grand Challenges": Clean and secure energy, Sustainable and low cost electronics and Smart nanomedicine. In order to focus our R&D activities we identified 5 different Research Lines (RLs) where several of our 8 Research Groups contribute. RL1: Sustainable energy conversion and storage systems; RL2: Superconductors for power applications; RL3: Oxide electronics; RL4: Molecular electronics; RL5: Multifunctional nanostructured biomaterials.

The objective of nurturing new research ideas through interdisciplinary collaborations has been strongly incentivized in the scope of FUNMAT. Both, through the internal high risk exploratory "Frontier Interdisciplinary Projects" (FIPs), or through our talent attraction programs (SO fellowships, COFUND PhD and postdoctoral calls, INPhINIT



- la Caixa PhD fellowships, etc.), we have been able to attract young scientists and to generate many new internal and external outstanding collaborative projects fully integrated into our FUNMAT Research Program. In 2017 we granted 9 new FIPs, including a new “proof-of-concept” category.

During 2017 our R&D activities have been already fully engaged in the 9 ERC Grants allocated up to now to ICMAB researchers and, additionally, we were awarded with several new outstanding European research projects. Particularly, ICMAB coordinated the first COFUND project allocated to any CSIC Institute devoted to “Functional Advanced Materials” and having the participation of the Institute of Microelectronics of Barcelona (IMB-CSIC), the Catalan Institute of Nanoscience and Nanotechnology (ICN2), the Catalonia Institute for Energy Research (IREC) and the Synchrotron ALBA. Other prestigious EU or international projects were also achieved: CARBAT (FET-Open); SMART-4-FABRY, FASTGRID and KARDIATool (LEIT) and a CERN project.

Overall, at the end of 2017 a total of 34 European or international projects were alive (15 new projects in 2017) which provide to ICMAB a total budget of 25.5 M€. Actually, in 2017 we reached the highest ever percentage of our budget on competitive funding: 64 % from a

total budget of 13.7 M€. Within the 7.6 M€ raised on research projects, 56 % came from Europe or international sources. We envision our progress in the success of attracting competitive funds to the decisive support of FUNMAT to build up a Strategic Project Managing Unit.

Concerning the FUNMAT priority “Training and talent attraction” we can stress that our Master and PhD Fellowships programs have been extremely successful in attracting the interest of young researchers from all around the world (26 countries). Our enhanced international visibility as an excellence research center is also helping to attract PhD students from China (8 Chinese PhD students in the first two years of FUNMAT). At the end of 2017 we had a total of 97 PhD fellows (46 % from abroad) and 58 postdocs (50 % from abroad). Overall, after two years of FUNMAT the ICMAB has more than 50 additional researchers (increase of approx. 40 %), together with 41 undergraduates and master students that worked at ICMAB during 2017. Also 16 of our PhD students completed the thesis. These numbers are a clear evidence of our enhanced attractiveness as an excellent research center which required an additional effort to make available laboratory and office spaces, mainly through the agreement achieved with MATGAS to extend the use of their neighbouring building. The scientific production of ICMAB researchers continues to be diverse

and of high quality, a total of 201 articles were published (89 % (SJR) of them in Q1 journals) with an average impact factor of the journals of 5.7 in 2017. We continue to increase the total number of citations (> 133.000 at the end of 2017) and our researchers are widely selected to lecture in international conferences as reference speakers.

You will find in this report a selection of highlights corresponding to outstanding publications of the different Research Lines. They cover contributions from novel materials, methodologies and devices for a transition to a more efficient energy paradigm (thermoelectrics, superconductors, batteries, solar cells) to inorganic and organic electronic or photonic materials and devices (ferroelectrics, antiferromagnets, piezoelectrics, multiferroics, photodetectors, transistors) or nanomaterials for diverse therapy, diagnostics and tissue repair challenges in nanomedicine (radiotherapy and cancer treatment, nanovesicles for bioimaging, biological evaluation of nanoparticles, electrodes for neural repair). You will also find in this report a thorough description of our efforts to invigorate the communication, outreach and technology transfer actions, including at all steps our efforts to implement an effective gender action plan. It is particularly worth to notice that the number of outreach activities and the ICMAB

activities related to Communication and Scientific Culture have been strongly increased during this year linked to the incorporation to the ICMAB staff of our Communication & Outreach Officer.

The international evaluation of the ICMAB activities by our Scientific Advisory Board (SAB) was celebrated through a second edition which focused particularly this year on the Research Lines “RL1: Sustainable Energy conversion and storage systems” and “RL3: Oxide electronics”, where they appreciated the high quality and excellence of the research being performed. The other three RLs are scheduled to be evaluated in the SAB edition of 2018. The overall evaluation about the implementation of the FUNMAT Severo Ochoa action and the enthusiasm of the ICMAB personnel was very positive.

In conclusion, we are very proud that the ICMAB has increased its vibrant vitality, both concerning the scientific activities and the warm atmosphere of ICMAB’s life as an international center of excellence. I’m sure that you will, at least partly, feel this ICMAB environment and enthusiasm all through this report. If you want to still have more information about the ICMAB activities you can access to the website version of our report (<https://resources.icmab.es/annualreport2017/>).

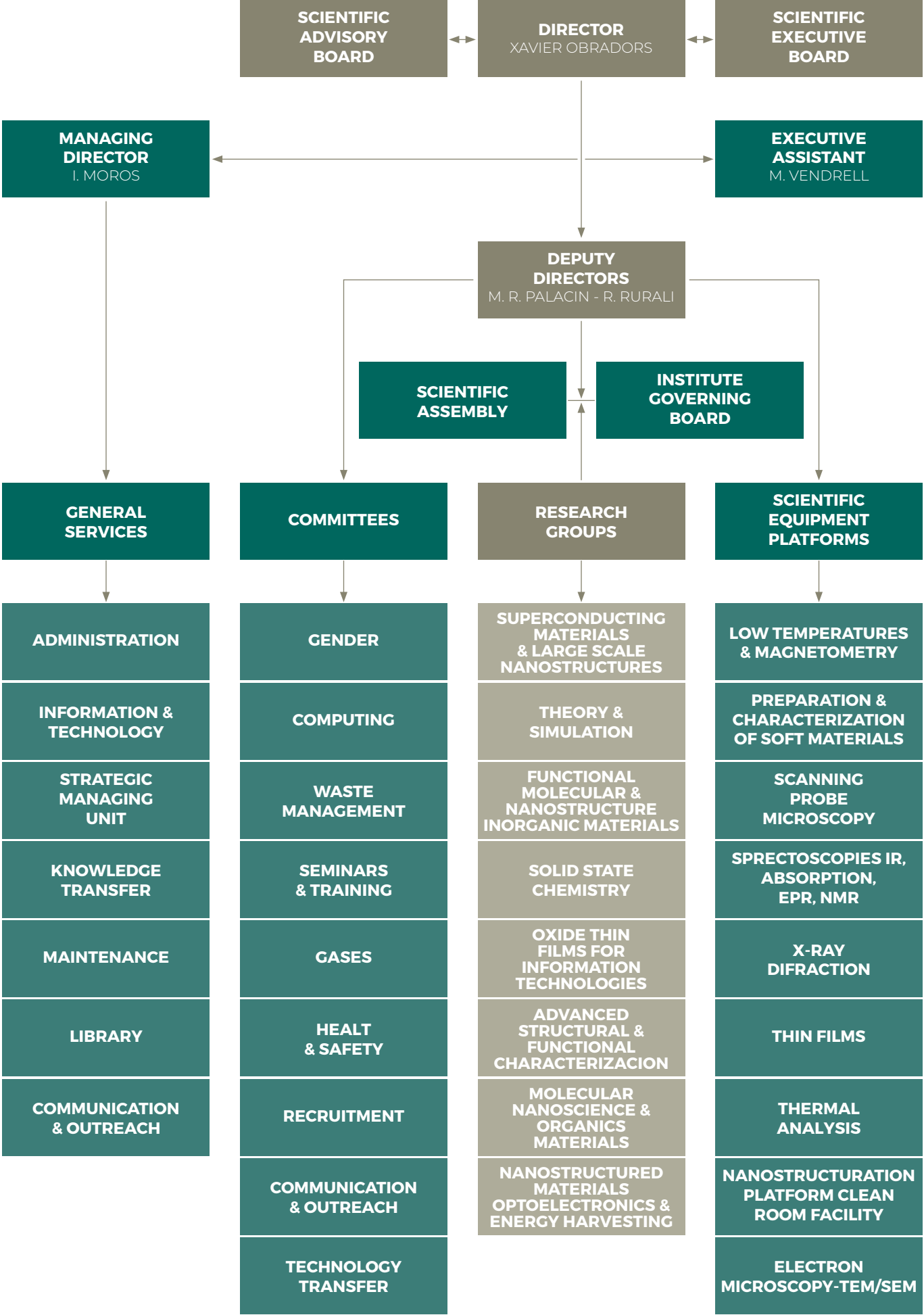
Enjoy the tour!

XAVIER OBRADORS

ICMAB Director



ORGANISATION





GOVERNANCE

DIRECTION TEAM

The ICMAB is led by Director, Xavier Obradors, and the Executive Board, formed by M. Rosa Palacín and Riccardo Rurali (Deputy Directors), and Imma Moros (Managing Director). Marta Vendrell is the Executive Assistant.

SCIENTIFIC ADVISORY BOARD (SAB)

INSTITUTE BOARD

Formed by the Director, the Deputy Directors, the Managing Director, the Heads of the Department, the Staff representatives and the PhD fellows' representative.

SCIENTIFIC EXECUTE BOARD (SEB)

Formed by 10 members, including the Direction team, the Strategic Managing Unit and the Research Lines coordinators: Mariano Campoy-Quiles (RL1), Teresa Puig (RL2), Josep Fontcuberta (RL3), Marta Mas-Torrent (RL4) and Immaculada Ratera (RL5).



SILKE CHRISTIANSEN
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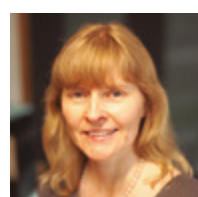
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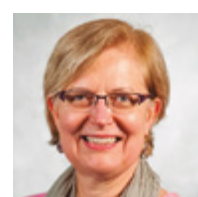
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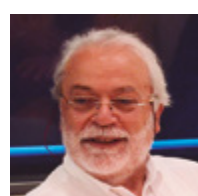
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NATALIE STINGELIN
from the School of Materials Science in Engineering at Georgia Institute of Technology (USA)

ICMAB STAFF

Personnel by categories

TOTAL PERSONNEL

332

59
PERMANENT
RESEARCH
STAFF

58
POSTDOC

97
PHD
RESEARCHERS

41
UNDERGRAD.
& MASTER
STUDENTS

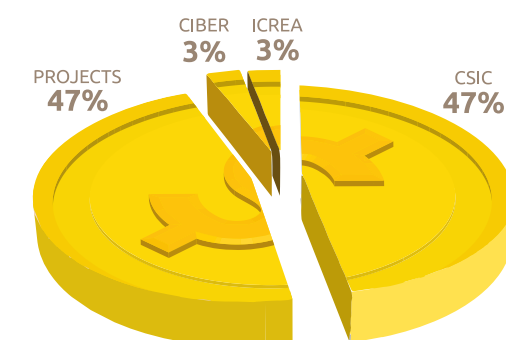
28
TECHNICAL
STAFF

14
SPIN-OFF
STAFF

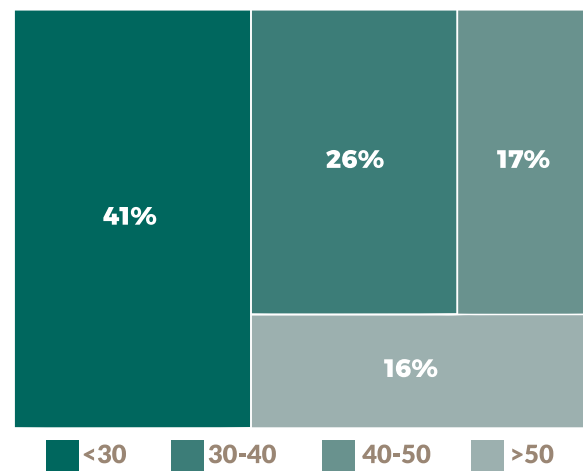
29
ADMIN &
MAINTENANCE

6
VISITORS

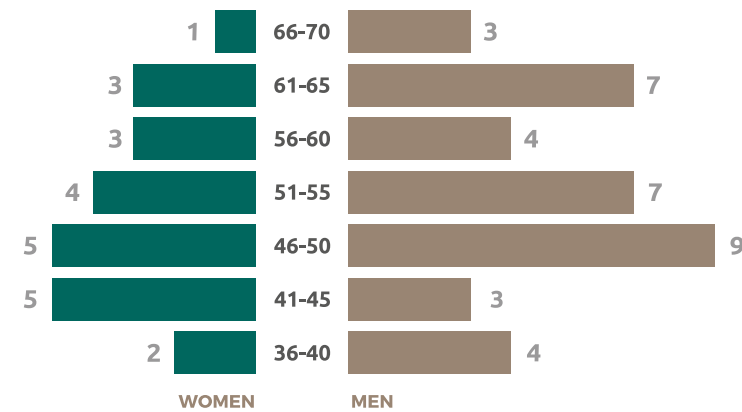
Personnel funded by



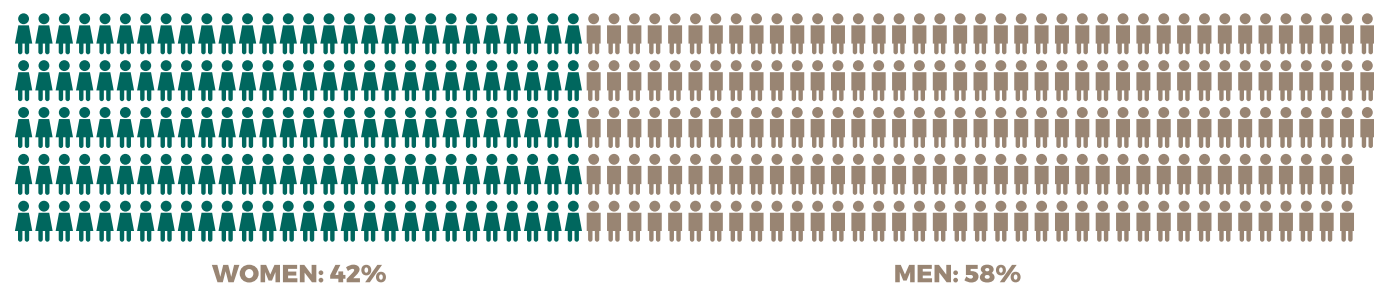
ICMAB Age



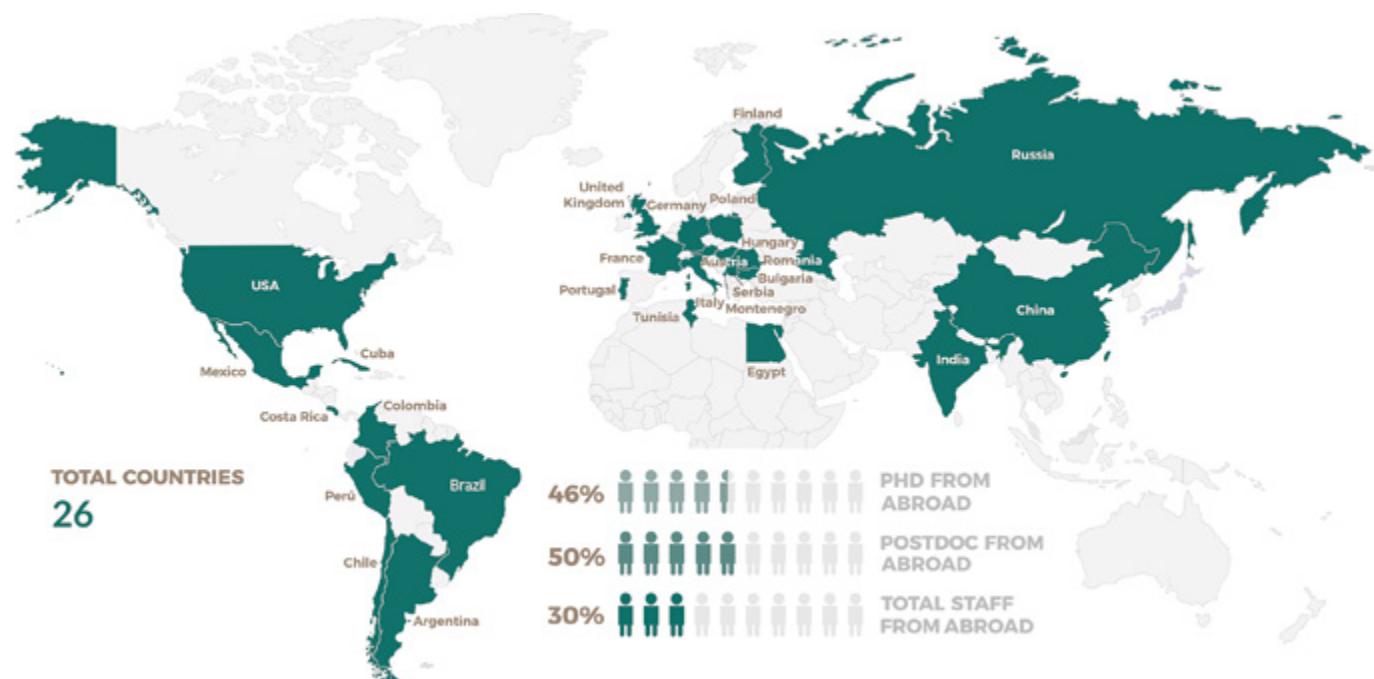
Permanent Researchers Age



Female / Male



Internationality



RESEARCH GROUPS

Research activities are carried out by multidisciplinary research groups, formed by senior scientists, PhD and postdoc researchers. In total, the Institute has 8 research groups, which cover most of the research topics in multifunctional advanced nanomaterials.

ADVANCED STRUCTURAL AND FUNCTIONAL CHARACTERIZATION

Crystallography of Magnetic and Electronic Oxides and Surfaces (CMEOS):

addressed to explore, understand and develop new strongly correlated materials of interest in fundamental condensed matter research and as novel materials for the Information technologies. The activities of the group are based on the application of chemical and magnetic crystallography methods to the investigation of emergent functional oxides. Combining an intensive use of Large Scale Facilities (such as neutron and synchrotron sources) with symmetry analysis methodologies, we investigate the symmetry-properties relationship associated to structural, magnetic or electronic orders in functional oxides (<https://departments.icmab.es/cmeos/>).

Prof. José Luis García-Muñoz

has a wide expertise on strongly correlated functional oxides, their preparation, fabrication and advanced characterization with emphasis on the application of scattering methods. Group leader of CMEOS, its current scientific interests include spin-charge-orbital order phenomena and instabilities in frustrated magnetic and electronic materials, the study at atomic-scale of physico-chemical mechanisms in materials for oxide electronics, and the symmetry phenomena in commensurate and incommensurate novel magnetoelectric multiferroics with strong coupling of the ferroic orders.

Dr. Javier Torrelles has been lately interested in elucidating the structure of the interface between titanium



oxide and water to understand the photocatalysis process. In general, he has a wide expertise on solving the geometric structure of crystals, oxides and thin films, and on determining the electric and magnetic properties of these compounds.

Crystallograph Group: addressed to explore, understand and develop new strongly correlated materials of interest in fundamental science, such as studies of intermolecular interactions, and in the improvement of methods for crystal structure determination from electron diffraction data. The group has developed the new through-the-substrate (tts) X-ray microdiffraction technique, integrated now at ALBA Synchrotron, and has a great expertise in nanocomposite porous materials, applied to different catalysis reactions (<https://departments.icmab.es/crystallography/>).

Prof. Carles Miravittles has always combined his research in crystallography and characterization of materials with multiple responsibilities during his career, such as Director and Founder of ICMAB (1986-2008). He is now Ad honorem Research Professor at ICMAB.

Prof. Elies Molins, PhD in Physics, is interested in how the microscopic structure of materials influences its macroscopic behavior. He is specialist on single crystal X-ray diffraction, Mössbauer spectroscopy and aerogels and related porous materials.

Prof. Jordi Rius Palleiro graduated in Geology and holds a PhD in Natural Sciences from the Philipps-Universität (Marburg). His main research area is Crystallography, more precisely the design and subsequent implementation of X-ray diffraction

phasing algorithms for the non-routine determination of relevant crystal structures in Chemistry and Mineralogy. Currently, he is involved, in collaboration with the ALBA synchrotron, in the development of the synchrotron tts-microdiffraction technique and its application to Materials Science and Cultural Heritage problems.

Dr. Xabier Mikel Turrillas, PhD in physics and Materials Science, is interested in material characterization by X-ray diffraction, to discover the microstructure of the materials and their properties. He is detached at ALBA Synchrotron, in the Experiments Division.

Dr. Monica Benito, PhD in Chemistry, is interested in the synthesis and characterization of aerogels, and their functionalization.

Dr. Ignasi Mata's research interests are Mössbauer spectroscopy and X-ray diffraction on pharmaceutical products, preparation of nanoporous materials for thermal insulation and catalysis, computational chemistry studies of intermolecular interactions in molecular crystals, and synthesis and characterization of co-crystals



FUNCTIONAL MOLECULAR AND NANOSTRUCTURED INORGANIC MATERIALS

Inorganic Materials & Catalysis Laboratory (LMI): the focus of the group's scientific activity is in the chemistry and applications of boron cages. Their geometric forms and the fact that they are made of a semi-metal, boron, give them unique properties largely unexplored. Today, the chemistry of boron clusters, has achieved a sufficient degree of maturity that has led to new applications, in many cases not attainable with conventional organic compounds. For instance boron clusters readily offer structural hollow spheres, something that is utterly difficult with organic compounds. Boron clusters are applied in this group in energy, environmental science, molecular electronics and medicine. At present, the LMI group is formed by four research staff members, three post-doc, eleven PhD candidates and one technician. The group is sustained by Regional, National and EU funding (<https://departments.icmab.es/lmi/>).

Prof. Francesc Teixidor graduated in Chemistry and got the PhD in the same area. He became interested in the boron clusters during his postdoctoral stay. Since then, he has contributed to their development understanding their bonding, developing methods of synthesis

and its applications. His current interests are in the electron transfer of metallacarboranes and their applications in energy and molecular electronics.

Prof. Clara Viñas graduate in Chemistry and in Pharmacy and got the PhD in Pharmacy. Her career has been developed in industry, institutional laboratories involved in food science analysis as well as environmental control and research laboratories. Her interest is in the development of new methods of synthesis and derivatization of boron clusters to be applied in medicine, biosensors, sustainable environment and energy.

Dr. Rosario Núñez, PhD in Chemistry, is interested in the chemistry of boron and silicon, including the design, preparation and characterization of boron cluster derivatives and new materials of interest in biomedicine especially in BNCT for cancer treatment, and electronics.

Dr. José Giner interests are focused on the synthesis, characterization and application of inorganic (boron based) and inorganic-organic hybrid solids. His focus for several years have been on the development of new carborane-based ligands or linkers for preparing a variety of molecular, supramolecular and polymeric materials. His areas of interest are new

concepts in Metal-Organic Framework (MOF) Chemistry, multifunctional molecular materials and crystal engineering.

Nanoparticles and Nanocomposites Group (NN):

this group has quite diverse research interests but with a focus in the rational synthesis of nanoparticles and nanocomposites and the study of their structural-functional properties including those related to the nano/bio interfaces. At present, the interdisciplinary NN team is formed by three principal investigators, two post-docs and eight PhD candidates that have secured competitive grants. NN has a running portfolio of seven projects. We envisage the integration of our materials in devices and products for nanomedicine, information technologies or energy and environment. The NN members participate actively of science outreach and gender equality initiatives. (<https://departments.icmab.es/nn/>, @NNgroupICMAB).

Prof. Anna Roig, graduated in Physics with a PhD in Materials Science. She is currently involved in two main research lines: i) nanoparticle synthesis and their validation for medical applications as drug delivery vehicles, contrast agents or in cell therapies and ii) bacterial cellulose-based materials.

Dr. Martí Gich, is a materials scientist with a background in industrial R&D. His current activities are focused in i) understanding functional properties in oxides and their applications in information technologies, ii) preparing nanostructured materials by soft chemistry and iii) integrating thin films on technological substrates by physical and chemical methods.

Dr. Anna Laromaine holds a Chemistry PhD and her scientific work encompasses chemistry, materials science and biology. She currently focuses in the production of bacterial cellulose and their composites for bio-applications and the evaluation of materials using approaches such as cell cultures and the nematode *C. elegans*.

Functional Nanomaterials and Surfaces (FunNanoSurf):

the group interests relate to the fields of nanoscience and nanotechnology, particularly the areas of molecular electronics, molecular magnetism and biology. We design molecular systems capable of providing inputs at the nano-scale and focus our efforts in the control and organization of such species on different surfaces/nanodevices. The main areas of expertise are (i) synthesis of functional molecules/polymers & supramolecular aggregates, (ii) characterization of our molecular-based materials and (iii) surface studies (<https://departments.icmab.es/funnanosurf/>).

Dr. Núria Aliaga-Alcalde's work focuses on the relevance and necessity of molecular design in nanoscience, where functional molecules play a key role since they provide homogeneous tunable nanometer-size units and properties ready to be exploited (as reliable sensors, switches, quantum computing materials or molecular electronics). Toward this main idea, key factors are the design of specific molecules (CCMoids, porphyrins and diketone systems) and their control and organization on surfaces/nanodevices where their properties can be tuned. So far, the results accomplished have shown the advantages of these systems as biomarkers (luminescent properties), molecular transistors (gateable molecular junctions) and as single-molecule magnets (SMMs).

Dr. Arántzazu González-Campo interests focus on the preparation of multifunctional responsive materials for biomedical and energy applications using supramolecular and surface chemistry. With this aim, she is currently involved in three different projects: i) the development of (bio) chemical functionalization of surfaces; ii) development of supramolecular-based responsive polymers and MOFs and ii) development of biocompatible sensors o biosensors.



MOLECULAR NANOSCIENCE AND ORGANIC MATERIALS (NANOMOL)

NANOMOL is a research group composed by several labs with wide expertise and recognized excellence in the synthesis, processing and study of molecular and polymeric materials with chemical, electronic, magnetic and biomedical properties. We continuously generate new knowledge in our basic and applied research projects regarding the micro and nano structuring of molecular materials. We offer this knowledge to improve the properties of products manufactured in diverse sectors, such as chemicals, pharmaceuticals and electronics, thereby contributing to increasing their added value (<https://projects.icmab.es/nanomol/>, @NanomolGroup).

Prof. Jaume Veciana and **Prof. Concepció Rovira** are the group leaders of NANOMOL.

Prof. Jaume Veciana has a long expertise in the design, synthesis, and processing of functional ((poly) radicals, electroactive, redox, bioactive, etc.) organic molecules/polymers as advanced functional molecular materials and their applications in molecular electronics

and spintronics and in molecular nanomedicina.

Prof. Concepció Rovira's interests are focused on the design, synthesis, and processing of functional organic molecules as advanced molecular materials and their applications in Molecular Electronics such as unimolecular electronics and spintronics and sensors based on conducting nanocomposite thin-films.

NANOMOL consists of four different labs devoted to a variety of research topics:

The research activities of **Dr. Nora Ventosa's** Lab are focused on the study and application of molecular soft materials for drug delivery and bioimaging. Green procedures using compressed fluids are developed to facilitate the scale-up of nanomedicines and reaching clinical testing.

Dr. Jose Vidal-Gancedo's Lab interests are focused in the design, synthesis and characterization of organic radicals and their application to study the radical behavior in different types of molecules,



macromolecules or materials based on them mainly focused on biological applications.

Dr. Imma Ratera's Lab interests are focused on the design and synthesis of novel multifunctional organic electroactive and radical molecules and their molecular and supramolecular chemistry. The group is interested in the properties of these molecules once nanostructured as self-assembled monolayer, organic nanoparticle or hydrogels towards applications in different fields such as molecular

electronics and biology. **Dr. Judith Guasch** is in this team.

Dr. Marta Mas-Torrent's Lab is focused on the design and synthesis/preparation of new functional molecular materials for their application in organic/molecular electronic devices. Our work ranges from fundamental studies in order to better understand materials properties to a more applied perspective aiming at developing proof-of-principle devices. Dr. Núria Crivillers is in this team (@MMTgroupICMAB).



MAGNETIC MATERIALS AND FUNCTIONAL OXIDES

Laboratory of Multifunctional Thin Films And Complex Structures (MULFOX): research group focused on the development and integration of new materials, basically nanometric oxide thin films, and the exploration of their use in photovoltaics, electronics, spintronics, data storage and computing. These broad and scientifically challenging objectives are currently major social demands, as silicon-based electronics is reaching its limit in size, speed and efficiency, and radically new approaches, energy sustainable, are needed. Specifically, current activities include i) the search for disruptive approaches to materials and methods in photovoltaic conversion, ii) development of materials and devices that, based on polar materials, may allow us to contribute to develop more efficient data storage and brain-inspired computing schemes and iii) explore data storage and data manipulation alternatives to current methods, by using non-dissipative currents or efficient plasmonic signals (<https://departments.icmab.es/mulfox/>).

Prof. Josep Fontcuberta, group leader, has an extensive expertise on functional oxide thin films and focuses his activities on exploiting their properties: magnetic, ferroelectric, electric, and optical properties. He is persuaded that oxides may play a very important role in future high-tech devices. Examples of ongoing projects include: ferroelectric materials for data storage and neuromorphic computing, oxide-based spintronic materials and devices, novel approaches to photoconversion and affordable and sustainable transparent conductors.

Dr. Lourdes Fàbrega research is focused on the development of cryogenic detectors made of superconductors, for applications in Space, materials analysis and quantum information. Her work involves design and fabrication of the devices, with special emphasis on the underlying physics of the superconducting state.

Dr. Florencio Sánchez holds a PhD in Physics and his research activities pivot around the development of



functional oxides thin films, mainly ferroelectric, with emphasis in their epitaxial growth and incorporation into complex heterostructures. Currently he has interest in the integration of functional oxides with silicon, and particularly in the epitaxial stabilization of ferroelectric hafnium oxide.

Dr. Gervasi Herranz's research is focused on functional oxide interfaces and photonics, especially in exploiting the optical properties of functional oxide interfaces, apart from their magnetic and transport properties. The celebrated phrase "the interface is the device" describes his research activity, which aims at uncovering new physical phenomena at the boundary of materials, for new concepts and applications.

Dr. Ferran Macià holds a PhD in Physics and has a background in mathematics and telecommunication engineering. His work and interests are magnetism and spin-dependence electron transport (spintronics) in mesoscopic systems. He believes science and technology must connect with

society so he collaborates with companies, teaches at universities and schools, and participates in social and cooperation projects.

Dr. Ignasi Fina is focused on new materials for electronic applications, with two main research lines: the study of magnetoelectric coupling in antiferromagnetic materials and the study of ferroelectric materials for photovoltaic and neuromorphic computing applications.



Advanced Characterisation and Nanostructured Materials (ACNM):

the group's main scientific goal is to generate both fundamental and applied knowledge for the implementation of functional oxide materials in novel technologies as spintronics. It focuses on functional properties, structural characterization of functional defects, nanodevices, complex oxide thin films, self-assembled materials and nanoparticles for life sciences (<https://departments.icmab.es/acnm/>, @Alcmab).

Prof. Benjamín Martínez, group leader, is an experimental physicist with broad interest in magnetism and magnetic materials. His current research interest is focused on the study of spin dependent phenomena in functional oxides covering both the preparation and characterization of complex oxide thin films and heterostructures and the analysis of their magnetotransport properties to foresee potential applications for new spintronic devices.

Dr. Lluís Balcells interests are focused on magnetic materials,

including thin films and nanoparticles, for applications in electronics and spintronics.

Dr. Felip Sandiumenge scientific interest is focused on the correlation between structure and function in oxide epitaxial films, with emphasis on the atomic structure and defect chemistry of crystalline defects such as dislocations and domain walls.

Dr. Carlos Frontera has a long experience in the structural characterization of materials using diffraction techniques (X-ray and neutrons). He has applied these techniques to a wide variety of systems in bulk, nanoparticles and thin films form.

Dr. Alberto Pomar has a PhD in Condensed Matter Physics. He is an experimental researcher with a core expertise in the electronic and magnetic properties of perovskite-based complex oxides. He is devoted to the development and understanding of new routes to nanostructuration and their implications in the final functional properties of the oxide thin films and heterostructures.



NANOSTRUCTURED MATERIALS FOR OPTOELECTRONICS AND ENERGY HARVESTING

Group of Physical Chemistry of Surfaces and Interfaces

(SURFACES): focused on unraveling and controlling the nanoscale structural and electronic properties of nanostructures and interfaces through surface engineering. Devoting special effort to organic materials, part of our investigation centers on organic semiconductors with relevance as active layers for electronic devices (such as organic solar cells and organic field effect transistors). Our research spans from fundamental issues in organic growth to the electronic response of metal-organic junctions within two main research activities: i) Design and growth of ultrathin organic layers and organic/organic heterojunctions and ii) Nanoscale properties of organic/electrode interfaces and devices (<https://departments.icmab.es/surfaces/>).

Prof. Carmen Ocal's main research field of interest is surface science: crystallography, growth, chemical functionalization as well as characterization including atomic

structure, mechanical and frictional (nanotribology) and electronic properties at the nanoscale. Her group has been always involved in developing strategies using Scanning Probe Microscopies in combination with diffraction and spectroscopic techniques.

Dr. Esther Barrena's research uncovers the structure-property relationships of organic semiconductors. Her research addresses fundamental interface properties at molecular-scale as well as the nanoscale characterization of organic films in devices (such as organic-field transistors and photovoltaics). Her expertise includes real-time x-ray diffraction, organic growth, self-assembly and scanning probe microscopies.

Dr. Albert Verdaguer's research is focused on the interaction of water with surfaces. The interest of the research includes studies of wetting at the nanoscale and the study and design of surfaces to control ice nucleation. He has been involved in the developing of new strategies in Scanning Probe Microscopies



to study the solid/liquid interface and more recently in chemical recognition modes.

Nanostructures materials for optoelectronics and energy harvesting (NANOPTO):

the group focuses on producing and characterizing advanced semiconducting structures with the main objective of understanding their fundamental behavior in order to tailor and improve their functionalities and empower different applications in the areas of optoelectronics, energy-related, and sensing devices. The group is divided into 4 different research activities: i) Optoelectronics of group-IV semiconductor nanostructures; ii) Organic-Inorganic Thermoelectrics; iii) Photonic Architectures for Light Management and iv) Organic Solar Cells (<https://departments.icmab.es/nanopto/>).

Dr. M. Isabel Alonso is senior scientist and department head. She is a materials physicist interested in semiconducting structures

(inorganic, organic, and hybrid) that can contribute to expand the development of modern optoelectronic, energy-related, and sensing devices. Her core expertise is the MBE growth of SiGe structures and the use of optical spectroscopy, mainly ellipsometry, Raman scattering, and photoluminescence.

Dr. Mariano Campoy-Quiles is PhD in experimental physics from the Imperial College London and currently tenured scientist at ICMAB-CSIC. His group aims at producing breakthrough scientific advances that strongly contribute to the development of clean energy technologies based on organic and hybrid materials, including photovoltaics and thermoelectrics.

Dr. Alejandro R. Goñi is ICREA Research Professor. He is an experimental physicist with broad interests and expertise in solid-state physics, optical spectroscopy (Raman scattering, photoluminescence, etc.), nano-science and technology, thermoelectricity, low-dimensional materials (quantum wells, wires and dots), and highly correlated electron

systems. He leads the group activities in high-pressure research and the physics of novel hybrid organic/inorganic perovskites.

Dr. Miquel Garriga is research scientist. His main research is in spectroscopic ellipsometry of anisotropic and multilayered materials, optical characterization of bulk semiconductors, organic and inorganic semiconductor heterostructures and high critical temperature superconductors.

Dr. Agustín Mihi is an expert in large area and low cost photonic crystal and plasmonic structures via unconventional nanofabrication techniques. His research group investigates the design, fabrication and characterization of photonic architectures that enhance light-matter interaction applied to emerging optoelectronic devices.

Dr. Sebastián Reparaz is a tenured track researcher with a strong background in nanoscale thermal transport and optical spectroscopy. His research focuses on studying the thermal properties of inorganic/organic nanostructures through advanced characterization techniques. In recent years he focused in developing novel thermal experimental methodologies based on contactless optical techniques.

Laser Processing Group (LPR):

The strategic research lines of the LPR group are focused on the manufacture of improved functional nanomaterials through innovative laser techniques, to be applied mainly in the fields of energy (batteries, supercapacitors, generation of H₂) and environment (photocatalysis). The current areas of work are (i) Laser surface processing

and (ii) Deposition and growth by MAPLE and LDW techniques, for fabricating supercapacitor electrodes and photocatalysts based on hybrid nanocomposites constituted by carbon nanotubes, reduced graphene oxide and transition metal oxides nanostructures. The scientific and technical objectives in the medium / long term are oriented towards innovation in laser techniques for obtaining new materials with improved performance, as well as the implementation of these technologies in next generation devices and industrial processes (<http://icmab.es/laserprocessing>).

Dr. Angel Perez del Pino and **Dr. Enikő György** are the managers of the group. They are specialists in i) Processing of functional nanomaterials by the laser techniques: pulsed laser deposition (PLD), surface processing, matrix assisted pulsed laser evaporation (MAPLE) and laser direct writing (LDW); ii) Study of laser-matter interactions, and iii) Advanced characterization of nanomaterials.



SOLID STATE CHEMISTRY

The research interests of the **Solid State Chemistry group** are centered in the areas of battery materials, inorganic and carbon nanomaterials, hybrid materials, biomaterials and nitride-based materials. The design of new inorganic phases, basing on crystal chemical criteria, mixed-valence character and their modification by chemical / electrochemical doping –cationic or anionic- and by changing the size and microstructure, are among our major objectives. The development of new synthetic methodologies, specific for each targeted phase, is also a defining feature of the group. The investigated materials include high power/high capacity electrodes for rechargeable batteries, electroactive materials for neural growth, drug delivery systems, inorganic nanowires, carbon nanotubes, luminescent and electronic materials and catalysts (<https://departments.icmab.es/ssc/>).

Prof. Nieves Casañ-Pastor

research focuses on intercalation reactions on mixed valence metal

oxides conducting polymers, and nanostructured carbon hybrids. Room temperature electrochemical intercalation and deposition yield new materials and properties. A special focus on new large charge capacity biocompatible electrodes for electrostimulation and tissue repair.

Prof. Concha Domingo is an expert in the use of supercritical CO₂ technology for materials processing. Her current research focuses on the construction of graphene oxide aerogels with multiple applications ranging from CO₂ capture to batteries.

Prof. Amparo Fuertes research interests focus on the design of new metal oxynitrides and nitrides as electronic materials, phosphors or photocatalysts. This is performed through the development of synthetic approaches and the understanding of correlations between chemical composition, bonding, crystal structure, anion order and physical properties.

Dr. Ana M. López-Periago research involves the design and synthesis



of metal-organic frameworks using supercritical CO₂, with applications in the area of gas separation and sustained drug release.

Prof. M. Rosa Palacín is an expert in battery materials research, involving both fundamental studies on synthesis-structure-property relationships and also more technological aspects. Her activity has covered both commercial technologies such as nickel and lithium based and also innovative chemistries such as sodium or multivalent systems.

Dr. Alexandre Ponrouch scientific achievements stem from his solid background in electrochemistry and practical expertise in energy storage research (fuel cells, supercapacitors and batteries). His work is now mainly focusing on rechargeable post lithium batteries including electrolyte formulation and interfacial processes.

Dr. Gerard Tobias main research interests focus on the development of nanomaterials for oncology applications. The targeted nanomaterials should allow not only ultrasensitive biomedical imaging,

to achieve an early diagnosis of the disease, but also a localized treatment of cancer.

Dr. Dino Tonti is an expert on the preparation of thin films, nanoparticles, templated and porous materials for energy applications, in particular rechargeable batteries. His current activity is oriented to the understanding of the basic electrochemical processes and the improvement of the reversibility of metal-air batteries.



SUPERCONDUCTING MATERIALS AND LARGE SCALE NANOSTRUCTURES (SUMAN)

The **SUMAN** Research Group has a wide expertise in the preparation and advanced characterization of nanostructured materials, mainly thin films of oxides. We have a core activity in high temperature superconducting (HTS) materials, particularly the cuprates, prepared with the thin film and coated conductor architectures and as nanocomposites. We continuously generate new approaches to process these materials with enhanced performances using chemical solution deposition (CSD) methodologies for low cost conductors. The correlation between physical properties and micro/nano structure is a distinguishing element of our research, evaluated by magnetic and transport properties at high magnetic fields and low temperatures and advanced TEM characterization. Power and electronic applications of HTS is a topic of general interest of the SUMAN group. More recently, other functional properties of thin film complex oxides have become also a relevant topic in the group, including oxides with metal – insulator transitions as elements for oxide electronics and ferroelectric oxide for photovoltaics. SUMAN is composed at present of 9 senior scientists having

complementary profiles (<https://departments.icmab.es/suman/>).

Prof. Teresa Puig, group leader, is an expert in superconducting materials, involving fundamental understanding, preparation and micro/nano structure-property relationships of cuprates. Her main activity focuses on film and nanocomposites growth by chemical solution deposition for high current conductors and applications. Scientific interest also extends to other functional properties of complex oxides.

Prof. Xavier Obradors scientific interests include materials preparation, particularly complex oxides, with controlled micro/nano structures and the comprehension of the physical mechanisms underlying their superconducting, magnetic and electronic properties. The development of high critical current conductors and their applications is one of the main focuses at present.

Dr. Narcís Mestres research focuses on understanding the growth mechanisms and functional properties of new complex oxides nanostructures, thin films and nanocomposites synthesized from chemical solutions, with potential impact in electronics, energy saving



and environmental science.

Dr. Xavier Granados contributes to the development of the new HTS engineering power devices, modelling, construction and testing, as well as instrumentation development for experimental research. He participates in Platforms as Futurred, GIA and EERA for energy storage, and Eurofusion.

Dr. Susagna Ricart scientific interests include study of chemical and thermal behavior of metalorganic salts in non-aqueous solutions for the CSD approach to superconducting layers. She is particularly expert on synthesis and characterization of nanoparticles, mainly of complex oxide and rare earth fluorides for further applications in the CSD nanocomposite ceramics, biochemistry and catalysis.

Dr. Anna Palau scientific interests are mainly focused on the study of the outstanding physical properties functional oxides and in particular vortex matter physics in high temperature superconductors. She has devoted much effort in the opportunities that hybrid superconductor/ferromagnetic structures and advanced nanofabrication technologies can bring to energy efficient electronic devices.

Dr. Mariona Coll scientific interests focus on the processing of functional oxide thin films and heterostructures by cost-effective chemical methods to give rise to novel and enhanced functionalities for energy applications ranging from photovoltaics to superconductivity. She is interested on the relevance of nanometer scale control of materials composition and structure on the device performance.

Dr. Jaume Gázquez research concentrates on establishing relations between the structure, chemistry and physical properties of transition-metal oxide nanostructures. In particular, he is interested in the role of reduced dimensionality at interfaces, and defects by sub-Angstrom resolution, and chemical mapping at atomic level with aberration corrected scanning transmission electron microscopy (STEM- EELS).

Dr. Joffre Gutiérrez expertise is in the field of vortex matter and dynamics in high and low temperature superconductors. In particular, the interactions between microstructure and vortices and how they affect the macroscopic response of superconductors. One of the main focuses is the application of high temperature superconductors to new technologies.



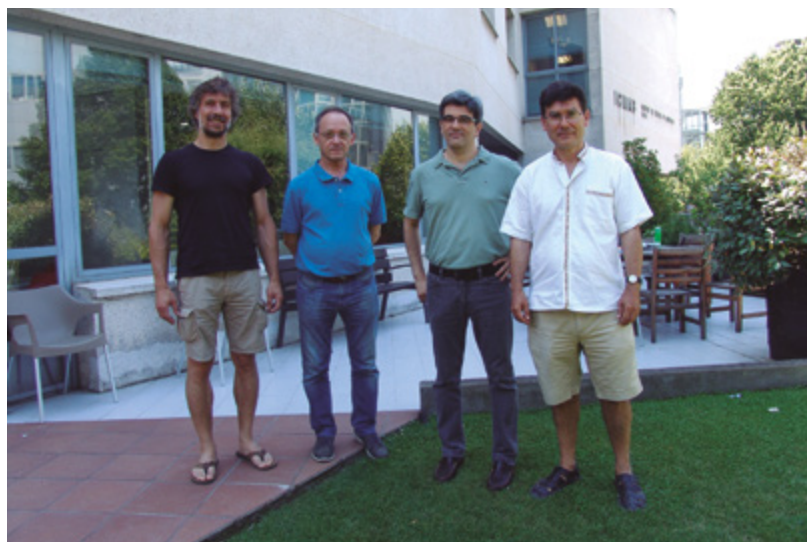
THEORY AND SIMULATION

The strategic lines of the **Theory and Simulation Group** are the simulation of soft-matter, novel functionalities in oxide-based systems, flexoelectricity, thermal transport, electronic and vibrational instabilities in low-dimensional systems and the development and applications of ab-initio simulation codes (<https://departments.icmab.es/mst/>).

Prof. Enric Canadell is mostly interested in the development of ideas to relate the structure and properties of solids and more especially low-dimensional conductors, in which field he developed the hidden nesting concept and the idea of two-band molecular conductors. More recently he has also been interested on the analysis of results of new tunneling techniques concerning two-gap superconductors, hybrid solids containing both molecular conductors and molecular rotors, charge ordering transitions in both extended and molecular solids, low temperature magnetoresistance oscillations in molecular metals,

single-component conductors, etc. **Dr. Riccardo Rurali** has become an expert on the theoretical study of impurities, ballistic electronic transport, and nanoscale thermal transport. He has an outstanding reputation in the field of semiconductor nanowires by which he is often contacted by leading international groups to carry out theoretical calculations to help understand their experimental results.

Dr. Massimiliano Stengel's research focuses on the development of frontier electronic-structure methods, and their application at tackling key fundamental and technological questions in ferroelectricity, magnetism, surface science and metal/oxide interfaces. In the past few years he has been particularly interested in perovskite thin films, and in particular in understanding how the reduced size affects their functional properties. Currently, his main thrust lies in the study of novel functionalities in oxide-based systems and in development of accurate modeling strategies



to bridge the gap between the microscopic and macroscopic worlds.

Dr. Alberto García is the director of the "Theory and Simulation" department. He is a member of the development group of the SIESTA program and one of his most active contributors. He has a wide experience in the development of ab-initio simulation methods and their applications in physics, materials science, and geophysics and has participated in international initiatives in scientific data management and computational frameworks (including GRID computing and XML formats and tools).

Dr. Jordi Faraudo's research focuses on the theory of soft matter, including systems as diverse as magnetic fluids, vesicles, membranes, nanochannels, thermoresponsive polymers and many others. He develops novel simulation techniques (for example, "on the fly" coarse-graining techniques for the simulation of self-assembly) to bridge the gap between the atomistic, nano, micro and macroscopic worlds. He also applies theoretical methods

to problems of particular interest for their experimental relevance in which an atomistic/molecular understanding is lacking.



SCIENTIFIC EQUIPMENT PLATFORMS

Research is supported by the Scientific Equipment Platforms that provide shared access to specialized and cross cutting equipment, services and expertise for the advanced technological preparation and characterization for all kinds of materials at different levels. It is made up of eleven technical facilities run by specialized technicians. These are open to external uses either from academia and industry, with conditions tailored to meet customer technology demands. The Scientific Coordinator of the Services is Prof. M. Rosa Palacín, also Deputy Director of the Institute.

X-ray diffraction lab

Technicians: Anna Crespi, Joan B. Esquiú and Javier Campos.
Scientist in charge: Jordi Rius.

Thermal Analysis Laboratory

Technicians: Roberta Ceravola (thermal analysis) and Julio Fraile (BET equipment).

Scientists in charge: Amparo Fuertes and Concepció Rovira.

Molecular Beam Epitaxy

Run by the scientist Isabel Alonso.

Spectroscopic Techniques Laboratory

Technicians: Vega Lloveras and Jaume Capell.

Scientists in charge: Rosario Núñez and José Vidal.

Thin Films

Technician: Raul Solanas.

Scientist in charge: Florencio Sánchez.

Electron microscopy service

Technicians: Judith Oró (TEM) and Anna Esther Carrillo.

Scientist in charge: Lluís Balcells.

Nanoquim Platform

Technicians: Neus Romà, Luigi Morrone, and Marta Riba.

Scientist in charge: Teresa Puig.

Preparation and Characterization of Soft Materials (SoftLab)

Technicians: Amable Bernabé, David Piña and Iván Martínez.

Scientist in charge: Nora Ventosa.

Low Temperatures and Magnetometry Service

Technician: Bernat Bozzo.

Scientist in charge: Benjamín Martínez.

Scanning Probe Microscopy (SPM)

Technicians: Maite Simón and Andrés Gómez.

Scientist in charge: Martí Gich.

Biomaterials and Cell Growth Laboratory (ICN2/ICMAB) (under construction)

Technician: Mario Juárez.

Scientist in charge: Imma Ratera and Anna Roig (ICMAB) and José Antonio Garrido (ICN2).



GENERAL SERVICES

Strategic Managing Unit

Jorge Pérez – Project Manager
Montse Salas – Project Manager

Knowledge Transfer Unit

Susana Garelik
Guillermo de Andrés

Communication & Outreach

Anna May Masnou

Administration

Immaculada Moros – General Manager
Patricia Moragues – Competitive Funding
José Ángel Burriel – Competitive Funding
María Rivera – Accounting
Rebeca Herrera – Accounting
M^a del Mar Astillero – Accounting
Antonio Miguel Socías – Accounting
Maribel Contreras – Accounting
Anna Fernández – Accounting
Joan Renau – Finance
Pietat Sierra Vela – Human Resources
Sonia Roldán – Human Resources

Information Technology

Joan Figuerola – Head of IT Service
Javier Rubio – Systems and Users Support
Ángel Elbaz – IT Support Staff
Albert Moreno – IT Support Staff
José Antonio Gómez – Webmaster

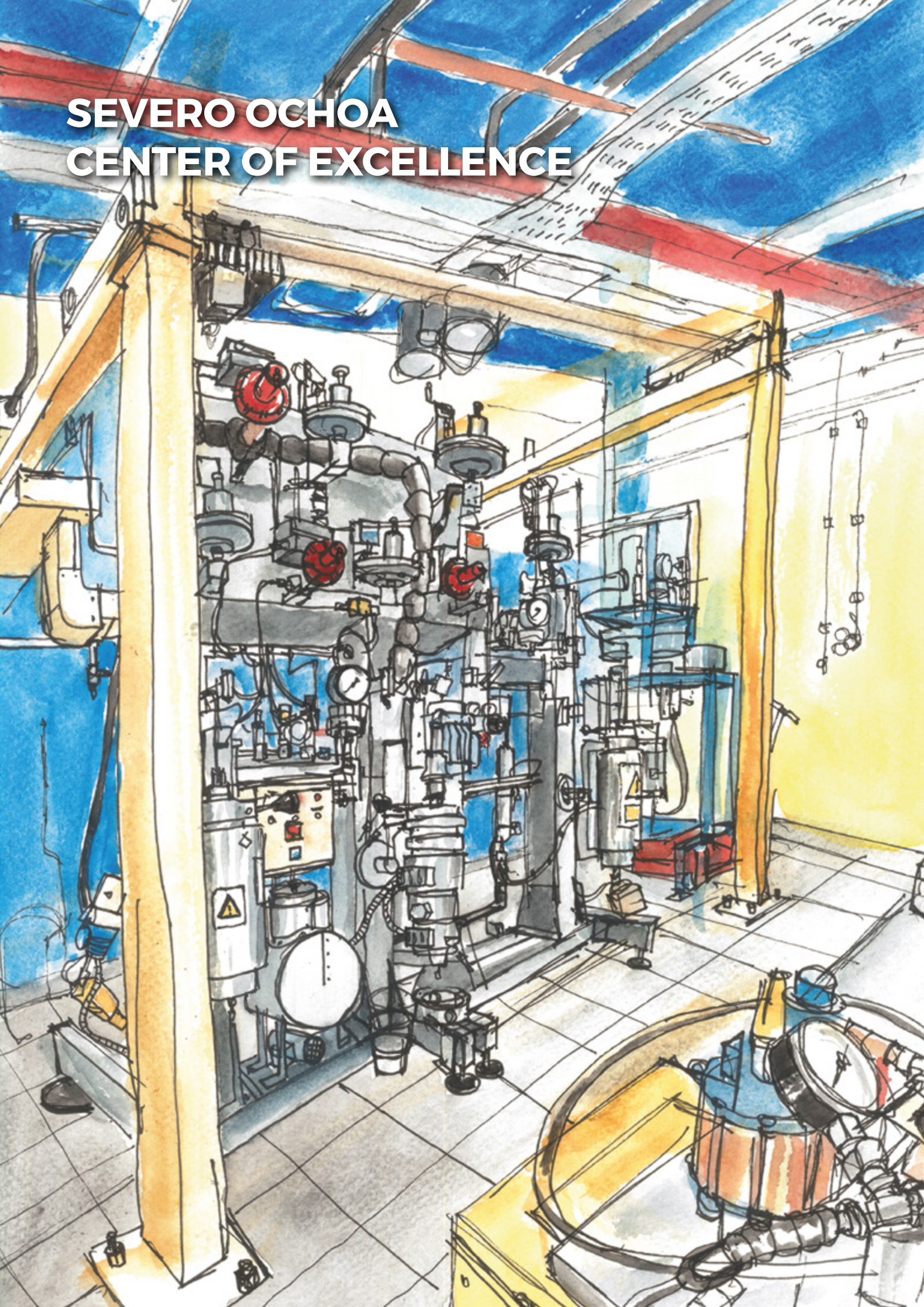
Library and Documentation

Alejandro Santos Botana

Maintenance

Toni Pons – Head of Maintenance
Oriol Sabater – Maintenance Support Staff
José Manuel Rodríguez – Maintenance Support Staff
José Ángel Algar – Maintenance Support Staff
Roberto Ibáñez – Maintenance Support Staff
Juan José Monis: Maintenance support staff

SEVERO OCHOA CENTER OF EXCELLENCE



CONSOLIDATION OF THE SEVERO OCHOA RESEARCH PROJECT 2016-2019: SMART FUNCTIONAL MATERIALS FOR SOCIAL GRAND CHALLENGES (FUNMAT)

The ICMAB became a Severo Ochoa Centre of Excellence in 2016, becoming one of the top research centers in Spain in Materials Science. The associated research programme brings together the institute's eight research groups in five priority research lines:

- RL1:** Sustainable energy conversion and storage systems
- RL2:** Superconductors for power applications
- RL3:** Oxide electronics
- RL4:** Molecular electronics
- RL5:** Multifunctional nanostructured biomaterials

These 5 RL are integrated into the three social grand challenges of the 21st Century, aligned with the main European Social Challenges in H2020:

- 1. CLEAN AND SECURE ENERGY**
- 2. SUSTAINABLE AND LOW COST ELECTRONICS**
- 3. SMART NANOMEDICINE**

The general objectives of the FUNMAT Severo Ochoa project are:

- Achieving a high scientific and technological impact.
- Strengthening the international ICMAB leadership in the functional materials area.
- Enhancing the fundraising capabilities of the ICMAB.
- Enhancing the activities related to outreach and the exploitation of research outcomes.
- Improving the training and recruiting activities of ICMAB to attract the best talent.
- Implementing a specific Gender Action Plan aimed to promote gender equality.





APPLICATION AREAS

CLEAN AND SECURE ENERGY

The Energy sector is facing a new worldwide paradigm with 20 % renewables and 20 % decrease of greenhouse emission for 2020. This requires new ways of producing, storing, transporting and stabilizing electricity. The ICMAB undertakes this challenge reinforcing our expertise in smart functional materials research and strategically developing cost-effective upscalable technologies, from materials choice all along the value chain process to proof-of-concept devices. Our roadmap promotes greener and cost-effective technologies strengthening materials growth from chemical methods and highlighting additive manufacturing technologies for large area materials at high performance/low cost.

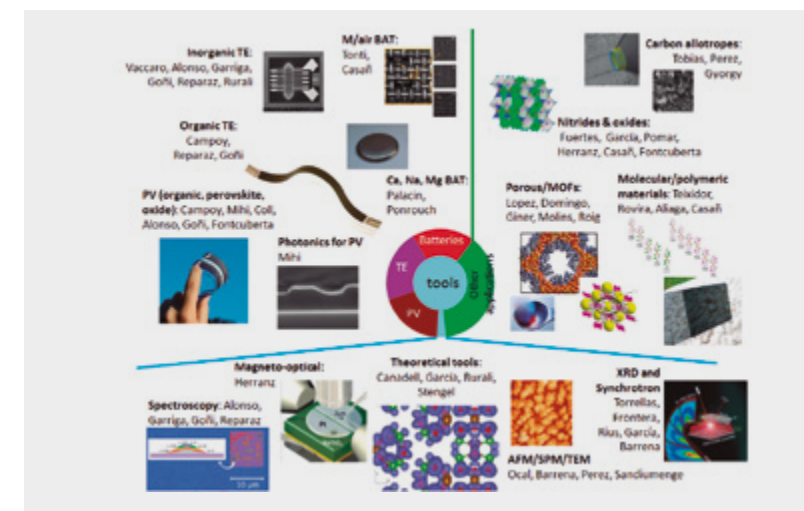
SMART AND SUSTAINABLE ELECTRONICS

Current needs in big-data handling are demanding new solutions for the dramatic energy consumption of current computing and data storage devices. Power dissipation and miniaturization are fundamental challenges for nanoelectronic circuits. We envisage sustainable and energy-efficiency approaches to electronics by working along two fronts: exploiting dissipation-less storage and information control by electric

fields and involving spin-only currents, rather than charge transport. The use of organic materials/molecules in devices will also provide important guidance towards a new-generation of memories. Great perspectives are expected for the development of devices exploiting the charge as well as the spin of the molecules.

SMART NANOMEDICINE

Academia and the innovative industry have directed its interests towards nanomedicine, whose technological breakthrough potentiality is widely acknowledged. It is envisaged that the unique properties of nanomaterials will make a strong impact contributing to solve some of the challenges of Health and Societal Wellbeing. FUNMAT will contribute to Nanomedicine, through improvement of drugs and medicines making them more selective, less toxic, and more efficient. It will also contribute to the advance of medical diagnosis by developing new contrast agents for medical imaging techniques. Further, the use of advanced materials and nanotechnology concepts in synergy with molecular biology will allow the generation of new tools for tissue engineering meaning a giant step for regenerative medicine.



MAIN HIGHLIGHTS AND ACTIVITIES OF RL1 AND RL3

IN 2017, THE SCIENTIFIC ADVISORY BOARD EVALUATED TWO OF THE FIVE RESEARCH LINES:

RL1: Sustainable energy conversion and storage systems

2017 MAIN HIGHLIGHTS

Photovoltaics: To enhance the energy conversion efficiency from light to electricity of organic photovoltaics (OPV) towards the 20 % goal, an ultrafast platform for the screening of the large library of organic materials has been developed within the ERC-FOREMAT, by coupling combinatorial samples with advanced spectroscopy. This fabrication platform can also be used to manufacture miniaturized spectrometers and polarization detectors. The full value chain in OPV will be further investigated in the H2020 ITN project SEPOMO. Moreover, the development of new scanning force tools that help to draw molecular-scale portraits of organic domains has also been achieved. Besides organics, other materials are being investigated for PV applications, including perovskites, boron-based, oxides, as well as nanostructured inorganics and

hybrid systems. A transversal strategy for enhancing light harvesting in thin film PV is the use of photonic structures, which are also been fabricated through low cost up-scalable soft lithography techniques (ERC-ENLIGHTMENT).

Thermoelectrics: Organic materials have low thermal conductivities and high Seebeck coefficients. To allow the increasing amount of doping needed to enhance the electrical conductivity and simultaneously preventing mechanical failure, we have introduced the ternary blend concept, in which a commodity polymer acts as binder and thus enables truly bendable thermoelectric devices. We are also targeting the controlled doping of nanocarbon materials as they are very promising candidates for thermoelectrics. We are exploring novel polymer/carbon strategies

and One 2017 granted FIP project is devoted to novel polymer/carbon nanotube strategies and the frontiers of thermal transport detection in nanostructures. In our attempt to take thermoelectrics towards higher TRLs, efforts are targeting the understanding of thermal interfaces, which play a key role in real life devices.

Batteries: The major focus is on development of sustainable post-lithium battery technologies based on abundant, non-toxic elements. Besides optimization of hard carbon anodes for Na-ion batteries (H2020 project NAIADES), and study of discharge products in Na-air batteries by X-ray imaging, efforts are being directed at consolidating research in multivalent technologies based on elements enabling the transfer of more than one electron. Within the framework of the ERC- CAMBAT, new electrolyte formulations enabling efficient deposition of Mg and Ca are being sought. Efforts to develop cathodes for Ca based batteries will be strengthened in the framework of the (FET-OPEN CARBAT) project. Finally, Zn-air batteries using aqueous electrolytes are revisited using a new cell concept.

Novel materials for alternative energy applications: A new family of bidimensional copper oxides produced hydrothermally show significant in plane ferromagnetism and electroactive properties and novel carbon/silica composite films show improved electrochemical sensing properties. Alternatively, processing of microporous metal organic frameworks (MOFs) using supercritical CO₂ is used, precisely, for CO₂ capture. Advanced

spectroscopic characterization of highly-porous MOF particles that spontaneously assemble into well-ordered 3D superstructures enabled the design and of photonic crystals. Contributions in the field of hydrogen production have also been published during 2017 related to synchrotron X-ray investigation of TiO₂ interfaces for photocatalysis and the development of Au/TiO₂ lyogels for hydrogen production. Finally, alternative materials that could find diverse uses in the field of energy include decorated semiconducting quantum dots which exhibit kinetic fluorescence switching.

2017 ACTIVITIES

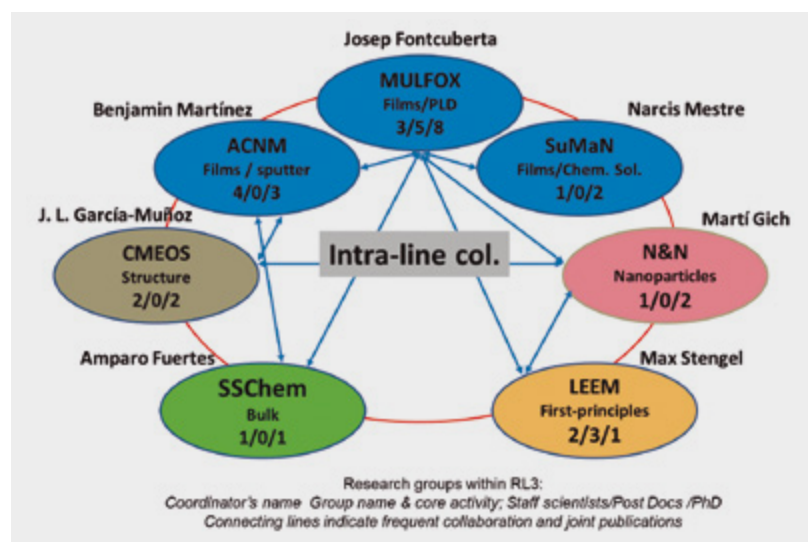
During 2017, two new labs associated to RLI have been completed through the funds obtained from two ERC grants (FOREMAT and ENLIGHTMENT). The first one consists on an assembly line for photovoltaic, thermoelectric and photonic devices, while the second contains a number of advanced tools for the characterization of photovoltaic, thermoelectric and structural properties. A third lab is being assembled for battery research associated to a third ERC grant (CAMBAT).

The scientific activities have resulted in many different contributions. A non-exhaustive list includes, over 60 papers published in high impact factor journals (including 1 Nat. Mater., 1 Nat. Chem., and 2 Adv. Mater.), 5 book chapters, more than 15 invited talks at international conferences, and several workshops organized (including one in emerging photovoltaics, and another on the

structure-performance nexus at the MRS in Boston), 2 patents filed, several contracts with the private sector (including Repsol, Toyota and Eurecat), and 3 PhD defences (OTE/OPV, nitrides and oxide PV). In terms of individual recognition, we would like to highlight that two researchers have obtained permanent positions (tenured scientist) and will focus their activities on thermoelectrics and oxide photovoltaics, and another two have been promoted (from Tenured to Research scientist). One of our staff (M. Coll) has been awarded the L'Oréal-Unesco prize for Women in Science 2017.

Several measures are underway to follow the advice of the SAB with respect to strategic cooperation with neighbouring technological players. On the one hand, negotiations are in place with technological centres in Catalonia to sign a Memorandum of Understanding to help bringing novel materials to more advanced TRLs. On the other hand, we are participating in different advanced networks, such as ALISTORE in battery research, ITN SEPOMO on organic photovoltaics, one Networks of Excellence of MINECO regarding emerging PV and we are starting to be more active in AMPEA. We are currently writing other proposals (ITN and Network of Excellence) in the topic of thermoelectricity. Finally, in terms of dissemination, our researchers have been very active, participating in Summer Schools (e.g. on Sodium Batteries in Sweden), with talks and workshops in Expominer, "Bojos per la Física" jointly organised with IFAE and ICN2, the ICMAB's kids day, as well as in several programs (Escolab) for high school students in which we taught them to build dye sensitized solar cells and batteries.





RL3: Oxide Electronics

2017 MAIN HIGHLIGHTS

Materials Preparation:

Integration of ferroelectric oxides on technological platforms and tuning of Polarization of BaTiO₃

by growth conditions rather than conventional substrate-induced strain control, suggesting an important role of point defects as a new knob to functionalize oxides.

New phase discovered in multiferroic ϵ -Fe₂O₃. This oxide was first demonstrated to be multiferroic at ICMAB and now a new magnetic phase of it has been discovered.

Nitride tuning of magnetic, optic and electric properties of transition metal perovskites. Oxynitrides may display radically different properties than their oxide counterparts. Hole doping has been achieved in LaCrO_{3-x}N_x and Sr₂FeWO₅N that allows tuning magnetic properties and, interestingly enough, the cationic order in the double perovskite is preserved during the topochemical nitridation.

Correlated cobalt oxides with spin-state and electronic instabilities.

The spin-state instabilities in Co(III)-based oxides were examined in relation to their conductivity, magnetic and structural transitions.

Advanced characterization:

Mapping Polar displacements mapped by HREM. The presence of polar displacements in otherwise non-polar LaAlO₃ films grown on SrTiO₃, has been observed and, based on first principle calculations, it has been shown that it results from a competition between distinct octahedral rotation patterns in the oxide in confined structures, in presence of a interface-related electric field.

A new scanning probe microscopy mode to study the piezoelectric response based on the direct piezoelectric effect (dielectric polarization under an applied mechanical stress). In contrast to

the widely used electromechanical characterization based in the inverse piezoelectric effect (mechanical deformation under an applied electric field), the new Direct Piezoelectric Force Microscopy allows a quantitative determination of the piezoelectric coefficients.

Magnetic symmetry and coupled internal orders in magnetoelectric and functional oxides.

Full symmetry analysis and description of internal orders and coupled modulations (crystal&magnetic ordering, charge and orbital ordering, spin-state ordering) in oxides with (i) metal-insulator transitions (ii) magnetoelectric properties and (iii) multiferroicity. Influence of distortion on the magnetic order and the magnetoelectric properties of frustrated R₂CoMnO₆ (R=Y, Ho, Tm, Yb and Lu) B-ordered perovskites. Magnetic crystallography of cycloidal multiferroics : discovery of different types of cycloidal flops and polarization rotations under magnetic field in cycloidal ferroelectrics.

Magnetic anisotropy and valence states in La₂Co_{1-x}Mn_{1+x}O₆ thin films studied by x-ray absorption spectroscopy techniques.

The structure of catalysis-active TiO₂ based surfaces. Using synchrotron surface diffraction the structure of the rutile TiO₂ (110) interface with water and that of the TiO₂ anatase (101) surface have been determined.

Devices and Functionalities:

Magnetodynamics driven by voltage-controlled surface acoustic waves (SAW). SAWs on piezo materials have been mapped using stroboscopic synchrotron light

and a photoemission microscope (PEEM). Simultaneous mapping of XMCD of micrometric objects grown on the piezo substrate has allowed to obtain dynamic views of elastic waves and magnetic anisotropy at unprecedented picosecond time scale.

Electric & mechanical switching of polarization.

Epitaxial BaTiO_{3- δ} /La_{0.7}Sr_{0.3}MnO₃ bilayers have been grown on Si with a columnar microstructure. This particular microstructure enables the flexoelectric switching of the BTO polarization and voltage controlled resistive switching, which can be also manipulated by a strain gradient. The combined electrical and mechanical control allows setting the system into three different configurations of polarization and resistive states.

Electric-field manipulation of magnetic states in antiferromagnetic systems, for the magnetic memories.

It has been discovered that some martensitic alloys displaying ferromagnetic/antiferromagnetic transitions, f.i. FeRh, can be used to hide magnetic information and its response can be modulated by voltage-controlled strains.

Fundamental understanding and modelling of oxide physics:

Flexoelectricity and gradient-related properties. Gradient-mediated couplings are materials functionalities that emerge from spatial variations of some order parameter (strain, polarization, magnetization, antiferrodistortive tilts), rather than the periodic bulk

phase itself. Gradients generally break inversion symmetry, and thereby produce an electrical polarization (P) even in materials that are nonpolar, hence their practical interest for applications. Our group is currently leading the way in this research thrust

Polar domain walls. Ferroelastic twin walls have received considerable attention in the past few years, as they are characterized by a net dipole moment even if the parent material is nonpolar. We have reported two new mechanisms that contribute to P: a direct “rotopolar” coupling to the gradients of the antiferrodistortive oxygen tilts, and a trilinear coupling that is mediated by the antiferroelectric displacement of the Ti atoms. These results open new avenues towards engineering pyroelectricity or piezoelectricity in nominally nonpolar ferroic materials.

2017 ACTIVITIES:

The scientific activity of RL3 has been made possible by gaining competitive financial resources from ERC (1), Spanish MINECO (5), IF-MSCA fellowship (1) and Severo Ochoa Excellence center -related FIP projects (3). This activity has resulted in a number of scientific papers published in top-ranked journals in the field. A non-exhaustive list includes: Nature Materials (2), Nature Comms (2), Adv. Funct. Mater. (1), Chem. Mater (1), Small (1), Phys. Rev. Lett. 82), ACS Applied Surface and Interfaces (1), Phys. Rev. Appl. (1), J. Phys. Chem. C (1); Sci. Reports (1), Phys. Chem. Chem. Phys. (1), Prog. Solid State Chem (1), etc. and a contributed chapter in a book. The activities have been

disseminated in major scientific forums by delivering Plenary (2), and Invited (13) lectures, in addition to about 30 oral presentations and specialized conferences and seminars at Laboratories and Universities. RL3 scientists have been chairing Conferences and Symposia (4) and been acting as Scientific Committee Members of several others. The international scientific visibility of RL3 has contributed to recruit a substantial number of Post Docs (4) and Pre-docs (9) including the prestigious InPhiT -La Caixa-Ochoa grant. This education activity has resulted in several PhDs defenses (3) and we have hosted Master and Graduates students for their projects and laboratory training (5). We are proud that one of the RL 3 members (Ignasi Fina) has been awarded by the “2017 Young Research Prize for Excellent trajectory” from the RSEF.



SOMM ALLIANCE

SOMMa is the alliance of Severo Ochoa centres and María de Maeztu units to promote Spanish Excellence in research and to enhance its social impact at national and international levels.

SOMMa was officially launched in October 2017. SOMMa brings together 25 centres and 16 units accredited through these excellence awards and aims to:

- **Increase the national and international visibility of the SO and MM programme as an “interdisciplinary and interconnected Spanish research ecosystem of excellence”**
- **Promote exchange of knowledge, technology and good practices among its members, the international scientific community and key stakeholders.**
- **Have a voice in Spanish science policy.**

- **Collaborate with other centres and universities to push forward Spanish science.**

The alliance’s starting activities comprised the establishment of its own governance, the launching of the website (somma.es) and the organisation of task forces to address the different objectives.

SOMMa is organized by a chair, co-chair and project manager, and by a steering committee in charge of different work packages. The ICMAB participates in “Work package 3: Outreach”, and helps in the organization of the 100xciencia meetings. In 2017, the meeting was held in Alicante, and its topic was “Co-creating value in scientific research”. The ICMAB Communication & Outreach Officer, Anna May Masnou, is also part of the SOMMa Editorial Board, which is in charge of the website and of the press releases of the SOMMa network.

STRATEGIC PRIORITY ACTIONS



FRONTIER INTERDISCIPLINARY PROJECTS (FIPs)

The FIP are an internal call of proposals for researchers of the Institute aimed for the development of high-risk exploratory projects of interdisciplinary character to generate cutting-edge research in the application areas of clean & secure energy, smart & sustainable electronics or smart nanomedicine. FIP projects aim to reinforce the internal links and scientific critical mass of ICMAB's researchers, and to contribute to strengthen the international leadership of the Institute in the area of functional materials.

In 2016 we granted 6 projects with a total of more than 400,000 € for the Institute researchers, allowing the contracts of 3 PhD fellows and 3 postdoctoral fellows within these projects. In 2017 we financed 9 projects with more than 550,000 €, 1 of which was in the new-created category "proof-of-concept", allowing

the contracts of 1 PhD fellow and 7 postdoctoral fellows.

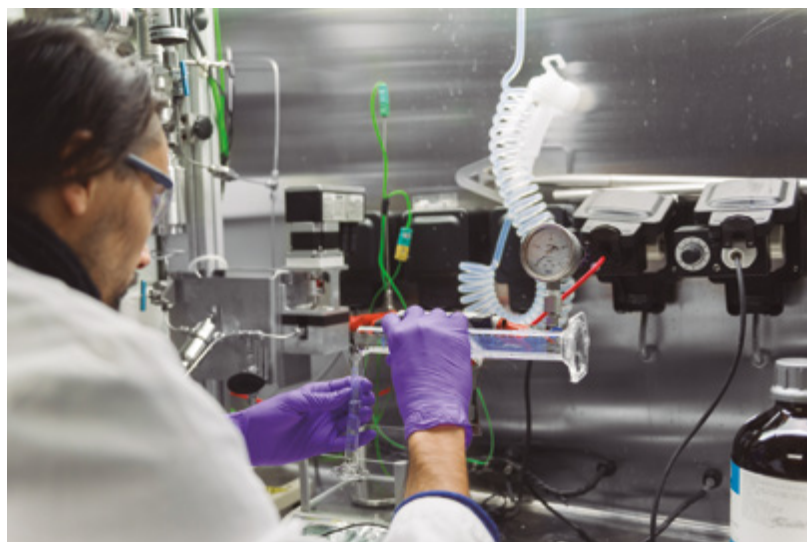
Individual:

- Jaume Gàzquez: "Revealing magnetism in real space at atomic resolution with aberrated electron probes" (MAGNETOPROBE)
- Jose Luis García-Muñoz: "Fabrication of high-temperature magnetoelectric multiferroic crystals with incommensurate magnetic spirals" (HOTMULTICRISTAL)
- Riccardo Rurali: "A oxide hybrid heat transistor" (OXHEAT)

Collaborative:

- Gervasi Herranz and Martí Gich: "Enabling Multifunctional Plasmonics on Hybrid Artificial Si-Integrated Systems" (EMPHASIS)
- Imma Ratera and Judith Guasch: "Biomimetic Lymph Nodes for Cancer Immunotherapy" (IMMUNODYNAMICS)





- Mariano Campoy-Quiles and Anna Roig: "Thermoelectric composites" (THERMOPAPER)
- Rosario Núñez and Gerard Tobias: "Boron Enriched Carbon nanoMAterials as Theranostic Agents for biomedical imaging and BNCT" (BECMATA)
- Sebastian Reparaz and Isabel Alonso: "Exploring the frontiers of thermal transport detection" (EXPLOTHRA)

Proof-of-concept (new category of 2017):

- Anna Laromaine: "Plant Nanohealing" (PNH)



TALENT ATTRACTION AND RECRUITING

The objectives of the talent attraction and recruiting actions are to improve our current training programs, to attract scientific talent, to educate, support and guide the young researchers and to boost our internationalization. The targets of the actions are the Master students, the PhD and postdoc fellows, and also the permanent researchers.

TOOLS & ACTIONS

• National and international calls (JdC, RyC, MSCA)

We support the already existing calls for pre-doc, postdoc and permanent researchers, including the Juan de la Cierva, Beatriz de Pinós, Ramón y Cajal and all the MSCA actions.

• Severo Ochoa Master internships

We have created a Master's students call, which was first launched in 2016 in collaboration with the CSIC, so that Master students can complete their Master's final research project in one of our ICMAB research groups. In 2016 we granted 7 scholarships for 3 months and 3,000 € each, and in 2017, 7 scholarships for 5 months and 5,000 € each.

• Own doctoral programme COFUND MSCA DOC-FAM

With this MSCA COFUND DOC-FAM project, coordinated by the ICMAB and with 5 more partners, we have incorporated 5 new PhD fellows in the first call in 2017 (financial assistance 33,000 €/year for 3 years). We also participate in the COFUND MSCA INPhINIT coordinated by "la Caixa" Foundation, hosting 3 PhD fellows (financial assistance 34,800 €/year for 3 years).

We also host PhD fellows from the National Programme for the Promotion of Talent and its Employability (MINEICO): 6 fellows from 2016 and 4 fellows from 2017 (financial assistance 18,000-20,600 € for 4 years).



• Postdoctoral actions

We are partners of the UAB-coordinated COFUND MSCA p-SPHERE for postdoctoral fellows. At the Institute we have 1 fellow from 2016 and 4 from 2017 (financial assistance 48,900 € for 3 years). We also support researchers in the preparation of proposals to MSCA-IF. In 2016 we submitted 5 proposals and 3 were awarded (1 reserve), and in 2017, 7 proposals were submitted, 1 awarded.

• Start-up package for new permanent researchers

We support the new permanent researchers with 25,000 € so that they can begin new projects.

• Support the participation in international conferences

We financially support the attendance to international conferences for PhD and postdoctoral fellows, so that they can present their research outside the walls of the ICMAB.



MOBILITY ACTIONS, TRAINING AND INTERNATIONALIZATION

ICMAB offers an excellent and solid scientific and technologic interdisciplinary training developed in an international environment, either for undergraduate, master students, PhD fellows, and postdoctoral researchers.

During 2017 there were 97 PhD fellows at ICMAB, 58 postdocs and 41 undergraduate and master students. Apart from the supervised guidance from the scientists, the Institute offers a continuous program of seminars and workshops to meet the demands of both staff and students.

• PhD theses

In total, by the end of 2017 the ICMAB graduates amounted 240.

- 16 PhD theses were defended in 2017.

• Seminars

We hosted many seminars during 2017:

- 19 ICMAB Periodical Lectures
- 21 Invited Seminars
- Four special seminars on patents, nanotechnology risks and women in science:

- *Gender and class inequality in social networking sites* (9 Feb): 60 attendees
- *FUNMAT Seminar: Basic concepts in patents: a practical approach* (June): 30 attendees
- *Seminar "The risks of nanotechnology"* (17 July): 50 attendees
- *"Re-reading Curie" by Xavier Roqué* (19 Dec): 60 attendees

• Conferences and meetings

The researchers have presented their results in more than 95 international meetings and 19 national meetings, and organized 5 international and 3 national conferences. In addition, they organized 2 annual meetings, participated in the SOMMa meeting and organized a meeting between illustrators and scientists:

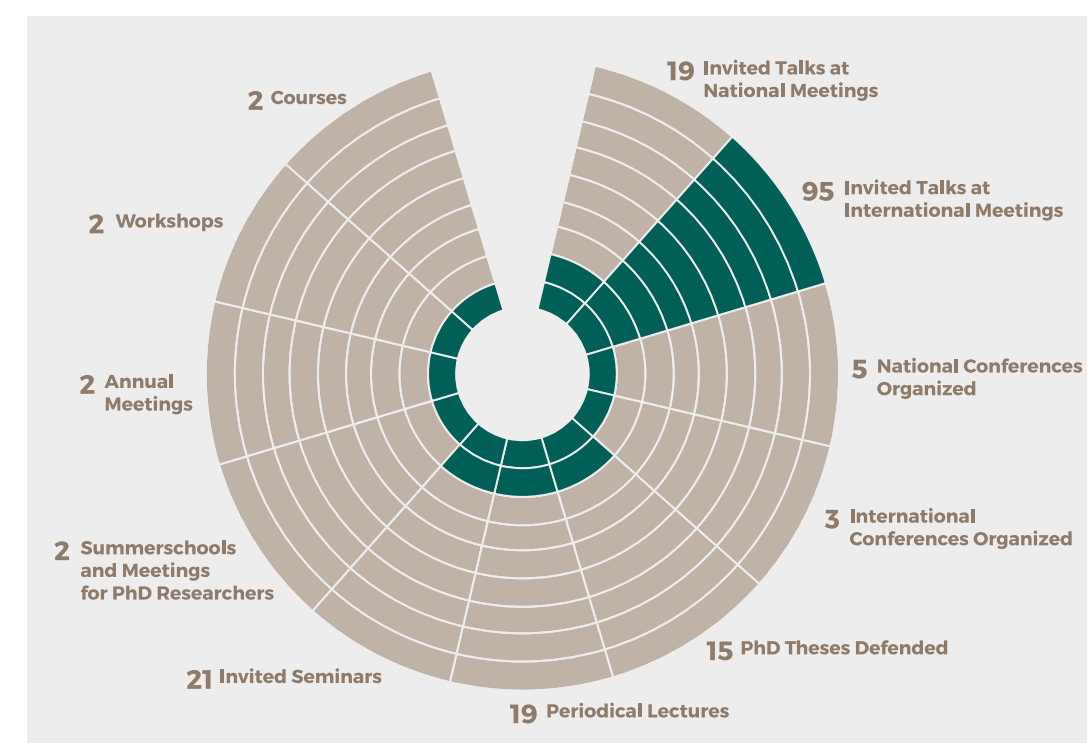


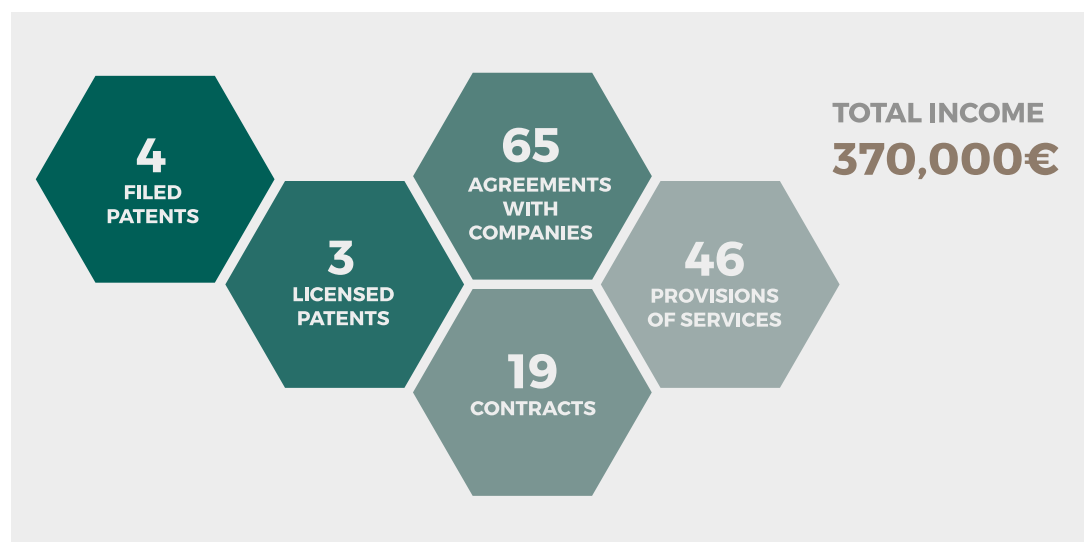
- NANOSELECT NOE Annual Meeting (10-12 July): 4 invited lectures, 24 talks by ICMAB researchers, 47 posters, organized by RL1, RL2 and RL3 researchers.
- 100xciencia.2: Co-creating value. Meeting of Severo Ochoa and María de Maeztu Centers focused on technology transfer on 2017 (2-3 Nov)
- Scientific Meeting of BNC-b PhD Students (7-8 Nov): 78 participants (49 posters, 29 talks), organized by PhD fellows of ICMAB, ICN2, UAB, ALBA Synchrotron, IMB-CNM (Barcelona NANOCLUSTER)
- Meeting between Illustrators and Scientists (29 Nov): 40 attendees

• Courses and workshops

We have organized 2 workshops, 4 courses and 1 summer school in 2017:

- III Workshop on Materials Characterization by Diffraction Methods (23 Jan)
- Workshop of the series Accelerator Magnets in High Temperature Superconductors (15-17 Feb)
- "Effective presentations, effective meetings and negotiation" course IL3 (April-June): 15 attendees, 6 sessions
- Course on emotional education (May): 30 attendees, 5 sessions
- Course of Advanced Web of Science (22 Nov)
- English courses: 50 attendees, several schedules.
- Summer School Materials for Biomedical Applications: MATBIO2017 (19-22 June): 16 invited speakers, 52 attendees from 18 Institutions (56 % female), 63 % PhD fellows, 22 % Master students, 11 % Postdoctoral fellows and 4 % Undergraduate, organized by RL5 researchers.





INVIGORATE THE TECHNOLOGY AND KNOWLEDGE TRANSFER PROGRAM: CONNECTING INDUSTRY WITH OUR EXCITING DEVELOPMENTS

The mission of the Technology Transfer Unit at ICMAB is to translate ICMAB research into social use via technology and knowledge transfer, through a process which provides social and economic benefits to ICMAB, Industry and the society.

To date we have filed and licensed a significant number of patents, and we are responsible of advising our researchers in IPR related matters. ICMAB has signed many contracts and collaborations with different types of companies, and, in addition, our researchers contribute by developing new knowledge in collaboration with our industrial partners in many European projects. Examples: CARBAT, Calcium based rechargeable batteries; MAGBBRIS, New magnetic biomaterials for brain repair and Imaging after Stroke; Smart-4-Fabry, New nanomedicine for the treatment of the Fabry rare disease.

We are approaching a quality improvement of our TT processes, in special for new opportunities marketing of our research results. For this reason, in 2017 we started the project "Review of technology transfer practices at ICMAB: assessing the technology transfer potentials along selected value chains" commissioned by the Fraunhofer- IMW.

In 2017, particularly, we signed the following contracts with the Industry

- Pharmaceutical companies: Interquim, Mohes and Medichem.
- Repsol and Toyota: for energy storage and batteries



- CEA-Commissariat à l'énergie atomique et aux énergies alternatives
- SRON-ESA: Optimization of a European Transition Edge Sensor Array
- Chimigraf (SMEs)
- Spin-offs: Nanomol, Oxolutia and Nanusens.
- Technological centers: Fundación Eurecat

We also participated in industrial national projects called "Retos colaboración", which are led by these companies: Praxis Pharmaceutical, Creaciones Aromáticas Industriales, Oxolutia, Pharma Mar, Almirall,

In 2017, we licensed the following patents

- CU2012-0112 " Vesículas que comprenden factor de crecimiento epidérmico y composiciones que las contienen". Licensed CIGB-CUBA
- Materiales de electrodo positivo en base de titanio para baterías recargables de calcio y celda que comprende los mismos. Licenced Toyota Motor Europe.
- One dimensional structure pre-calciated materials as positive electrode for rechargeable calcium

batteries and cell comprising the same. Licensed Toyota Motor Europe.

And we filed the following ones

- Materiales de electrodo positivo en base de titanio para baterías recargables de calcio y celda que comprende los mismos. M^a Rosa Palacín Peiró and Toyota Motor Europe.
- One dimensional structure pre-calciated materials as positive electrode for rechargeable calcium batteries and cell comprising the same. M^a Rosa Palacín Peiró and Toyota Motor Europe.
- Minimally-invasive continuous clinical monitoring of small molecules with analytical accuracy. José Vidal Gancedo, Technion Research & Development Foundation Ltd. and Universität Ulm. Registered: USA, US62/577775
- Insect repulsion and/or barrier arrangement and method for repelling insects. Elies Molins, Biogents AG and ISGlobal. Registered: Germany and Europe: EP17208300.



INVIGORATE THE COMMUNICATION & OUTREACH PROGRAM

One of the main missions of ICMAB is to encourage scientific vocations and increase the general scientific knowledge of the society. Throughout last year, ICMAB continued to offer public engagement and science education activities. A Communication & Outreach Officer was hired in April 2017 to invigorate the communication program. Its main function is to support the dissemination of the research activity and the impact of the work developed by the ICMAB community.

Press

The ICMAB was deeply engaged with the media in connection with the new findings published by our scientists in high-profile journals and institutional and outreach activities, which led to articles in the press and online media as well as participation by scientists in radio or TV programmes. In particular, our press releases have made it to La Vanguardia, El Periódico, Agencia SINC, Hipertextual, Madrimasd or Nanowerk, to name a few.

Activities for students

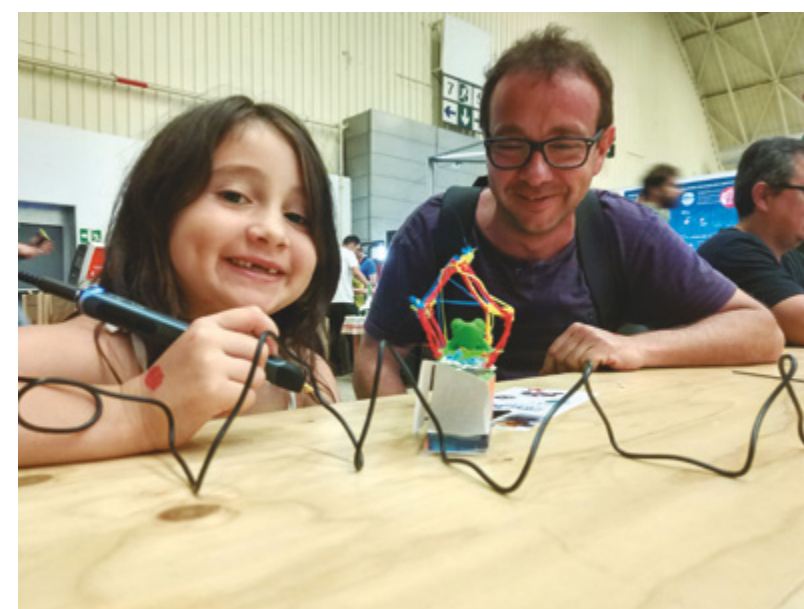
- A researcher in your classroom (8 sessions in 2017)
- **Joves i Ciència** (6 students),

Programa Argó UAB (6 students) and **Societat Catalana de Química** (3 students): stays at ICMAB during July

- **Bojos per la física** - Mad for physics (Fundació Catalunya La Pedrera) (10 June)
- **ESCOLAB** - School visits at our center (10 visits in 2017)
- Theater play for Women in Science day: Madame Châtelet and her followers at Instagram (Feb-March)

Outreach activities

- Participation in schools for retired people (**FUB+GRAN**) (March)
- **Nanoscience and Nanotechnology Festival**
- 10alamenos9**: organized by many

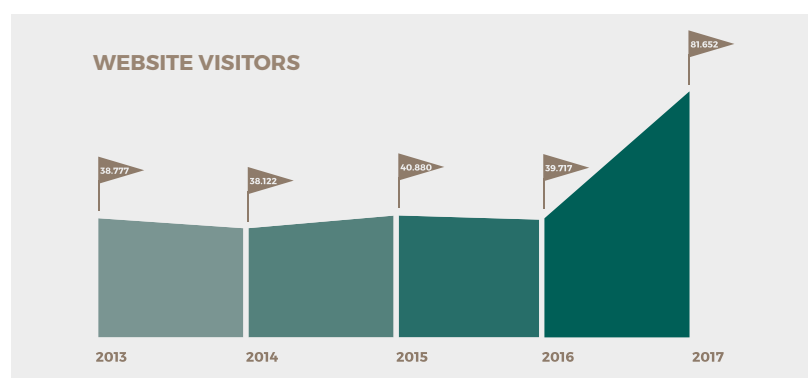


research centers and universities. Talks, seminars, workshops... around nanotechnology. (April)

- Participation in science fairs:
 - **YoMo** - Youth Mobile Festival (Feb)
 - **Saló de l'Ensenyament** (March)
 - 10alamenos9 - Nanoscience and Nanotechnology Festival (April)
 - **Festa de la Ciència a Barcelona - Science Festival in Barcelona** (May)
 - **Exporecerca** (May)
 - **Pint of Science Festival** (May)
 - **Barcelona Maker Faire** (June)
 - **Ciència en Acció** (Oct)
 - **Expominer** (Nov)
 - **Setmana de la ciència** - Science week (Nov)

Website and social networks

There is a 100 % increase in the number of users of our website, and a 30% increase in the number of sessions between 2016 and 2017. To be highlighted, on May 2017, we quadrupled the number of users. In addition, the ICMAB rose from the thirteenth to the fourth place in the "Research centres websites ranking" out of a total of 139 CSIC institutes websites. In addition, a 30% increase in followers has been observed in our main social networks, Twitter, Facebook and Instagram, in the same period.



Mailing & Intranet

We have updated the Agenda of events, the intranet documents, and created a weekly newsletter with the upcoming seminars and meetings at the ICMAB and at the institutes of the BNC-b and with the latest news.

Celebrations

We have organized a retirement reception (Vladimir Laukhin), the Institute's Anniversary Party, the Christmas party, the Kids' Day and the photo contest FOTICMAB for our staff.

Corporate image & merchandising

We have prepared institutional presentations and posters with information of our RLs, a catalogue and flyers of our activities and of our job opportunities and a welcoming pack for our staff (old-timers and newcomers) consisting of a mug and a bag.



INVIGORATE THE PROJECT MANAGING PROGRAM

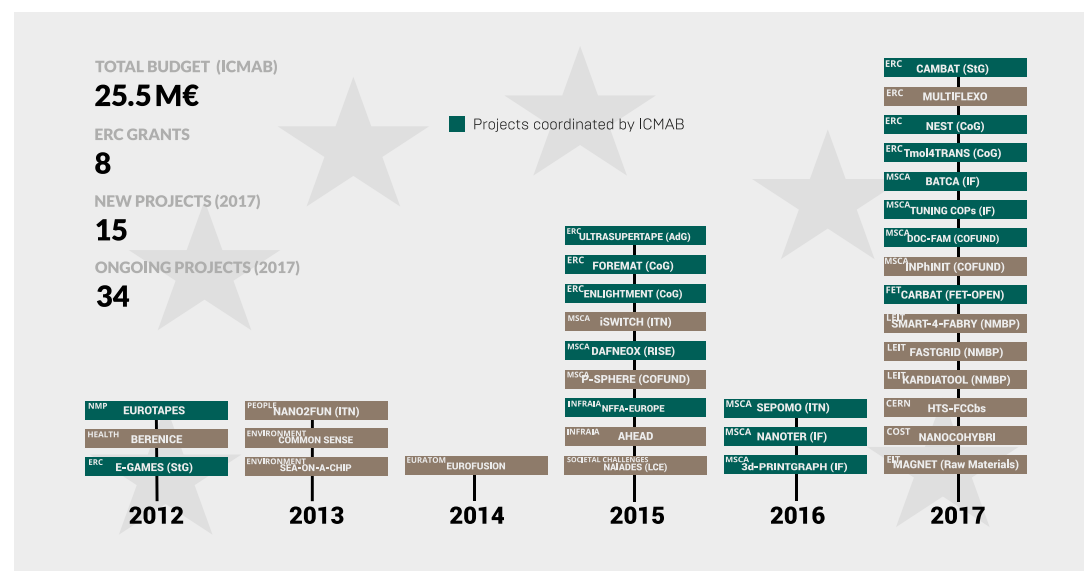
Strategic Managing Unit

The Strategic Managing Unit, responsible for the implementation of the funding obtained by the Institute, was created in 2016 to reinforce the strategic projects, support all the initiatives related to the Severo Ochoa FUNMAT governance and initiatives, coordinate with the Managing Director the expenditures control and justification, promote the achievement of strategic projects complementing the FUNMAT actions and provide support to researchers in preparing, submitting and reporting new projects and grants. In close collaboration with ICMAB's governing bodies and the other available Units, it promotes a continuous development strategy to position ICMAB as one of the leading European Research Centers in Materials Science. Among its main objectives, the Unit is responsible for the constant

search for new funding opportunities focusing on the strategic and innovation objectives of our Severo Ochoa FUNMAT project with the aim of enhancing ICMAB's scientific excellence, with an open-minded approach to detect new opportunities for our researchers. In 2017 the Unit was formed by Jorge Pérez and Montse Salas.

Research Projects

The ICMAB is leading several collaborative research projects funded by the European Commission under its Framework Programmes and several national (RETOS and I+D Excelencia) and regional projects. This continued leadership results in high visibility, a strong reputation as well as relevant scientific and innovation output. In 2017 there was an extraordinary increase in the success of international grant attraction, mainly coming from EU projects from H2020. At the end of



2017, we had 34 EU ongoing projects: 15 of them started in 2017, among them 4 new ERC Grants, 1 COFUND MSCA coordinated by ICMAB (DOC-FAM) and 1 FET-OPEN (CARBAT). The total number of ERC grants increased to 8 in 2017.

ERC PROJECTS

· Advanced Grants

Teresa Puig (2015) Ultrafast growth of ultrahigh performance superconducting tapes (ULTRASUPERTAPE)

· Consolidator Grants

Mariano Campoy-Quiles (2015)

Finding a needle in a haystack: efficient identification of high performing organic energy materials (FOREMAT)

Gerard Tobias (2017)

Nanoengineering of Radioactive Seeds for Cancer Therapy and Diagnosis (NEST)

Núria Aliaga (2017)

Efficient electronic transport at room temperature by T-shaped molecules in graphene based chemically modified three-terminal nanodevices (Tmol4TRANS)

Massimiliano Stengel (2017)

Hierarchical multiscale modeling of flexoelectricity and related materials properties from first principles (MULTIFLEXO)

· Starting Grants

Marta Mas-Torrent (2012)

Surface self-assembled molecular electronic devices: logic gates, memories and sensors (e-GAMES)

Agustín Mihi (2015)

Photonic electrodes for enhanced light management in Optoelectronic devices (ENLIGHTMENT)

Alexandre Ponrouch (2017)

Calcium and Magnesium metal anode based batteries (CAMBAT)

· Proof-of-concept

Marta Mas-Torrent (2014)

Large Area Organic Devices with Bar-Assisted Meniscus Shearing Technology

COFUND MSCA DOC-FAM

The Institute of Materials Science of Barcelona (ICMAB-CSIC) coordinates the first MSCA-COFUND programme awarded to CSIC. The doctoral fellowship programme DOC-FAM (DOctoral training programme in Functional Advanced Materials) will

allow the mobility of 22 Early Stage Researchers in the field of functional advanced materials, 9 of them will be recruited by the ICMAB. The first call of the project was on October 2017, and the first fellows will be incorporated during the second semester of 2018.

The other participants in DOC-FAM programme are the Institute of Microelectronics of Barcelona (IMB-CNM-CSIC), the Catalan Institute of Nanoscience and Nanotechnology (ICN2), the Catalonia Institute for Energy Research (IREC) and the ALBA Synchrotron. The duration of the programme is 5 years and involves a budget of 3,453,120 €. Half of this budget will be supported by the 1,726,560€ EC grant, while the other half will be cofunded by the project participants.

NFFA EUROPE

ICMAB is one of the host institutions of the NFFA-Europe (Nanofoundries for fine analysis) project for the synthesis and characterization at the nanoscale across Europe, which started in 2015 and will last until the end of 2018. During 2017, ICMAB has participated in the following way: we have received 14 users to our facilities, from France, Italy, Greece, India, Switzerland and Russia. The installations used until now have been: scanning electron microscopy (SEM), transmission electron microscopy (TEM), atomic force microscopy (AFM), X-ray diffraction (XRD), electron paramagnetic resonance (EPR), atomic laser deposition (ALD), magnetometry by Superconducting Quantum Interference Devices (SQUID) and ellipsometry.

A Summer School devoted to "NFFA available instruments and techniques" took place at the Engineering School of the Autonomous University of Barcelona (UAB) between July 18-22, 2017. As part of the school, visits to all the relevant infrastructures at the UAB Campus involved in the NFFA-Europe-transnational access were programmed. ICMAB-CSIC received 30 students from all over Europe, which were given a brief introduction of the Institute activities and then had the opportunity to visit some of the laboratories participating in the project, including the Cleanroom facility and the Raman, AFM and Low Temperature and Magnetometry laboratories.



CREATION OF NEW COMMITTEES

An interesting Severo Ochoa action is the formation of three new committees on **Recruiting, Seminars & Training**, and **Gender Equality**. These committees are integrated by members of each research lines and have the support of the Severo Ochoa project managers. In 2017, two other committees were created, the **Technology Transfer** committee, and the **Communication & Outreach** committee. These new committees were added to the already existing committees of the Institute: **Health & Safety, Computing, Gases** and **Waste Management**.



WOMEN IN SCIENCE

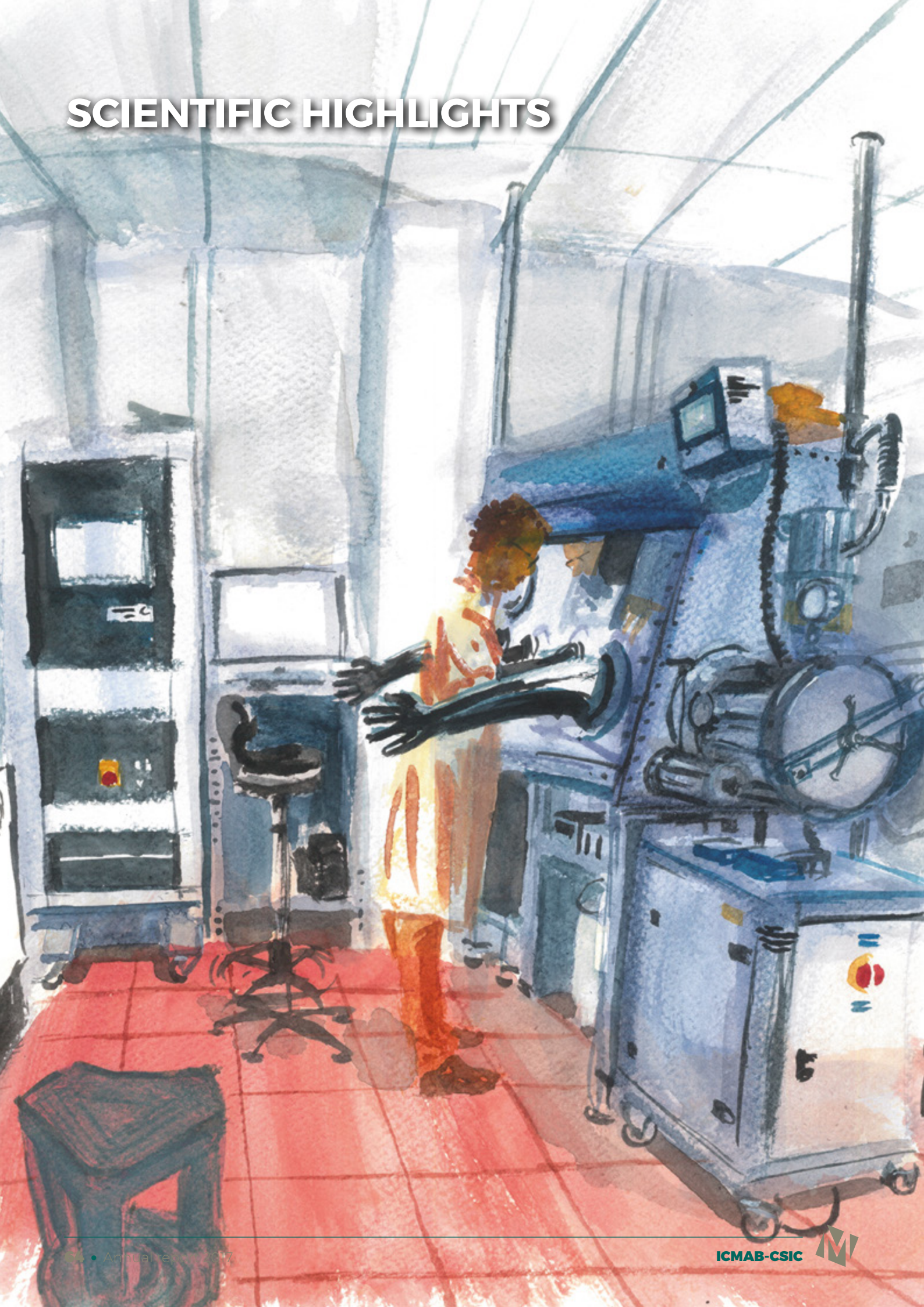
At ICMAB we promote equal opportunities for men and women and boost women's advancement in scientific careers. With this in mind, we carry out multiple initiatives to give visibility to our female scientists and to promote science in young girls:

- We have created a newly **Gender Equality Committee**, in which all the scientific communities are represented, and whose main goal is the recognition and strengthening of equal opportunities within the Institute and the design, implementation and evaluation of positive action measures against discrimination. In addition, to eliminate gender bias in recruitment processes, attract and recruit female scientists, improve work-life balance, promote career development and establish and disseminate gender-sensitive practices.
- We enjoy celebrating the **International Day of Women and Girls in Science** and, therefore, a series of leisure activities aimed at generating a reflection and debate were organized. The dramatized

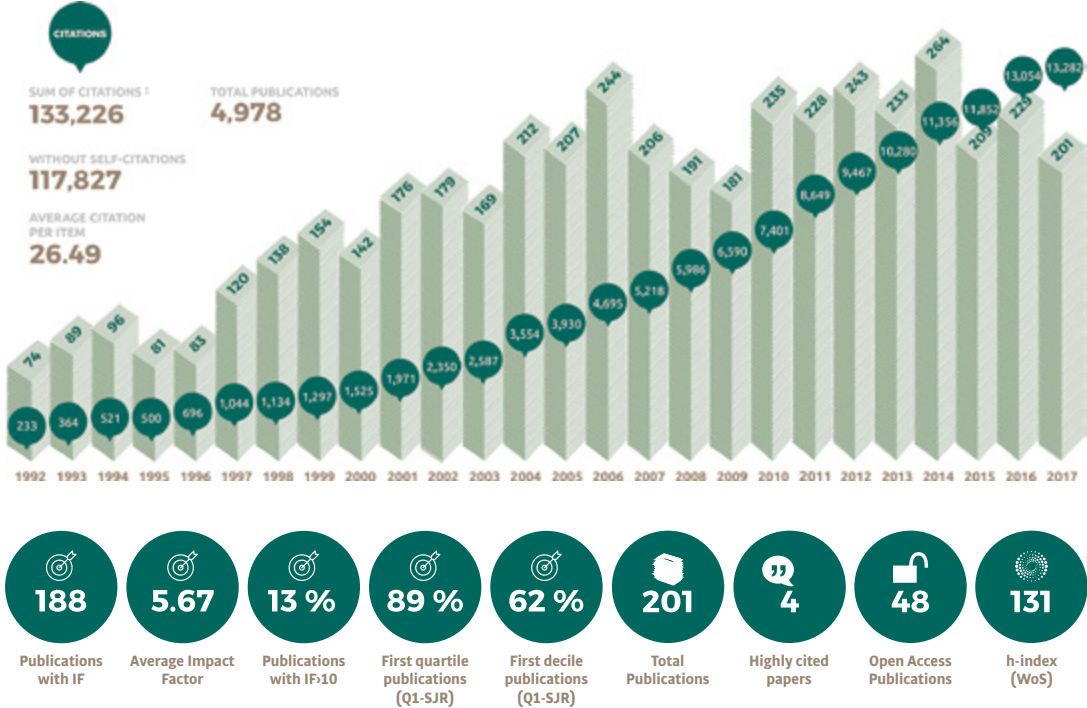
reading "Madame Châtelet and her Instagram followers", to make visible the scientific women throughout history; public conference about "Gender and class inequality in social networking sites" and a public conference about "Re-reading Marie Curie".

- In 2017 the ICMAB participated in the summer school "**Diversity in the Cultures of Physics**" for young women physicists, with a seminar and a visit to our installations with a gender dimension view.
- We encourage all the scientists to participate in different activities and awards. As a matter of fact, Mariona Coll was awarded with one of the **Research Awards "For Women in Science" from l'Oréal-UNESCO** in 2017 for her project on new materials for photovoltaics.

SCIENTIFIC HIGHLIGHTS



PUBLICATIONS 1992 - 2017
Source: Web of Science-Core Collection 12/06/2018



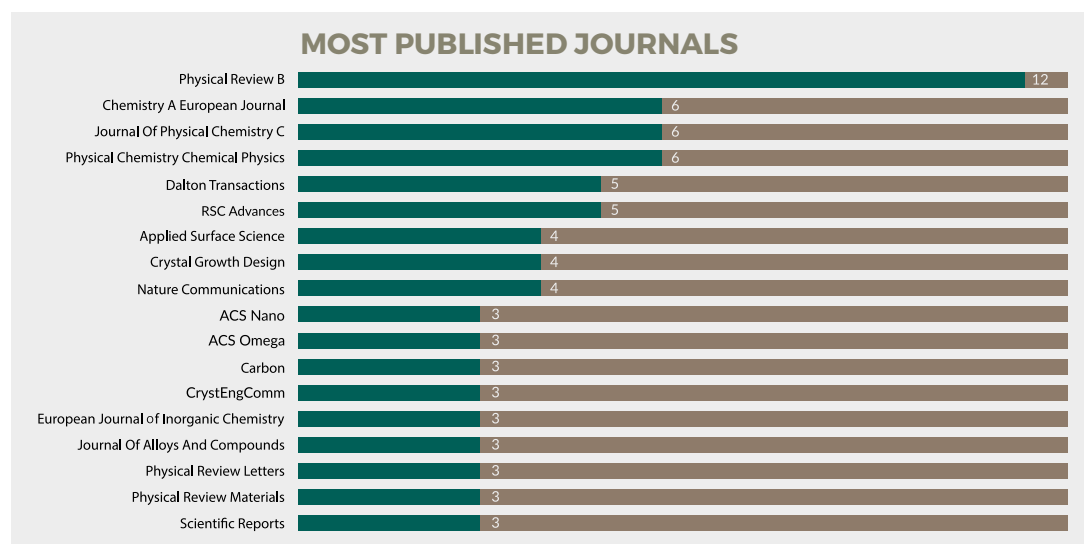
SCIENTIFIC OUTPUTS

ICMAB confirmed its leadership in excellence in science in the Nature Index 2017. The Institute was the first in the ranking among the CSIC centers, and the fourth among the research centers in Catalonia and Spain. CSIC was the first research institute in Spain, and was ranked in the top 10 research institutes in Europe, and in the top 50 of the world. The Nature Index database, which tracks the author affiliations collected from high quality scientific articles published in 68 high-quality science journals independently selected by a panel of active scientists, is an indicator of an institution impact compared to other ones in the world. The Nature Index 2017 was based on published research articles from 1 February 2016 to 31 January 2017.

Our Institute is characterized by its high quality research outcomes and by its highly talented people. At the end of 2017, we counted with nearly 5,000 publications, and more than 130,000 citations, with an average ratio of more than 26 citations per paper and a total h index of 131. In 2017 ICMAB researchers published 201 articles in international scientific journals, with an average impact factor of 5.67. 89 % (SJR) of the papers were in first quartile (Q1) journals, and 13 % were published in

journals with impact factor above 10; 48 were published in Open Access journals, and around 70 % are now in the Digital CSIC, the institutional repository of the Spanish National Research Council, which organizes, preserves and provides open access to CSIC research outputs. Moreover, 4 of the publications of 2017 are considered at this moment “highly cited papers” by the Web of Science, i.e. there are in the top 1 % mostly cited in their category and year worldwide.





TOP 10

The list of the top 10 articles published in the highest impact factor (IF) journals, by ICMAB researchers during the year 2017 are the following:

Number 1 published in Nature, with IF 40.14

Conflicting evidence for ferroelectricity.

D'Avino, Gabriele; Souto, Manuel; Masino, Matteo; Fischer, Jonas K. H.; Ratera, Imma; Fontrodona, Xavier; Giovannetti, Gianluca; Verstraete, Matthieu J.; Painelli, Anna; Lunkenheimer, Peter; Veciana, Jaume; Girlando, Alberto. NATURE, JUL 13 2017, 547, 7662, E9-E13. DOI: 10.1038/nature22801.

Number 2 and 3 published in Nature Materials, with IF 39.74

Structure of a model TiO₂ photocatalytic interface.

Hussain, H.; Tocci, G.; Woolcot, T.; Torrelles, X.; Pang, C. L.; Humphrey, D. S.; Yim, C. M.; Grinter, D. C.; Cabailh, G.; Bikondoa, O.; Lindsay, R.; Zegenhagen, J.; Michaelides, A.; Thornton, G.. NATURE MATERIALS, APR 2017, 16, 4, 461. DOI: 10.1038/NMAT4793.

Functional electronic inversion layers at ferroelectric domain walls. Mundy, J. A.; Schaab, J.; Kumagai,

Y.; Cano, A.; Stengel, M.; Krug, I. P.; Gottlob, D. M.; Doganay, H.; Holtz, M. E.; Held, R.; Yan, Z.; Bourret, E.; Schneider, C. M.; Schlom, D. G.; Muller, D. A.; Ramesh, R.; Spaldin, N. A.; Meier, D. NATURE MATERIALS, JUN 2017, 16, 6, 622. DOI: 10.1038/NMAT4878.

Number 4 published in Chemical Society Reviews, with IF 38.62

Self-assembled monolayers in organic electronics.

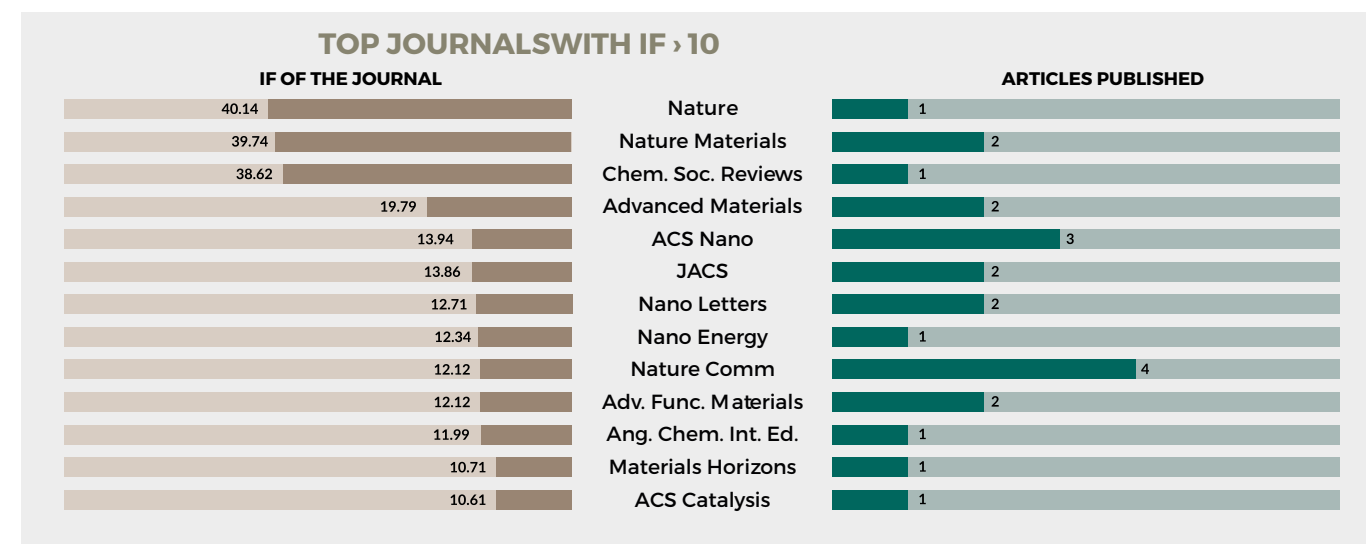
Casalini, Stefano; Bortolotti, Carlo Augusto; Leonardi, Francesca; Biscarini, Fabio. CHEMICAL SOCIETY REVIEWS, JAN 7 2017, 46, 1, 40-71. DOI: 10.1039/c6cs00509h.

Number 5 and 6 published in Advanced Materials, with IF 19.79

Polymer: Fullerene Bimolecular Crystals for Near-Infrared Spectroscopic Photodetectors.

Tang, Zheng; Ma, Zaifei; Sanchez-Diaz, Antonio; Ullbrich, Sascha; Liu, Yuan; Siegmund, Bernhard; Mischok, Andreas; Leo, Karl; Campoy-Quiles, Mariano; Li, Weiwei; Vandewal, Koen. ADVANCED MATERIALS, SEP 6 2017, 29, 33, 1702184. DOI: 10.1002/adma.201702184.

Biomimetic Inspired Core-Canopy Quantum Dots: Ions Trapped in Voids Induce Kinetic Fluorescence Switching.



Arpita Saha, Elena Oleshkevich, Clara Vinas, and Francesc Teixidor. ADVANCED MATERIALS, DEC 13 2017, 29, 46, 1704238. DOI: 10.1002/adma.201704238.

Number 7, 8 and 9 published in ACS Nano, with IF 13.94.

Redox-Induced Gating of the Exchange Interactions in a Single Organic Diradical.

Gaudenzi, Rocco; de Bruijkere, Joeri; Reta, Daniel; Moreira, Iberio de P. R.; Rovira, Concepcio; Veciana, Jaume; van der Zant, Herre S. J.; Burzuri, Enrique. ACS NANO, JUN 2017, 11, 6, 5879-5883. DOI: 10.1021/acsnano.7b01578.

Pressure-Responsive, Surfactant-Free CO₂-Based Nanostructured Fluids.

Grimaldi, Natascia; Elena Rojas, Paula; Stehle, Simon; Cordoba, Alba; Schweins, Ralf; Sala, Santi; Luelsdorf, Stefan; Pina, David; Veciana, Jaume; Faraudo, Jordi; Triolo, Alessandro; Braeuer, Andreas Siegfried; Ventosa, Nora. ACS NANO, NOV 2017, 11, 11, 10774-10784. DOI: 10.1021/acsnano.7b02500.

Ion Transport across Biological Membranes by Carborane-Capped Gold Nanoparticles.

Grzelczak, Danks, Klipp, Belic, Zaulet, Kunstmann-Olsen, Bradley, Tsukuda, Viñas, Teixidor, Abramson, and Brust.

ACS NANO, 2017, 11, 12, 12492-12499. DOI: 10.1021/acsnano.7b06660

Number 10 and 11 (Bonus!) published in the Journal of the American Chemical Society, with IF 13.86.

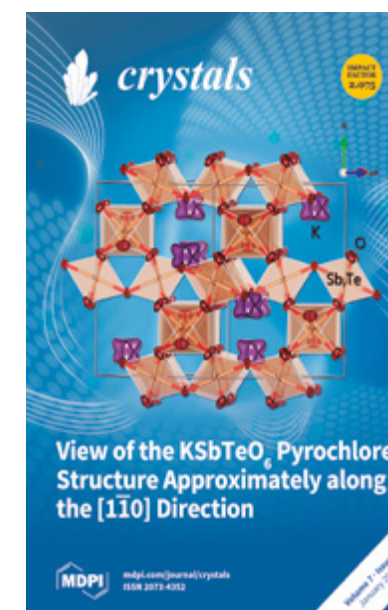
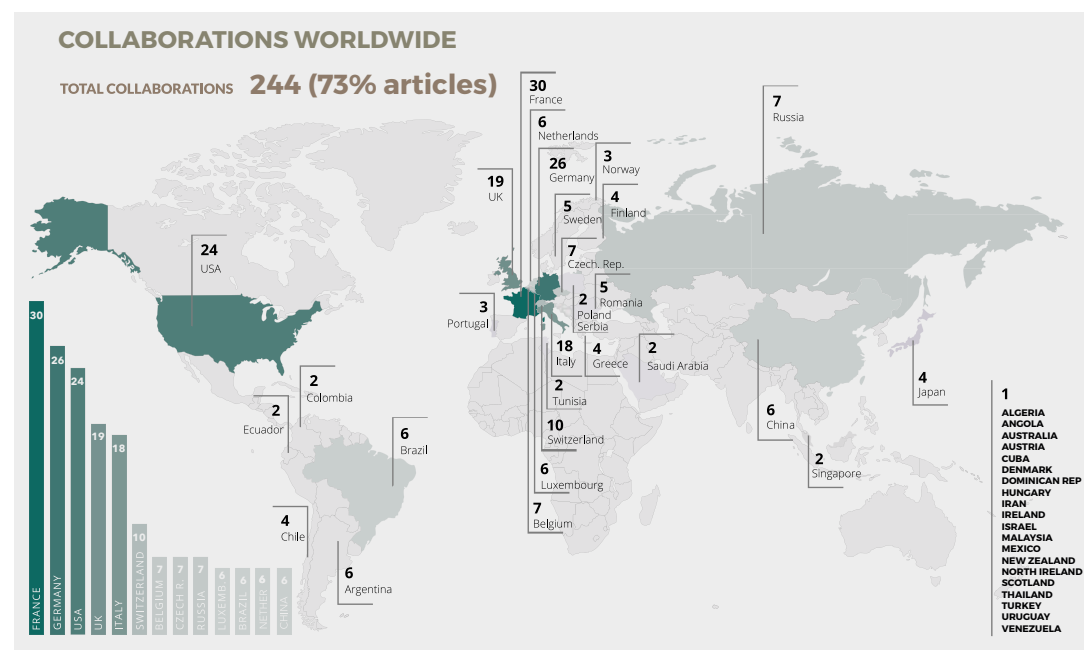
Tuning the Rectification Ratio by Changing the Electronic Nature (Open-Shell and Closed-Shell) in Donor Acceptor Self-Assembled Monolayers.

Souto, Manuel; Yuan, Li; Morales, Dayana C.; Jiang, Li; Ratera, Imma; Nijhuis, Christian A.; Veciana, Jaume. JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, MAR 29 2017, 139, 12, 4262-4265. DOI: 10.1021/jacs.6b12601.

Operative Mechanism of Hole-Assisted Negative Charge Motion in Ground States of Radical-Anion Molecular Wires.

Franco, Carlos; Mayorga Burrezo, Paula; Lloveras, Vega; Caballero, Ruben; Alcon, Isaac; Bromley, Stefan T.; Mas-Torrent, Marta; Langa, Fernando; Lopez Navarrete, Juan T.; Rovira, Concepcio; Casado, Juan; Veciana, Jaume. JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, JAN 18 2017, 139, 2, 686-692. DOI: 10.1021/jacs.6b08649.

*IF: Impact Factor 2016 Journal Citation Reports, Thomson Reuters

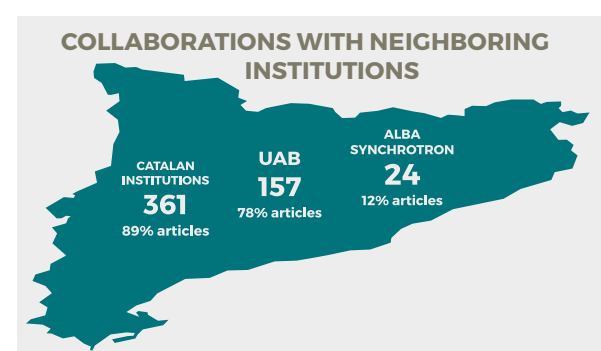
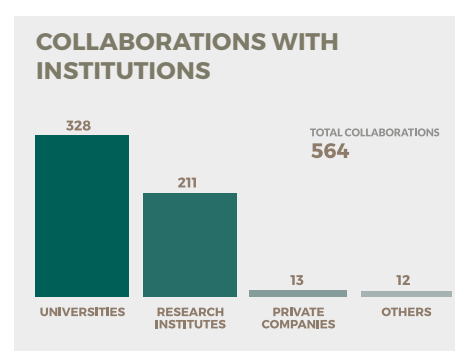
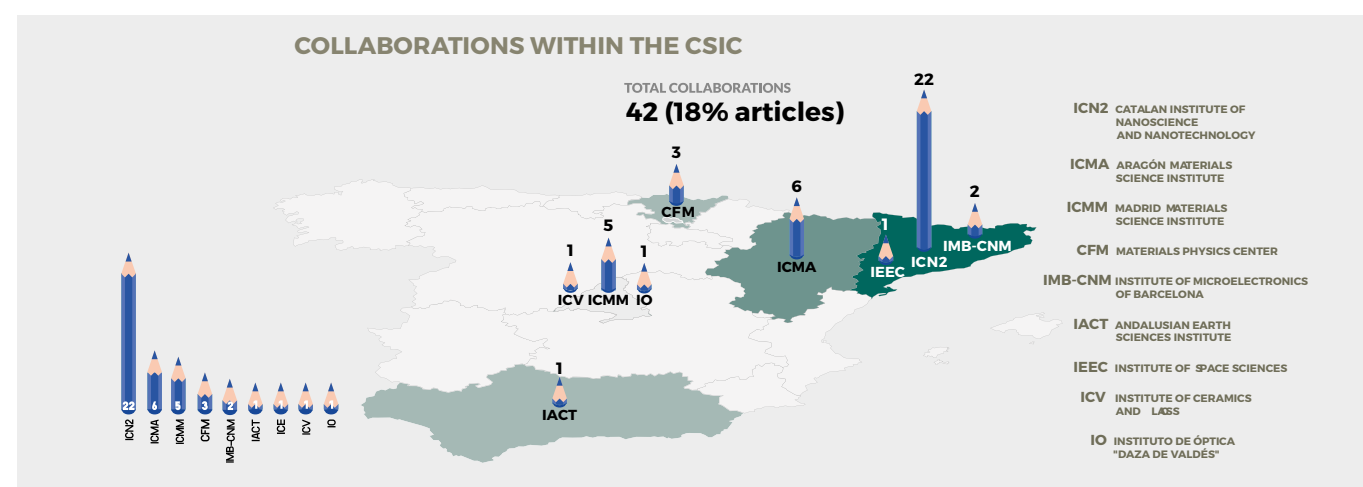


Potassium Disorder in the Defect Pyrochlore K₂Sb₂Te₆: A Neutron Diffraction Study.

José Antonio Alonso, Sergio Mayer,
Horacio Falcón, Xabier Turrillas
and María Teresa Fernández-Díaz.
Crystals, 7(1), 24, 2017. DOI: 10.3390/
cryst7010024

SCIENTIFIC COLLABORATIONS

The internationality and interdisciplinary of our researchers is also confirmed by the high number of collaborations with other countries' institutions (244, representing 73 % of the articles, and also with Universities and CSIC centers (UAB, UPC, UB, UG, IMB-CNM, ICMA, IEEC...), BIST Centers (ICFO, IRB, CRG, ICN2, ICIQ, IFAE, IBEC), other Severo Ochoa and María de Maeztu centers (CRAG, BSC, GSE, DCEXS-UPF, ICCUB-UB, BGSMath, DTIC-UPF, ICTA) and Hospitals and Large Scale facilities (Vall d'Hebron, ALBA Synchrotron), in Catalonia, and with international collaborations in universities and research centers all over the world.



Electric and Mechanical Switching of Ferroelectric and Resistive States in Semiconducting BaTiO_{3-δ} Films on Silicon.

Andrés Gómez, José Manuel
Vila-Fungueiriño, Rahma Moalla,
Guillaume Saint-Girons, Jaume
Gázquez, María Varela, Romain
Bachelet, Martí Gich, Francisco
Rivadulla, Adrián Carretero-Genevri-
er. *SMALL*, 13, 39, 2017. DOI: 10.1002/
small.201701614



Carborane–stilbene dyads: the influence of substituents and cluster isomers on photoluminescence properties

A. Ferrer-Ugalde, J. Cabrera-González, E. J. Juárez-Pérez, F. Teixidor, E. Pérez-Inestrosa, J. M. Montenegro, R. Sillanpää, M. Haukkad and R. Núñez. Dalton Transactions, 46, 2091-2104, 2017. DOI: 10.1039/C6DT04003A

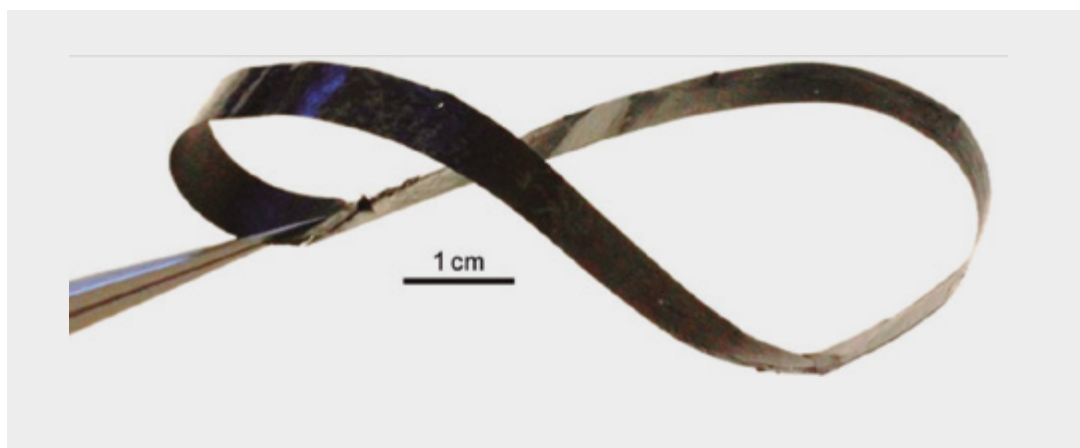
FLEXIBLE ORGANIC THERMOELECTRICS

We show that ternary mixing of semiconducting polymers and dopants embedded in a flexible matrix is an efficient approach to retain flexibility in highly doped organic thermoelectrics.

DAVID KIEFER,¹ LIYANG YU,^{1,2} ERIK FRANSSON,¹ ANDRÉS GÓMEZ,³ DANIEL PRIMETZHOFFER,⁴ ARAM AMASSIAN,² MARIANO CAMPOY-QUILES,³ AND CHRISTIAN MÜLLER¹

[1] A Solution-Doped Polymer Semiconductor: Insulator Blend for Thermoelectrics. *Advanced Science*, 2017, 4 (1), 1600203

FIGURE
Flexible thermoelectric tape based on PEO matrix, P3HT semiconductor doped with F4TCNQ dopant.



Materials that can convert waste heat into electricity via the thermoelectric effect are currently being considered key elements in the transition to a more efficient energy paradigm. Organic thermoelectrics offer the prospect of low cost, as well as low toxicity for low temperature applications. Organic semiconductors have low thermal conductivities and reasonable Seebeck coefficients, and thus most efforts are placed on increasing their electrical conductivity. Doping with molecular dopants is an efficient way of doing so, which, however, turns films brittle. In this contribution, we propose the use of ternary mixing to improve the mechanical properties of highly doped organic semiconductors.

Poly(ethylene oxide) (PEO) is demonstrated to be a suitable matrix polymer for the solution-doped conjugated polymer poly(3-hexylthiophene), P3HT. The polarity of the insulator combined with carefully chosen processing conditions permits the fabrication of tens of micrometer-thick films that feature a fine distribution of the F4TCNQ dopant:semiconductor complex.

The resulting ternary exhibits higher doping efficiency from 20 % to 40 % compared to binaries, while the thermal conductivity remains low $0.3 \text{ W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$. Free-standing, mechanically robust tapes (see Figure) illustrate the versatility of the developed dopant:semiconductor:insulator ternary blends. These tapes can resist strains of over 300 %, compared to less than 10 % for the binaries.

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A SUNDIAL THAT WORKS IN THE SHADE

Multiple polarization sensitive photodetectors can be prepared on a single substrate by controlling solvent evaporation during the deposition of conjugated polymer films.

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[1] Controlled Pinning of Conjugated Polymer Spherulites and Its Application in Detectors. *Advanced Optical Materials*, 2017, 5 (19), 1700276

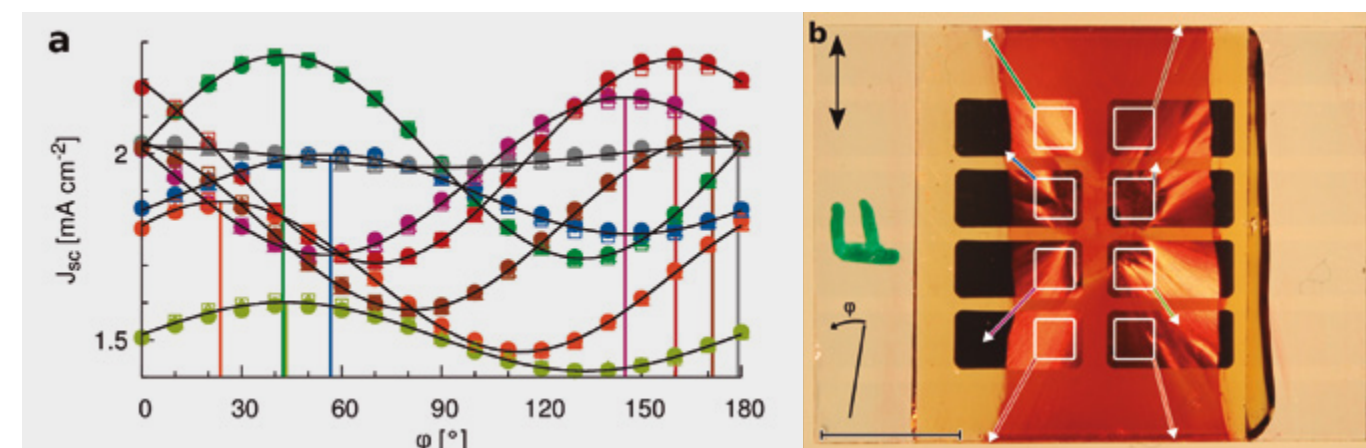


FIGURE
Photograph of a device containing 8 cells (right) as well as the corresponding polarization dependent photocurrents (left).

Typically, thin printed or coated films of conjugated polymers are optically isotropic, since at the nanoscale, the polymer chains are oriented randomly. By using additives that serve as nucleation sites during processing, large-scale orientation in the form of fibers or spherulites, circular polycrystalline crystallites, can be achieved. However, the resulting macroscopic orientation is still not well-controlled, because of the stochastic nature of nucleation. In this work, we show that by controlling solvent evaporation, the location of initial nucleation can be controlled, resulting in predictable and repeatable orientation of square-centimeter sized samples. Incorporating these films into the active layer of organic photovoltaic devices such as those shown in the Figure, multiple photodetectors with distinct polarization dependence on a single substrate can be manufactured. By measuring the photocurrent of several subcells, the intensity as well as the polarization state of the incident light can be determined, which allows these devices to be used as polarization sensors.

While direct sunlight is not polarized, the sky, like all reflected light, in fact is. The degree and orientation of this polarization depend on the position of the sun. By pointing this sensor towards the sky, these devices, like sundials, allow to determine the time of day, yet do not need direct line of sight towards the sun.

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SYNTHESIS OF NANOMETRIC ZIF-8 BY A SUSTAINABLE SUPERCRITICAL ROUTE

ZIF-8 nanometric particles are prepared via an environmentally friendly method using supercritical CO₂, aimed to minimize the environmental impact of the existing technologies for the synthesis of metal organic frameworks.

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JULIO FRAILE, GERARD TOBIAS, CONCEPCIÓN DOMINGO

[1] Supercritical CO₂ for the synthesis of nanometric ZIF-8 and loading with hyperbranched aminopolymers. Applications in CO₂ capture. **Journal of CO₂ Utilization**, 2017, 18, 147-155

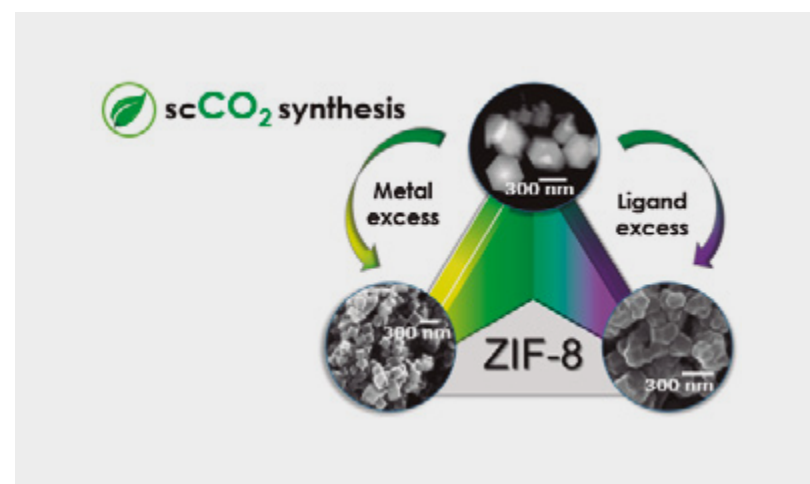


FIGURE
A straight and high yield precipitation of empty-pore ZIF-8 nanopowder with tunable morphology is achieved via an environmentally friendly supercritical CO₂ method.

During the last few years, microporous coordination polymers, or three-dimensional metal-organic frameworks (3D MOFs), with zeolitic topologies have become a major focus of research in advanced functional materials. These novel materials have relevance in diverse sorption applications, such as CO₂ capture or gas separation, heterogeneous catalysis and sustained drug release, to name some. ZIF-8, with formula [Zn(2-methylimidazole)₂] and sodalite topology, is currently one of the most extensively investigated zeolitic imidazole frameworks (ZIFs), a subclass of MOFs. The conventional solvothermal procedure described to synthesize ZIF-8 requires the use of dimethylformamide (DMF) and a heating period of 24 h at 140 °C. Micrometric particles are thus precipitated, but DMF molecules remain trapped inside the pore space and must be removed by solvent exchange in methanol, followed by vacuum drying; the whole preparation method lasting several days. For practical applications and a feasible scale-up, the development of

environmentally friendly, one-pot synthetic methods of fine particles of ZIF-8 is desirable. The process should afford the formation of ZIF-8 as a dry and empty-pore powder in a high yield, with the use of minimal amounts of expensive imidazole, whilst avoiding the need of additives or organic solvents. All these requirements have been successfully fulfilled in this work by using exclusively a green solvent, supercritical CO₂ (scCO₂), as the reaction medium (Figure).

These process characteristics would enable the scaling-up, while promoting their industrial use. By using a stoichiometric molar ratio of reagents, a post-synthesis washing step was not necessary and high yields were achieved. Microporous particles of nanometric sizes are either precipitated as dispersed primary particles or assembled into hierarchical macroporous structures. Remarkably, a crystalline sample of ZIF-8 constituted by particles in the size range of 100-300 nm and a BET specific surface area as high as 1700 m²·g⁻¹ was prepared by the proposed green process.

The reported protocol opens up new perspectives for the production of MOF nanoparticles in a cost efficient and environmentally friendly manner, and is expected to have significant implications for the development of MOFs sorption applications.

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LIGHT OUT OF SILICON

We use state-of-the-art theoretical calculations to show how to design silicon-based materials that can emit light.

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& RICCARDO RURALI⁴

[1] Optical Emission in Hexagonal SiGe Nanowires. **Nano Letters**, 2017, 17, 4753-4758

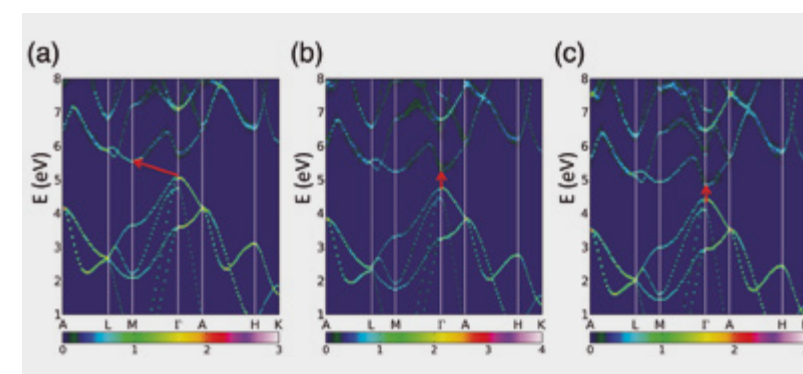


FIGURE
Band structures obtained with a band unfolding technique for (a) Si_{0.8}Ge_{0.2}, (b) Si_{0.7}Ge_{0.3} and (c) Si_{0.6}Ge_{0.4}. The bandgap becomes direct for hexagonal Si_{1-x}Ge_x alloys with $x \geq 0.3$.

According to a quote of uncertain attribution “The easiest way to get light out of silicon (Si) is taking a Si wafer, drill a hole into it and put a light bulb behind it!” This paradoxical sentence intends to highlight in, admittedly, a funny way how disappointing the many research efforts to make silicon a material for photonics have been thus far. Indeed, efficient light emission is not among the many remarkable properties of silicon and this limitation has hindered the development of silicon-based optoelectronic devices. Considerable work has been done to find optically active materials that are fully compatible with silicon technology, but clearly the *Holy Grail* keeps on being the luminescence out of bulk monocrystalline silicon. The reason for the poor emission efficiency of Si is the indirect nature of its fundamental bandgap. When electrons are excited to the conduction band, their decay to the valence band with the emission of a photon must involve a transfer of momentum to the crystal lattice by means of a phonon a quantum of lattice vibration to guarantee its conservation. The need to absorb or emit a phonon makes the photon emission process so slow that in practice most of the recombinations will happen non-radiatively.

Recent advances in the synthetic growth of nanowires have given access to crystal phases that in bulk are only observed under extreme pressure conditions. The advent of these novel Si polymorphs, such as hexagonal Si, promises to overcome some of the limitations that have kept Si out of the photonic arena thus far. The bandgap of hexagonal Si is smaller than the one of cubic Si but is still indirect. On the other hand, hexagonal Ge is predicted to have a direct bandgap. This fact could have important implications with respect to the long-standing goal of designing a Si-based light-emitting material as it suggests that a hexagonal Si_{1-x}Ge_x alloy could become a direct bandgap semiconductor for sufficiently high Ge content, x. We have used state-of-the-art theoretical modeling to predict the electronic and optical properties of hexagonal Si_{1-x}Ge_x nanowires, show that the bandgap can become direct, and assess which is the minimum Ge content for this to happen (Figure). We compute the optical properties demonstrating that the direct radiative transition is permitted and that it will be the dominant recombination mechanism. Further increasing the Ge content beyond the minimum threshold needed to obtain a direct bandgap allows tuning the emission at expenses of a larger lattice mismatch with pure Si, providing a way to tune the absorption spectrum for versatile photovoltaic applications.

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CHEMICAL MAPPING OF COMPOUNDS DISCHARGED IN ALKALI METAL-OXYGEN BATTERIES BY X-RAY TRANSMISSION MICROSCOPY

A novel analysis method has been developed to observe the spatial arrangement of different compounds forming discharge deposits in cathodes of aprotic metal-oxygen batteries. The images revealed unexpectedly complex architectures

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TEÓFILO ROJO,^{2,6} DINO TONTI¹

[1] Discharge products of ionic liquid-based Li-O₂ batteries observed by energy dependent soft x-ray transmission microscopy. **Journal of Power Sources**, 2017, **359**, 234–241

[2] Architecture of Na-O₂ Battery Deposits Revealed by Transmission X-ray Microscopy. **Nano Energy**, 2017, **37**, 224–231

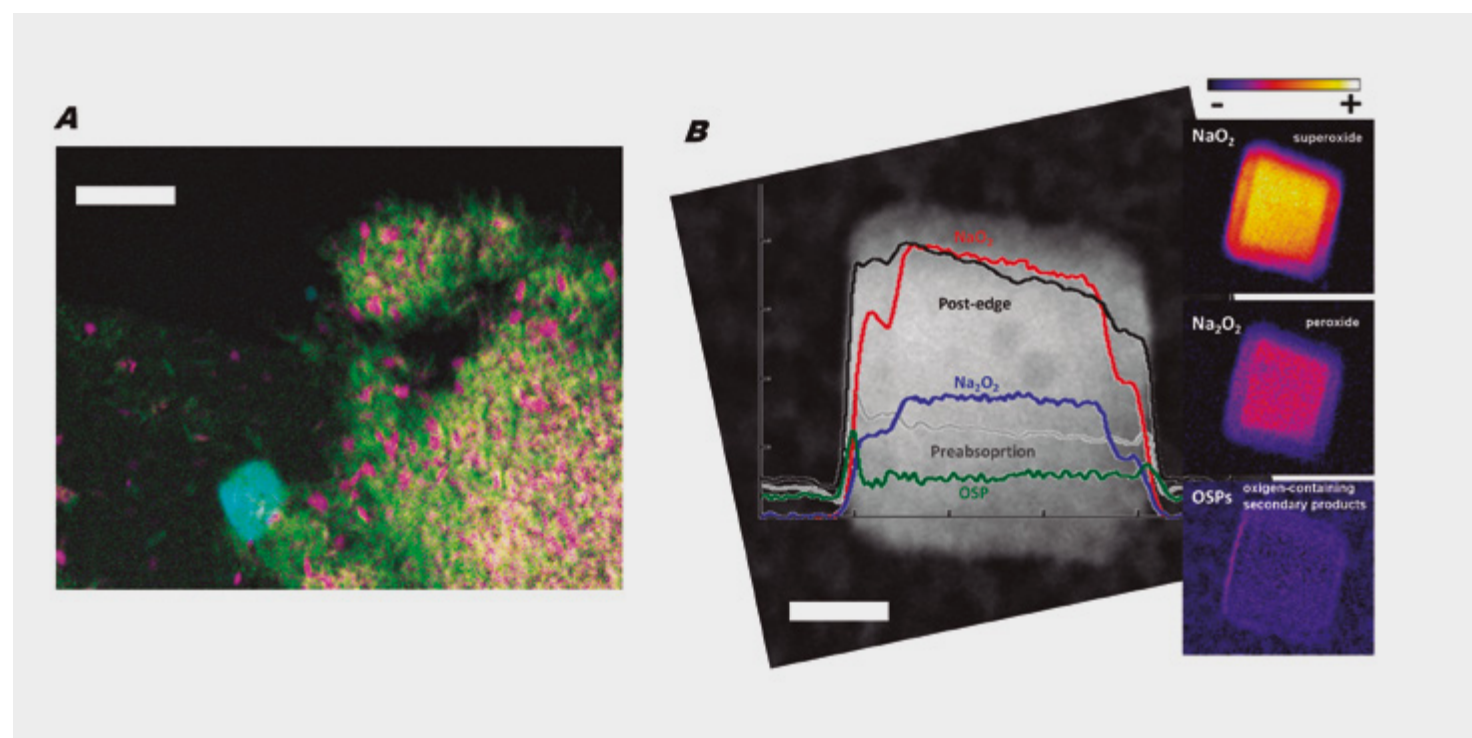


FIGURE
X-ray transmission microscopy maps of deposits on discharged metal-oxygen cathodes, bar corresponds to 1 μm . A) Li/O₂ cathode; components are represented in different colors: superoxide (yellow), peroxide (magenta), hydroxide (green), and ice (cyan). B) Na/O₂. Left: concentration profiles of the different compounds along the discharge product (cubic-shaped) of a sodium-oxygen battery. Right: maps of oxygen distribution.

microscopy available at the MISTRAL beamline of the ALBA synchrotron. This technique allows distinguishing at the nanoscale between different regions of the deposits formed, according to the quantity and the chemical state of the oxygen present. Soft X-ray spectromicroscopy offers excellent sensitivity to oxygen and other light elements, high energy resolution, low noise and larger penetration depth, which makes it possible to detect compounds even if not crystalline, or to study micrometric particles, overcoming limits of more conventional techniques. Unprecedented detail of the architecture of typical deposits, which allows a better understanding of their formation mechanisms, the influence of parasite reactions, and possible obstacles to their dissolution expected during charging, are achieved.

In a work published on Journal of Power Sources [1], the higher stability of room temperature ionic liquid electrolytes in Li/O₂ batteries has been explained by the absence of decomposition products such as carbonates, which instead rapidly form when the sample is exposed to air. The deposits (Figure A) also show separate LiOH particles, likely favored by water traces, which however do not appear as a barrier to peroxide dissolution.

In a report in the journal Nano Energy [2], both products expected in Na/O₂ batteries (sodium peroxide and superoxide) have actually been identified in discharged electrodes, and decompose almost simultaneously while charging. In addition to these two oxides, a complex structure of several layers formed by electrolyte decomposition products is observed at their surface (Figure B). Even if the complete deposit decomposition may explain the

superior cycle life compared to lithium-oxygen batteries, these findings indicate that further improvements in the electrolyte formulation are required for a long-term stability.

In general, these observations reveal a much more complex reality compared to what expected by the ideal discharge/charge reactions, but the information provided by this tool offers possibilities to elaborate strategies for more efficient metal-air batteries.

The search for the next-generation batteries has recently focused on rechargeable metal-oxygen batteries, considered very attractive as room-temperature devices with high theoretical energy densities (comparable to gasoline) for application in electrical vehicles. These batteries when using aprotic electrolytes form oxides during the discharging process, which then ideally decompose into the metal ions and oxygen when charging. Lithium-oxygen systems have been largely studied, as they promise highest energy density and an exceptional specific capacity. However, recent studies found that solid products that are difficult to remove are formed, diminishing the battery

performance. The extent of these side reactions strongly depend on the electrolyte composition.

Sodium-oxygen batteries can be an interesting alternative given the earth-abundance of sodium, and especially because they often show a more attractive cycle life. Most authors report that no sodium peroxide (Na₂O₂) is formed during the discharge process; instead, sodium superoxide (NaO₂) is formed. This compound forms in only one-electron transfer step and is believed to decompose more easily upon charging.

We have analyzed the discharge products of these batteries by adapting energy-dependent transmission soft X-ray

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AN ATOMISTIC INTERACTION MODEL OF THE WATER-TITANIUM DIOXIDE INTERFACE TO EXPLORE MECHANISMS OF PHOTOCATALYSIS

Atomic scale understanding of liquid-water interaction with photocatalytic interfaces by surface X-ray diffraction and local probe techniques

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[1] Structure of a model TiO₂ photocatalytic interface.
Nature Materials, 2017, 16 (4), 461-466

FIGURE
Selected reflections (CTRs: Crystal Truncation Rods) from surface x-ray diffraction measurements (SXRD) together with the proposed models. a, Structure factors corresponding to the adjustment of the different TiO₂ (110) surfaces for (0,1,1), (1,2,1) and (2,1,1) CTRs. The error bars in black, red and blue represent the experimental data of the surface measured in vacuum (UHV), immersion in water, and exposure to a drop of water, respectively, while the continuous lines correspond to the data calculated by each of the models. The vertical notches on the x-axis show the Bragg peaks. b-d, Ball model for clean samples / UHV, immersion and exposure to a drop of water, respectively. e, Representative model of the rutile TiO₂ interface (110) with water.

Understanding the interaction of water with titanium dioxide (TiO₂) surfaces is crucial due to the important implications of TiO₂ in many usages, including solar energy conversion through photocatalytic water splitting. The significant technological advances in this field contrast with the poor knowledge of the processes occurring on their surfaces at atomic scale, needed to boost performance.

Numerous studies on TiO₂/water interfaces have provided an atomic-level understanding of this interface, although the emphasis has been on the gas-phase water interface with TiO₂. However, it is clear that the liquid/solid interface is more relevant for practical applications. We employ a novel approach to provide the first quantitative structure of a well-defined metal oxide/water interface, which also represents a model of the interface present in the rutile TiO₂ photocatalyst. More specifically, we perform both ex-situ and in-situ measurements of the liquid water/TiO₂ interface in an aerobic environment, formed by either temporarily immersing a rutile TiO₂ surface into water or by depositing a water droplet on top.

The surfaces were characterized using scanning tunnelling microscopy techniques (STM) at UCL and Surface X-ray diffraction (SXRD) measurements at the European Synchrotron Radiation Facility (ESRF) in Grenoble. These techniques provide the potential means to elucidate the structure of this model photocatalytic interface at a quantitative level, which is formed by terminal hydroxyls in contact with the TiO₂ surface layer. STM measurements evidence the formation of an ordered hydroxyl overlayer formed after dipping that covers the 50 % of the surface oxide. The SXRD results identify the bonding sites

with five-fold coordinated Ti atoms. This model together with density functional theory calculations suggest a mechanism for the way in which these hydroxyl molecules align on the metal oxide surface as a half monolayer, corresponding to a (2 x 1) structure: thought to be through the mixed dissociation of O₂ and H₂O on a rutile surface containing point defects. Stability of the overlayer was shown to rely on a competition between charge transfer arising from the presence of defects and the surface distortion due to the adsorption of the hydroxyls.

Figure (a) shows selected SXRD results in the form of crystal truncation rods (CTRs) recorded from the H₂O_{dip} surface together with those from the as-prepared UHV (Ultra High Vacuum) surface. Proposed models (b,c,d), for clean, H₂O_{dip} and H₂O_{drop} surfaces are supported by DFT calculations. Figure 1 (e) shows the water/TiO₂ interface model derived from experiment and theory. The water/TiO₂(110)-(2x1) interface has not been anticipated in aqueous environment and is different from what has been established for water on TiO₂(110) under UHV conditions

The model photocatalytic interface provided from accurate experimental data lays the foundations to the investigation of the elementary steps involved in water splitting under operating aqueous conditions. This may ultimately lead to an atomistic-level understanding of the photocatalytic process of water splitting, which would allow the design of more efficient devices.

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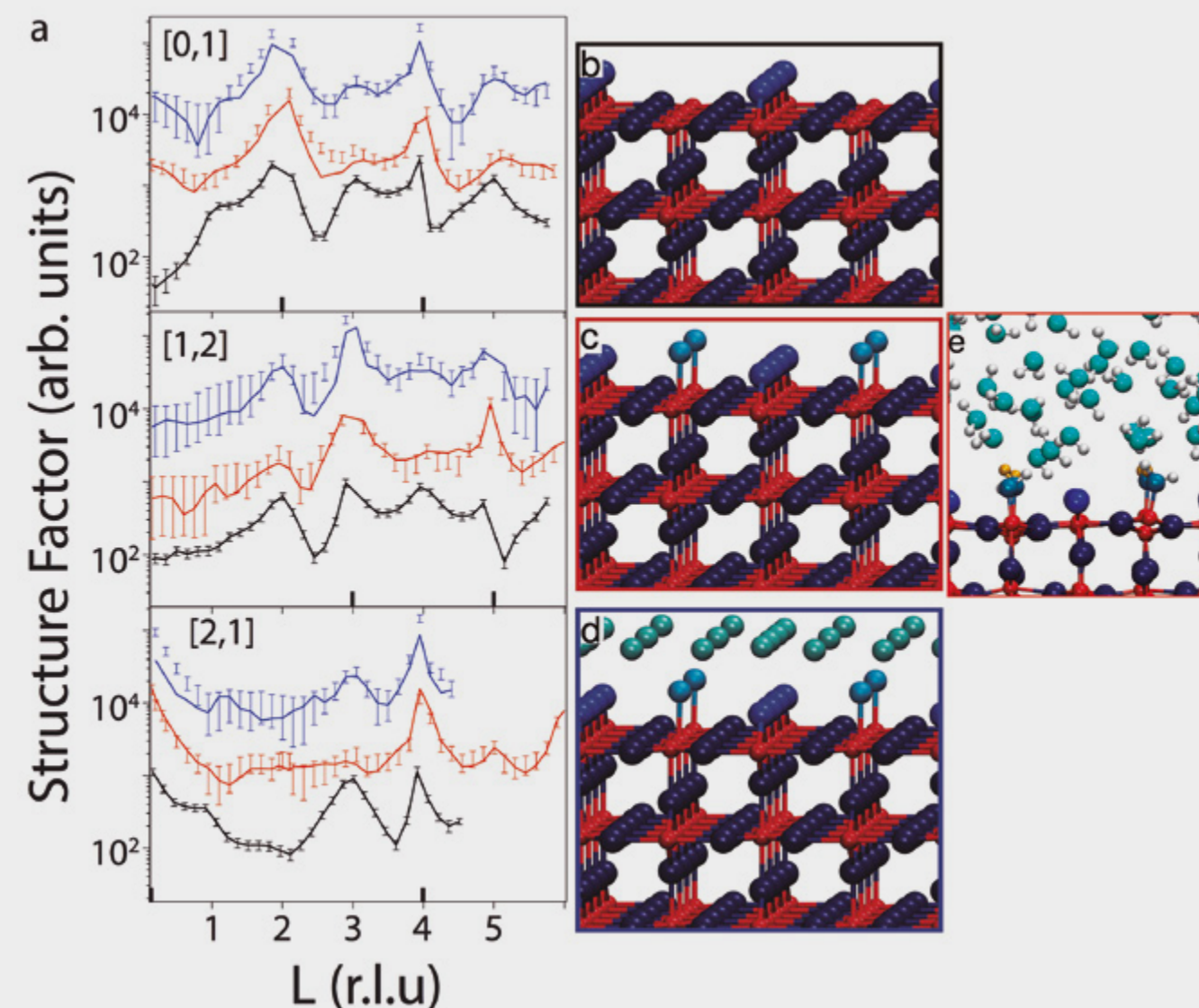
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⁶Corrosion and Protection Centre, School of Materials, The University of Manchester, UK

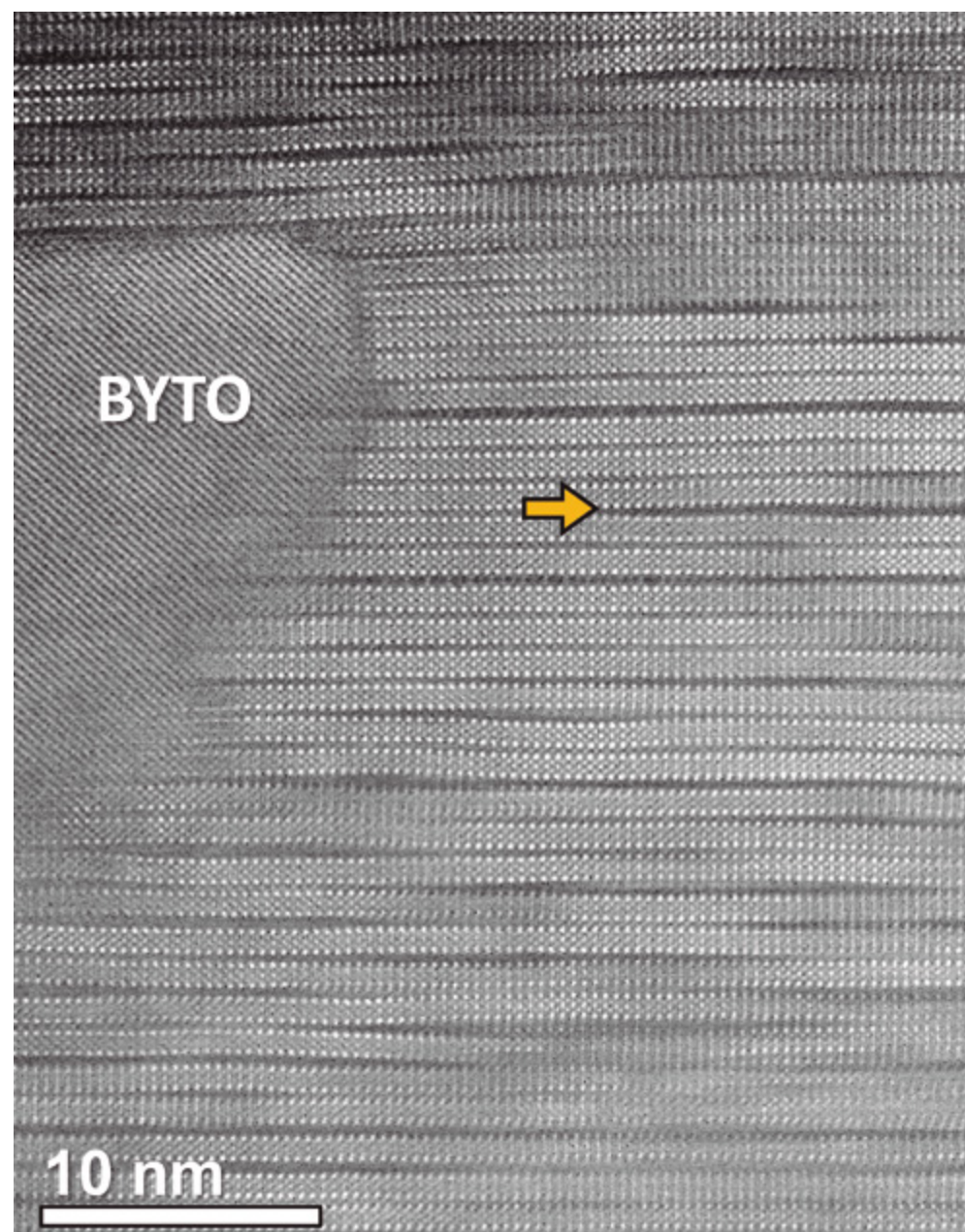


UNRAVELLING OPPORTUNITIES OF SOLUTION-DERIVED SUPERCONDUCTING NANOCOMPOSITES

YBCO superconducting nanocomposites formed by chemical solution deposition method: study of individual defects, formation of hybrid superconducting-ferromagnetic nanocomposites and optimization of oxygenation kinetics

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FIGURE
Z-contrast STEM image from YBCO nanocomposite with Ba_2YTaO_6 nanoparticles surrounded by a large amount of Y248 defects. The yellow arrow shows one of the Y248 defects.



[1] Hybrid $\text{YBa}_2\text{Cu}_3\text{O}_7$ Superconducting-Ferromagnetic Nanocomposite Thin Films Prepared from Colloidal Chemical Solutions. **Adv. Electron. Mater.** **2017**, **3**, 1700037

[2] Probing localized strain in solution-derived $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ nanocomposite thin films. **Phys. Rev. Materials**, **2017**, **1**, 024801

[3] Untangling surface oxygen exchange effects in $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ thin films by electrical conductivity relaxation. **Phys. Chem. Chem. Phys.**, **2017**, **19**, 14129

The outstanding field of superconducting nanocomposites has demonstrated, in the last decade, the power of artificially induce controlled pinning centres in $\text{YBa}_2\text{Cu}_3\text{O}_7$ (YBCO) films with scalable techniques. Methodologies based on physical and chemical approaches have incorporated these strategies for growth of long length coated conductors, i.e. epitaxial multilayers with an active superconducting film grown on flexible substrates.

Nowadays, several companies have introduced superconducting nanocomposites in their production lines. Yet, chemical solution deposition (CSD) has been one of the most powerful methodologies for its low cost. In these three articles we unravel some of the powerfulness of the CSD method to reach high superconducting properties by a thorough understanding of the process consequences. In particular, we use scanning transmission electron microscopy (STEM) to study the atomic structure of most relevant individual defects in solution-derived YBCO nanocomposites. The inclusion of incoherent secondary phase nanoparticles within the YBCO matrix dramatically increases the density of $\text{YBa}_2\text{Cu}_4\text{O}_8$ (Y248) intergrowths. Its formation is found to trigger a concatenation of strain-derived interactions with other defects and the concomitant nucleation of intrinsic defects, which weave a web of randomly distributed nanostrained regions that profoundly transform the vortex-pinning landscape of CSD YBCO nanocomposite thin films [1]. We then extend this study to demonstrate the capability of the CSD route to grow hybrid YBCO-ferromagnetic nanocomposite epitaxial films from preformed spinel ferrite (MFe_2O_4 , M = Mn, Co) nanoparticles.

Results show that during the YBCO growth process, most of the nanoparticles evolve to ferromagnetic double-perovskite phases ($\text{YBaCu}_{2-x-y}\text{Fe}_x\text{Co}_y\text{O}_5/\text{YBaCoFeO}_5$). The hybrid nanocomposites described opens the study of fundamental questions like magnetic vortex pinning in superconducting/ferromagnetic heterostructures [2].

Finally, we show that the oxygenation kinetics of YBCO films, one of the most relevant processes for ensuring high critical currents but also one of the less studied ones, is limited by surface exchange process of oxygen molecules prior to bulk diffusion into the films. We have used electrical conductivity relaxation measurements to determine the most likely rate limiting step and established a strategy to accelerate the oxygenation kinetics at low temperatures based on the catalytic influence of Ag coatings, thus allowing us to strongly decrease the oxygenation temperature of YBCO films [3].

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STRAY MAGNETIC FIELD COMPETITION IN SUPERCONDUCTOR-FERROMAGNETIC HYBRID SYSTEMS

We elucidate the interplay between superconducting-ferromagnetic stray magnetic fields in hybrid systems, formed by an inhomogeneous superconducting film combined with ferromagnetic nano-rods.

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[1] Competition between Superconductor - Ferromagnetic stray magnetic fields in YBa₂Cu₃O_{7-x} films pierced with Co nano-rods. **Scientific Reports, 2017, 7, 5663**

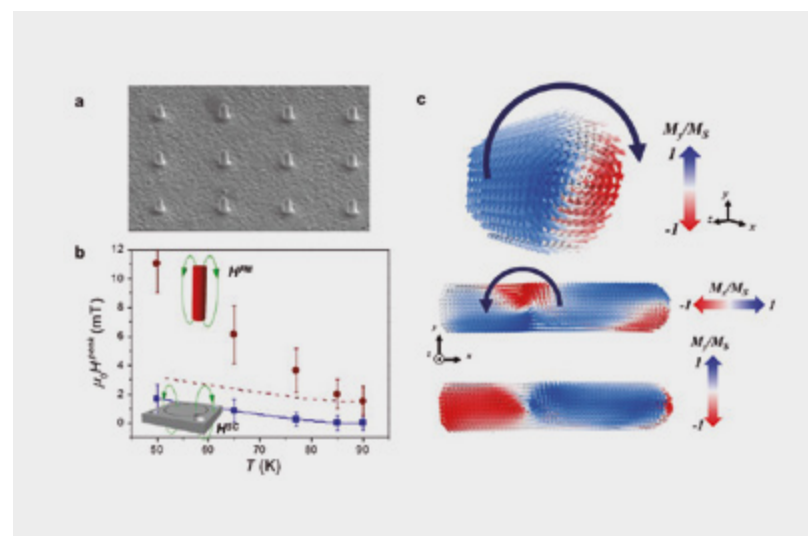


FIGURE
(a) Tilted SEM picture of SC-FM hybrid system.
(b) Temperature dependence of SC and FM stray magnetic fields. Dashed line shows the expected dependence without SC-FM interactions.
(c) Micromagnetic simulations showing the 3D remanent magnetic state of a Co nano-rod.

The understanding of cooperative phenomena in superconductor (SC)-ferromagnetic (FM) systems has a crucial role from a fundamental point of view and in practical applications. Exploring novel interactions in SC-FM hybrid systems can lead to the design of novel physical properties and complementary unique functionalities.

In this work we investigate specially designed hybrid systems based on high temperature SC (YBa₂Cu₃O_{7-x}) films, patterned with antidots, and filled with FM (Co) nano-rods, grown by focused electron beam induced deposition (FEBID) (Figure-1a). These systems exhibit novel SC-FM interactions arising from the synergic influence of stray magnetic fields coming from Co nano-rods, H^{FM} , and trapped inhomogeneous magnetic fields generated by supercurrent loops, H^{SC} , (Figure 1-b). Direct competition between these two stray magnetic fields is possible since the patterned YBa₂Cu₃O_{7-x} films are able to

generate large SC trapped fields, essentially negligible in conventional low temperature superconductors. Besides, Co nano-rods grown by FEBID offer the possibility to produce complex three-dimensional (3D) spin textures, which provide a third dimension in controlling magnetic states at the nanoscale (Figure 1-c).

We have combined electric transport measurements with X-ray photoemission electron microscopy (X-PEEM) and micromagnetic simulations to elucidate the interplay between competing SC-FM phenomena. We show that both the superconducting properties of the SC film and 3D magnetic state of FM nano-rods can be tuned by cooperative non-homogeneous SC-FM stray fields.

The work opens up a new avenue for the ad-hoc design of hybrid systems in which the magnetic field cooperation can yield new functionalities and phenomena such as the possibility of tailoring pinning of vortices in the superconductor or 3D magnetic domains in the nano-rods, which will be important for the operation of fluxonic and spintronic devices.

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THERMAL AND ELECTRIC CONTROL OF HIDDEN AND SLOW DYNAMIC MAGNETIC STATES

Magnetic states can be hidden and retrieved either by thermal and electric means at near room temperature in iron-rhodium (FeRh) films

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[1] Electric-Field-Adjustable time-dependent magnetoelectric response in martensitic FeRh alloy. **ACS applied materials & interfaces, 2017, 9 (18), 15577-15582**

[2] Hidden Magnetic States Emergent Under Electric Field, In A Room Temperature Composite Magnetoelectric Multiferroic. **Scientific Reports, 2017, 7 (1), 15460**

FIGURE
Sketch of the hiding process by thermal means. Bar code filling corresponds to real magnetic domain images collected at high (top) and low (bottom) temperature and plotted using the same color scale for the ferromagnetic (visible) and antiferromagnetic (invisible) states, respectively



Information that requires being stored for a long time is usually stored in different sorts of magnetic media: hard disks, tapes, etc. The appearance of magnetic memories has encompassed the appearance of illicit copies, which must be avoided in the case of very sensitive information, i.e. information contained in credit cards, identification cards, or certificates of authenticity. Information can be mathematically encrypted. However, industry demands higher degree of security by hiding magnetic information at the materials level. In this work [1,2] we show that magnetic information can be stored in iron-rhodium (FeRh) films. FeRh is ferromagnetic at high temperature ($\approx 100^\circ\text{C}$) and therefore magnetic information can be stored in it. However, at room temperature it is antiferromagnetic, thus magnetically invisible. We use this uncommon property to store, hide and retrieve magnetic information. Store and retrieving processes are done at high temperature, where the ferromagnetic state sets in. The hiding process is demonstrated to be possible either by thermal or electric means (Figure). The former is performed by simply cooling down the material at room temperature. The latter can be done using piezoelectric materials as a substrate for the FeRh film. Electric field applied to the piezoelectric substrate causes deformation on the FeRh that is used to unbalance the amount of ferromagnetic and antiferromagnetic regions in the material. We have also observed that the formation of the antiferromagnetic phase at expenses of the ferromagnetic ones, if the effect is mediated by electric field, is extremely slow at the scale of seconds. Therefore, information is only seen by short period of time.

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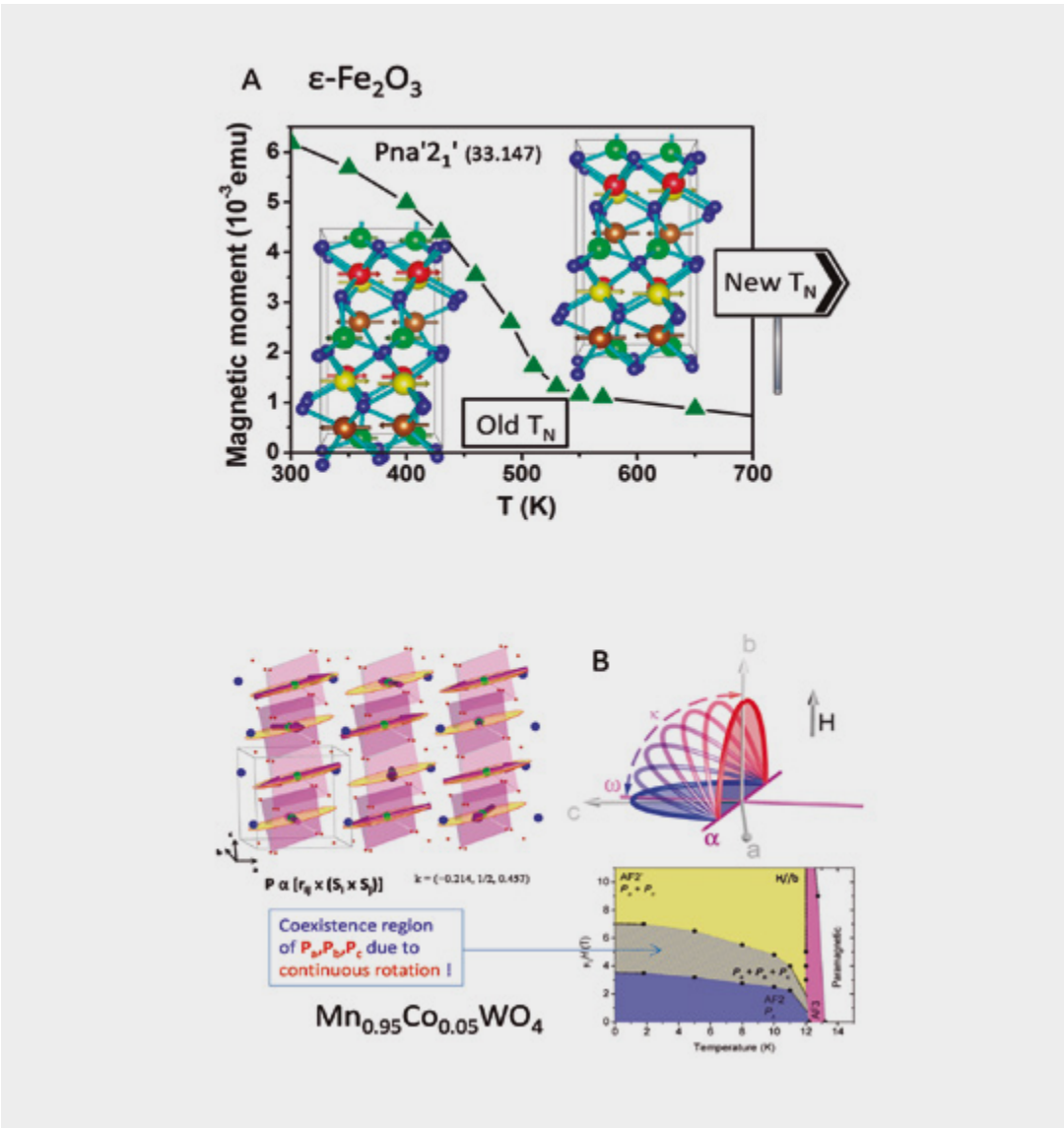
MAGNETIC CRYSTALLOGRAPHY OF MULTIFERROIC OXIDES PRESENTING SPIN-ORBIT COUPLING

Unveiled new functional ordered magnetic phases at high temperatures or under external magnetic fields in frustrated multiferroic oxides using neutron and synchrotron techniques

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[1] Unveiling a new high-temperature ordered magnetic phase in ϵ -Fe₂O₃. **Chemistry of Materials** 29 (2017) 9705-9713
[2] Magnetic field-induced phase transitions and phase diagrams of Mn_{0.95}Co_{0.05}WO₄ multiferroic with cycloidal spin structure. **Physical Review B** 96(10) (2017) 104435

FIGURE
A: The temperature dependence of the magnetization at 50 kOe in ϵ -Fe₂O₃ and the two distinct ferrimagnetic orderings identified below and above 500 K.
B: Cycloidal magnetic ground state of ferroelectric Mn_{0.95}Co_{0.05}WO₄. Easy α and hard ω magnetic axes within the ac plane. For $H//b$ a flop of the magnetic moments from the ab to the $\omega\omega$ plane occurs continuously via a rotation of the cycloidal plane around the α axis ("angular phase").



In improper multiferroics, magnetism is coupled to ferroelectricity (FE) so that the configuration of magnetic moments may be modified by an external electric field and, conversely, the electrically polar state may be magnetically switched. Together with their potential interest as fundamental components in electronic devices such as energy-efficient FE random access memories, understanding the interplay between magnetism and ferroelectricity is of interest in fundamental research into quantum matter. New findings are presented in two relevant magnetoelectric compounds (ϵ -Fe₂O₃ and Mn_{0.95}Co_{0.05}WO₄) that exhibit magnetic frustration and significant spin-orbit coupling. Iron oxides have been studied for many decades because of their biochemical, magnetic, catalytic, or multiferroic properties. The acentric (Pna2₁) ϵ -Fe₂O₃ has four different Fe sites, and it shows a huge RT coercivity, 20 kOe, very attractive for high-density magnetic recording or high-frequency electromagnetic absorption applications, in addition to magnetoelectric and multiferroic properties. Our study of ferrimagnetic ϵ -Fe₂O₃ refutes the current belief that its magnetic ordering occurs around 500 K (below that of hematite, magnetite or maghemite). Whereas the magnetization of ϵ -Fe₂O₃ nanoparticles, its coercivity and remanence sharply drop and virtually vanish around 500 K, our neutron diffraction study reveals the presence of a new ferrimagnetic order well above 500 K with Pna'2₁' magnetic symmetry, but only involving two of the four Fe³⁺ sublattices. So, the presence of a new high-temperature ferrimagnetic phase with T_{N1} ~ 850 K was unveiled. Moreover, synchrotron results confirm that ϵ -Fe₂O₃ presents a huge spontaneous magnetostriction at the hard-soft transition near T_{N2} ~ 500K, where the hard phase is presumably stimulated by a nonzero orbital angular moment. These findings in ϵ -Fe₂O₃ may open the door to further expand the working range of this multifunctional iron oxide. The spin-orbit coupling is also the responsible for the non-collinear incommensurate magnetic orders that generate chiral ferroelectric phases in frustrated Mn_{1-x}Co_xWO₄ multiferroics. So, the ground state of Mn_{0.95}Co_{0.05}WO₄ is a ferroelectric phase induced by cycloidal spin ordering of the metal ions. In this improper multiferroic the complete magnetoelectric

phase diagrams for magnetic fields applied along distinct directions in relation to the cycloidal spin structure have been determined and described. Neutron diffraction (<12T), polarization and magnetic measurements (<60T) were performed on oriented quality single crystals, revealing how the field-induced magnetic structures evolve together with the corresponding evolution of the electric polarization P. The existence of nonpolar sinusoidal phases (for which P=0) was observed preceding the spin-flip transitions into the paramagnetic state. At moderate fields, not only the relevant field-induced magnetic structures up to 12 Tesla were solved but, in addition, the ways they proceed were tracked by single crystal neutron diffraction, identifying and refining some appealing intermediate spin and ferroelectric configurations. So, if the direction of the field is applied along the easy-axis α in the cycloidal plane an abrupt spin-flop transition occurs to a state perpendicular to the field direction. However, we have proved that when the magnetic field is applied perpendicular to α in the cycloidal plane, then the flop occurs continuously via a "continuous rotation of the cycloidal plane around α " (and of the electric polarization vector), producing what we have called an angular cycloidal phase.

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DIRECT PIEZOELECTRIC FORCE MICROSCOPY: A NEW RELIABLE SCANNING PROBE MICROSCOPY MODE TO STUDY FERROELECTRICS AT THE NANOSCALE

Direct Piezoelectric Force Microscopy is a new approach to study ferroelectrics with nanoscale resolution based on the direct piezoelectric effect, providing a stable, reliable and quantitative characterization platform

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[1] Piezogenerated charge mapping through direct piezoelectric force microscopy. **Nature Communications, 2017, 8, 1113.**

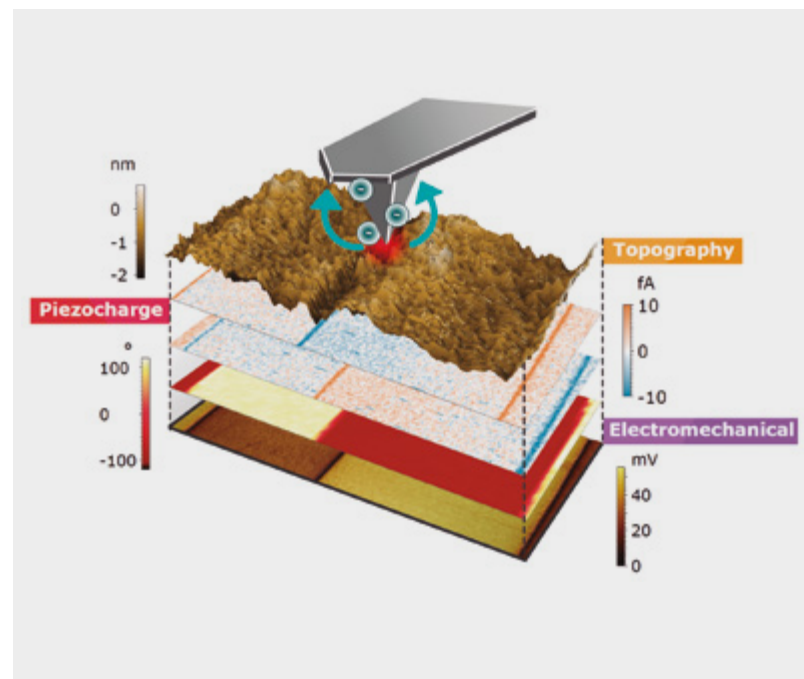


FIGURE 3D composition mapping obtained from the new DPFM mode. Both the piezo-generated charge, the electromechanical behavior and topography are obtained for a sample composed of Periodically Poled Lithium Niobate (PPLN).

The piezoelectric effect, the dielectric polarization of non-centrosymmetric crystals under a mechanical stress, was discovered by the Curie brothers in 1880. Also, they shortly after reported the predicted converse effect, i.e. that a piezoelectric material would be mechanically strained by an applied electric field. Since those early discoveries, the unique ability of piezoelectrics and ferroelectrics for interconverting mechanical and electric energy has endlessly inspired technological developments and these materials are found in many everyday applications. Yet, the basic understanding of piezoelectricity and ferroelectricity is challenged and reshaped by findings that come along with new developments in

the materials characterization. Namely, the characterization technique Piezoresponse Force Microscopy (PFM) has brought a new perspectives of the complexity and properties of ferroelectric materials. PFM exploits the converse piezoelectric effect by measuring the material deformation under an AC electric field applied through a contacting cantilever tip. Despite the high potential of the technique, it cannot be used to distinguish ferroelectricity from a Material Under Test (MUT) nor it can be used as a quantification technique. Overcoming these limitations prompted us to investigate on new characterization techniques based into AFM to measure piezoelectricity and ferroelectricity in a reliable manner, with nanoscale resolution. By using an AFM tip, a strain is applied to the material while a specific low leakage current amplifier collects the piezo-generated charge built up by piezoelectric effect. The mode provides simultaneous acquisition of topography channel, electromechanical response and piezo-generated charge build up (Figure). From this approach, we introduce a new AFM mode called Direct Piezoelectric Force Microscopy (DPFM), opening a new page into the portfolio of characterization techniques based in AFM.

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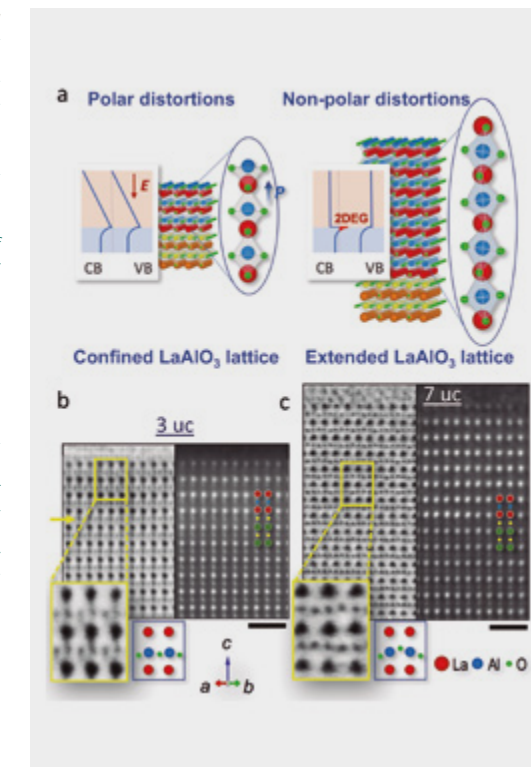
COMPETING STRUCTURAL PHASES IN QUANTUM CONFINED PEROVSKITES

Scanning transmission electron microscopy (STEM) and first-principle models demonstrate the competition between structural phases intertwined with transport properties in a quantum-confined perovskite system

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[1] Competition between Polar and Nonpolar Lattice Distortions in Oxide Quantum Wells: New Critical Thickness at Polar Interfaces. **Physical Review Letters, 2017, 119, 106102**

FIGURE (a) Polar and nonpolar antiferrodistortive (AFD) tilts in $\text{LaAlO}_3/\text{SrTiO}_3$ heterostructures. Schematic structures of the polar displacements and octahedral tilts in LaAlO_3 film of thicknesses below and above the critical one for 2DEG formation in SrTiO_3 : < 4 u.c. (left panel) and > 4 u.c. (right panel), respectively. (b-c) Atomic-scale mapping of the interface. Upper panel, b-c) Z-contrast (right) and ADF (left) simultaneously acquired STEM images of 3- and 7-uc-thick $\text{LaAlO}_3/\text{SrTiO}_3$ samples, respectively, viewed along the [110] zone axis. The [110] pseudocubic projection allows visualizing the buckling of the O sublattice. Lower panel, zoomed out regions of the ADF images of the 3- and 7-uc-thick LaAlO_3 layers along with schematics of the LaAlO_3 structure showing the distortions revealed by the ADF images, being La in red, Al in blue and O in green. Scale bar, 1 nm.



The broad family of perovskites hosts an extraordinary range of functional properties embracing, among others, magnetism, ferroelectricity or superconductivity. A clue to this astonishing versatility is the capability of perovskites to admit distortions from the ideal cubic reference structure, which leads to different deformations, such as buckling, tilting, rotations or elongations of the octahedral structural units. In turn, these lattice deformations modulate the ionic bonds between the constituent atomic species, fine-tuning the physical properties. Overall, two basic lattice distortions permeate the structural phase diagram of oxide perovskites: antiferrodistortive (AFD)

rotations and tilts of the oxygen octahedral network and polar ferroelectric modes. With some notable exceptions, these two order parameters rarely coexist in a bulk crystal, and understanding their competition is a lively area of active research. We analyzed such competition in a particular system, the $\text{LaAlO}_3/\text{SrTiO}_3$ interface. What makes this system particularly interesting is that -unlike most perovskites- polar structures and AFD-distorted structures are very close in energy and there is a genuine competition between these lattice distortions. Interestingly, by exploiting quantum confinement we shifted the balance between AFD and polar modes and selectively stabilize one of the two phases. These results, confirmed by combining scanning transmission electron microscopy (STEM) and first-principles-based models, demonstrate the existence of a crossover between states in which AFD rotations prevail, to strongly polar states with no AFD tilts. Remarkably, these structural changes are concomitant with a metal-insulator transition that leads to the emergence of a highly conductive 2DEG. This observation beautifully illustrates how sensitive perovskite are to lattice distortions and provide plentiful insights towards nanoscale control of material properties.

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MAGNETISM GOES SURFING

The article presents a direct imaging of the simultaneous evolution of both strain and magnetization dynamics of nanostructures at the picosecond time scale

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[1] Direct imaging of delayed magneto-dynamic modes induced by surface acoustic waves. **Nature Communications, 2017, 8, 407**

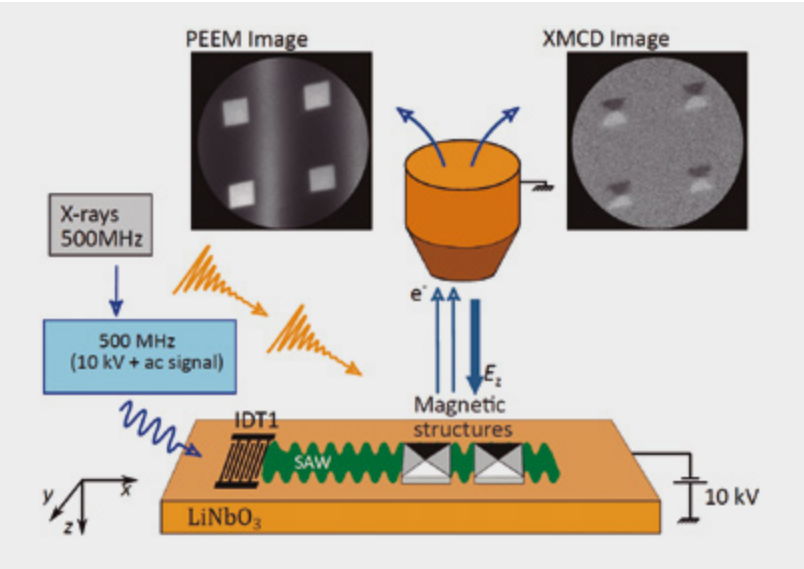


FIGURE Schematic plot of the experimental set-up. Circularly polarized X-rays illuminate the sample in the form of 20 ps pulses with a repetition rate of 500 MHz. The inter-digital transducer, IDT1, of the hybrid device receives an AC electric signal of the same frequency, which is phase locked to the synchrotron repetition rate, generating a piezoelectric surface acoustic wave that propagates through the substrate (LiNbO₃) and interacts with the magnetic nanostructures. The phase-resolved variation of the piezoelectric voltage at the surface sample is probed with the PEEM, as well as the magnetization contrast along the X-ray propagation direction arising from the XMCD effect. The two images show four 2x2 μm² Ni squares in presence of a piezoelectric wave. The PEEM image shows black and white stripes indicating the sign of the piezoelectric voltage whereas the XMCD image of the same structures shows magnetic-domain structures within the micrometric squares.

Magnetization states in magnetic materials are fundamental building blocks for constructing memory, computing, and further communication devices at the nanoscale. Static magnetization states such as magnetic domains are being used in non-volatile memories, whereas dynamic excitations—spin-waves—might serve to transmit signals and encode information in future electronic devices. Collective magnetization states are traditionally modified through magnetic fields created with electrical currents, which entail heat dissipation and stray fields. A promising strategy for handling high-speed magnetic moment variation at the nanoscale together

with low-power dissipation is the use of electric fields. Although direct effects of electric fields on magnetic states are weak, electric fields can be used to induce strain and elastic deformations in a nanoscale magnetic material that might result in changes of magnetic properties as shown mostly by static experiments. Surface acoustic waves (SAWs) are propagating strain waves that can be generated through oscillating electric fields at the surface of piezoelectric materials. SAWs have been used to induce magnetization oscillations in magnetic materials and to achieve assisted reversal of the magnetic moment but no direct measurement of the coupling were done so far. A direct measurement of the dynamic coupling between SAWs and magnetization requires resolving simultaneously strain and magnetization signals at the relevant time and space scales, which are picosecond and nanometer scales respectively. This article describes the effect of dynamic strain accompanying a surface acoustic wave on magnetic nanoelements. A technique based on stroboscopic X-ray microscopy is used to image simultaneously the evolution of both strain and magnetization at the nanometer and picosecond timescales (see figure). The study shows that there is a delayed response of the magnetization to the dynamic strain, adjustable by the magnetic material properties. The presented quantitative measurements provide an insight into dynamic magnetoelastic coupling in nanostructures with implications in the design of strain-controlled nano-devices.

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NOVEL FUNCTIONALITIES AT FERROIC DOMAIN WALLS

Our studies are based on first-principles density-functional theory calculations, which we combine with continuum models in a "multiscale" fashion to bridge the gap between the microscopic and macroscopic worlds

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[1] Macroscopic Polarization from Antiferrodistortive Cycloids in Ferroelastic SrTiO₃. **Phys. Rev. Lett., 2017, 119,137601**
[2] Functional electronic inversion layers at ferroelectric domain walls. **Nature Materials, 2017, 16, 622-627**

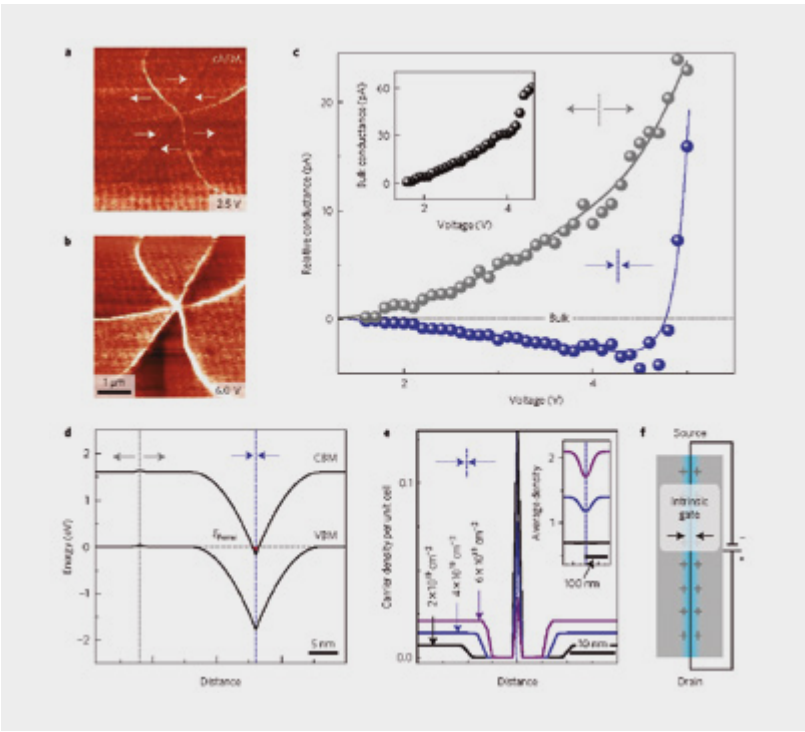


FIGURE Electrical transport measurements (a-c) and band-structure simulations (d-e) of the "head-to-head" and "tail-to-tail" domain walls in ErMnO₃. (f) schematically illustrates a possible device application.

Materials that at low temperature undergo a spontaneous ordering of their magnetic moment, electrical dipoles or elastic strain are called "ferroics" (or "multiferroics", if at least two of the above degrees of freedom coexist). These "order parameters", however, seldom crystallize in a homogeneous phase across the whole sample, but form instead multiple domains separated by thin "walls", or boundaries. While domain walls occupy a very small volume fraction of the crystal, they often display properties that markedly differ from those of the homogeneous domains. Such emergent behavior might enable, on one hand, useful functionalities (e.g. piezoelectricity) in materials where they should be forbidden by symmetry or, on the other hand, they could pave the way for new paradigms in nanoelectronics, where the domain wall itself could play the role of a

device element. In this highlight we present two illuminating examples of both ideas. The first publication is a theoretical study of the polar "twin" walls in SrTiO₃. SrTiO₃, an ubiquitous material in oxide research, undergoes a ferroelastic phase transition at 105 K, but remains nonpolar all the way down to cryogenic temperatures. An electrical dipole, however, forms at the walls; here we identify (and quantify) the mechanisms that are responsible for its appearance. The second publication is a combined experimental and theoretical work that demonstrates how domain walls in ErMnO₃, a hexagonal manganite, can emulate device elements such as transistors or diodes. In particular, the "head-to-head" arrangement of the polarization at the wall results in a local depletion of carriers, and hence in a suppressed conductivity at low voltage (Figure). At higher voltages, however, the conductivity undergoes an abrupt increase, analogously to the band inversion regime in semiconductor devices.

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AN ORGANIC MINIATURE SPECTROPHOTOMETER

Infrared photodetectors of tunable spectral response are fabricated by enhancing the charge transfer absorption of an organic blend in an optical cavity resonator

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[1] Polymer: Fullerene Bimolecular Crystals for Near-Infrared Spectroscopic Photodetectors. *Advanced Materials*, 2017, 29 (33), 1702184

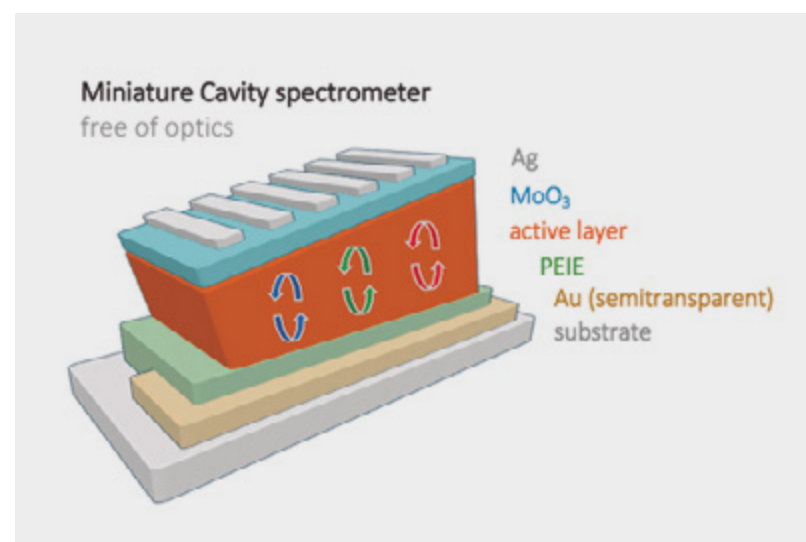


FIGURE
Miniature cavity spectrometer based on an active layer of two organic semiconductors that form a co-crystal structure, and thus have a large charge transfer absorption in the infrared. Wavelength selection is done by shaping the active layer as a thickness wedge.

Spectroscopic photodetection is a powerful tool in disciplines such as scientific research, food industry, medical diagnosis, industrial process monitoring, or agriculture. Typical spectrophotometers are bulky pieces of equipment and thus an integrated, miniaturized version could broaden the uses of this important tool. Here, we advance a solution for this by using organic semiconductor blends embedded into optical microcavity resonator structures. Conventional inorganic commercial detectors are based on band to band absorption in semiconductors (HOMO-LUMO transitions in organics). These detectors are not wavelength selective, as they show electrical response for all wavelengths where absorption is efficient. Spectral selection can be obtained by using optical structures with resonating behavior, such as microcavities. This type of device consists of an active layer sandwiched between two metal electrodes, one of

which is semitransparent. In microcavities, the central wavelength is determined by the thickness of the active layer, and the width of the spectral response is inversely proportional to the absorption of the material. For this reason, typical organic or inorganic absorbers would only work right at the absorption edge. In this work, we use the broad and very small absorption of the charge transfer state between two molecules, an electron donor, and an electron acceptor. This absorption is typically three orders of magnitude smaller than band to band absorption in organics. Because the exact energy of the charge transfer state strongly depends on the local morphology of the two molecules, the band is very broad and thus, the potential spectral range exploited is wide. The wavelength absorbed is adjusted by changing the thickness of the optical cavity. A possible application of these photodetectors, featured in the article, is a mini-UV-Vis spectrophotometer. For this, we have created a microcavity array on a single substrate, each pixel having a different resonating frequency by means of an active layer thickness gradient (wedge) across the substrate. The device of a few centimeters in length (see figure) is used as a portable UV-Vis spectrophotometer. Other potential uses are in the field of integrated electronics, in lab-on-a-chip applications, in colorimetry, or in thermal sensors, which require devices much smaller and portable than the current ones.

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BORON CLUSTERS AS FLUORESCENCE-TUNING MOIETIES IN SINGLE MOLECULES AND OCTASILSESQUIOXANE-BASED HYBRIDS

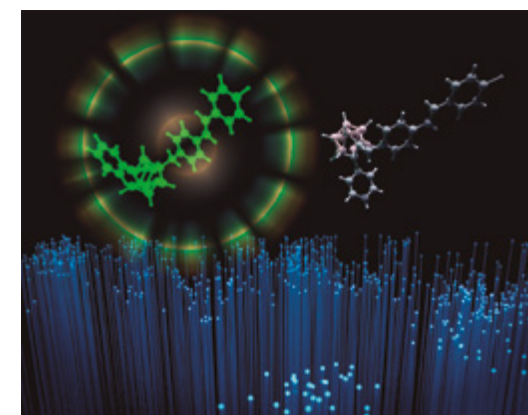
The studies presented here are aimed to demonstrate the role of carborane groups to tailor the luminescence properties of many fluorophores, and the potential of these clusters to prepare fluorescent thermally-stable nanohybrids

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[1] Fluorescent carborane-vinylstilbene functionalised octasilsesquioxanes: synthesis, structural, thermal and photophysical properties. *J. Mater. Chem. C*, 2017, 5, 10211-10219

[2] Carborane-stilbene dyads: the influence of substituents and cluster isomers on photoluminescence properties. *Dalton Trans.*, 2017, 46, 2091-2104

FIGURE
Representation of the fluorescence behavior of *m*- and *o*-carborane derivatives after UV irradiation (cover of the issue).



Carborane clusters are three-dimensional compounds with electron delocalisation, highly polarisable σ -aromaticity, thermal and chemical stability and geometrical diversity. During the last years, our group and others have been interested in the development of carborane-containing luminescent systems, and especially in deciphering the role of these carboranes in their photoluminescence properties. Discrete styrene-containing *ortho*- and *meta*-carborane derivatives substituted at the second carbon cluster atom (C_c) with -Me or -Ph groups, resulted to be exceptional starting compounds to prepare stilbene-containing carborane dyads (Slb-Cb) (Figure), and fluorescent boron-rich hybrids (POSS-Cb) based on the octasilsesquioxane core (T_8). These two sets of compounds were prepared *via* Heck coupling reaction. What is the role of the carborane and its substituent in their photoluminescence (PL) behaviour? It has been demonstrated that the fluorescence efficiency of Slb-Cb depends on the isomer (*o*- and *m*-); all the *m*-carborane derivatives display similar PL quantum yields (~30 %), regardless of the substituent at the second

C_c , being significantly more fluorescent than their *o*- counterparts. Furthermore, for the Me-*o*-carborane derivatives an important enhancement of the fluorescence was observed (15 %), whereas for those bearing the Ph-*o*-carborane unit, a severe fluorescence quenching occurred (0.07 %). In contrast, only the latter exhibited a notable PL emission in films, which is attributed to an aggregation-induced emission phenomenon.

In POSS-Cb the presence of the carborane moiety plays a key role in tuning the fluorescence emission of the nanohybrids. Noticeably, the unsubstituted *o*-carborane derivative has a much higher quantum yield in solution (59 %) than its two counterparts, whereas the Ph-*m*-carborane exhibited a significant higher emission than its homologous Ph-*o*-carborane. Contrarily, in all cases the emission was largely quenched in solid state (4-7 %) due to intermolecular interactions. It is noteworthy that all POSS-Cb displayed a considerable increase in the thermal stability with respect to the pristine POSS, as shown by TGA. In conclusion, we have proven that it is possible to modulate the PL properties of these carborane-containing dyads and POSS, by changing the C_c substituent and the carborane isomer.

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CONTROL OF THE DEVICE PERFORMANCE IN ORGANIC FIELD-EFFECT TRANSISTORS PREPARED BY SOLUTION-SHEARING: POLYMORPHISM AND SURFACE DOPING

The influence of polymorphism on the performance of organic field-effect transistors is investigated. Further, the surface doping of these devices is achieved employing an aqueous solution of Hg^{2+} cations

SERGI GALINDO, QIAOMING ZHANG, ADRIÁN TAMAYO, FRANCESCA LEONARDI, STEFANO CASALINI, MARTA MAS-TORRENT

[1] Mercury-Mediated Organic Semiconductor Surface Doping Monitored by Electrolyte-Gated Field-Effect Transistors. **Adv. Funct. Mater.** **2017**, **27** (46), 1703899.
[2] Control of Polymorphism and Morphology in Solution Sheared Organic Field-Effect Transistors. **Adv. Funct. Mater.** **2017**, **27**(25), 1700526.

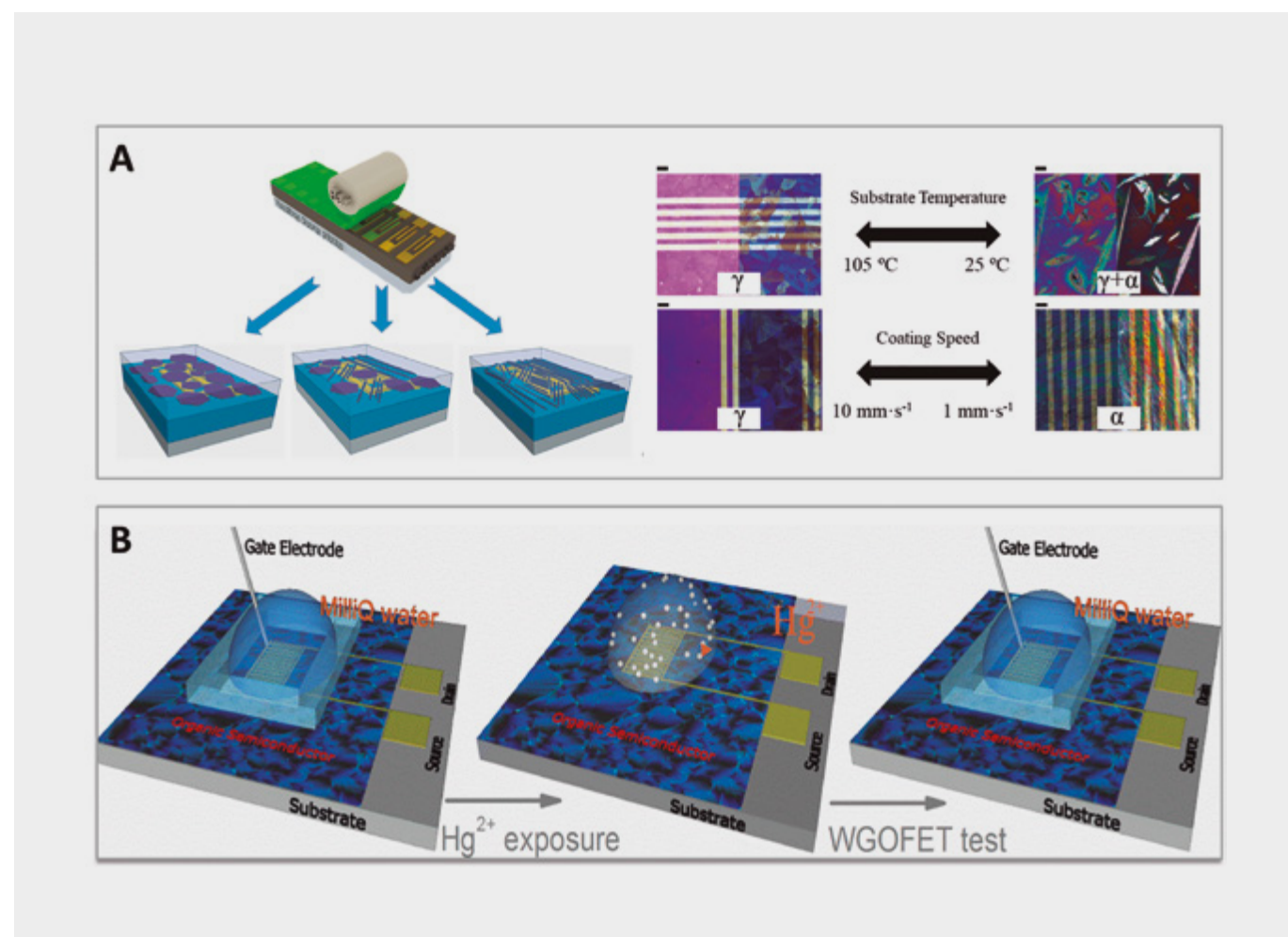


FIGURE
A) Conceptual illustration of how crystal growth process and polymorph formation can be programmed during solution shearing process by varying the substrate temperature or the coating speed and representative optical microscopy images of some of the films prepared (left and right parts of the images correspond to with and without polarizer). Scale bar: 100 μm . B) Schematic procedure of the surface transfer doping process: WGO-FET architecture measured in MilliQ water, exposition to Hg^{2+} solutions and WGO-FET setup for device characterization after Hg^{2+} treatment.

During the last decades, small molecule organic semiconductors have been successfully used as active layer in organic field-effect transistors (OFETs). Despite the high mobility achieved so far with organic molecules, in order to progress in the field it is crucial to find techniques to process them from solution compatible with up-scaling and to achieve high device reproducibility. We have recently shown that the bar-assisted solution shearing (BAMS) of an organic semiconductor blended with the insulating polymer polystyrene (PS) gives rise to highly crystalline thin films that show ideal OFET characteristics. Now, we have performed two more studies that are focusing on further controlling the performance of these devices.

To achieve a high device-to-device reproducibility it is essential to control the morphology and polymorphism of the active layer of OFETs. Indeed, polymorphism is often encountered in small molecule organic semiconductors since the presence of weak van der Waals intermolecular interactions makes these materials prone to structural modifications. We report that varying the deposition parameters (i.e., speed and temperature) or the solution formulation (i.e., semiconductor/binder polymer ratio) is possible to modify the crystallization regime and control the film morphology and semiconductor polymorphism (Figure-A). Hence, it is demonstrated that the control of the thermodynamics and kinetics of the crystallization process is key for the optimization of the device performance [1]. A viable way to achieve fine-control of the electronic properties of organic semiconductors is by chemical doping. Surface doping is particularly appealing in OFETs, where charge transport takes place at the first monolayers close to the dielectric surface. However, due to fabrication restrictions that OFET architecture imparts, this is extremely challenging. Here, we demonstrate that mercury cations, Hg^{2+} , can be exploited to control doping levels at the top surface of a thin film of a p-type

organic semiconductor (OSC) blended with polystyrene. Water-gated field-effect transistors (WGO-FETs), which have its conductive channel at the top surface of the organic thin film, turn out to be a powerful tool for monitoring the process. A positive shift of the threshold voltage is observed in the devices upon Hg^{2+} exposure. Remarkably, this interaction has been proved to be specific to Hg^{2+} with respect to other divalent cations and sensitive down to nanomolar concentrations. Hence, this work also opens new perspectives for employing organic electronic transducers in portable sensors for the detection of an extremely harmful water pollutant without the need of using specific receptors [2].

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A FAITHFUL SCANNING PROBE MICROSCOPY STRATEGY TO DRAW AT THE MOLECULAR SCALE THE LANDSCAPE OF DOMAIN BOUNDARIES IN ORGANIC THIN FILMS

Establishing structure–property relationships in organic devices requires accurately defining the thin-film crystallographic details. An unconventional mode of scanning force microscopy called transverse shear microscopy (TSM) becomes the unbeatable tool to reveal grain boundaries with nanometer resolution.

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[1] A molecular-scale portrait of domain imaging in organic surfaces. *Nanoscale*, 2017, 9, 5589–5596

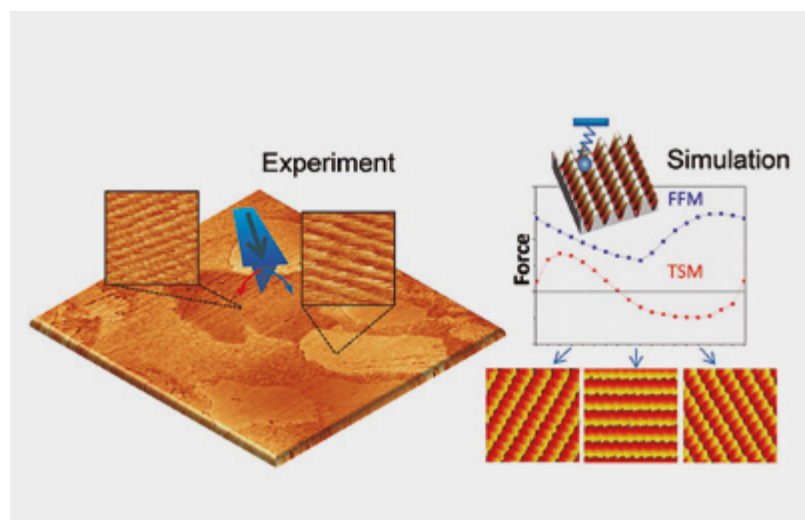


FIGURE Left: The novel lateral force imaging mode (cantilever torsion when scan parallel to its axis) of the scanning probe microscopy is illustrated by true TSM images of PTCDI-C8 islands on SiO₂. The different contrasts observed in the large image correspond to islands exhibiting rotated domains as evidenced by the small images showing molecular scale resolution (saw-tooth like). Right: Calculated FFM and TSM signals as a function of domain orientation and simulated images for three cases.

Thin films made out of small molecules often present polycrystalline morphologies characterized by significant amounts of grain boundaries which are detrimental for the operation of organic electronic devices. It is, therefore, of outstanding importance to have experimental tools able to provide a spatially-resolved structural characterization of the organic films at the dimensions level of such defects. From this point of view, during years we have already demonstrated that the friction force microscopy (FFM), where the torsion of the cantilever is sensed when the tip scans perpendicular to its axis, is a valuable tool to reveal structural details of molecular films which are difficult to visualize using other techniques. However, for most crystalline organic semiconductors, the FFM signal does not exhibit a noticeable dependence with the crystallographic directions of the surface. Recently we have been able to

demonstrate that, when scanning instead parallel to the cantilever axis, the recorded torsion signal can exhibit an important dependence on the azimuthal orientation of a crystalline surface. This non-common imaging mode is referred to as transverse shear microscopy (TSM). In our investigation we combine theory with FFM and TSM experiments at the molecular scale for the organic semiconductor N,N'-dioctyl-3,4:9,10-perylene tetracarboxylicdiimide (PTCDI-C8). Perylene diimide (PTCDI) derivatives are considered among the most promising and versatile materials to fabricate n-channel OFETs.

Our benchmark consists of sub-monolayer amounts of PTCDI-C8 deposited on SiO₂, so that bare substrate regions are used as in-situ reference and lattice-resolved images acquired on top of molecular islands with diverse domain orientations are available without the need of rotating the sample (Figure). We demonstrate that the lateral forces measured at a molecular scale in TSM, as in FFM, have a dissipative origin and arise from the stick-slip response of the tip elastically driven over the periodic atomic surface potential. We provide understanding of the observed TSM anisotropy in relation with the surface structure symmetry and give full information of the domain distribution in these thin organic films.

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ORGANIC RADICALS AS ACTIVE COMPONENTS OF MOLECULAR ELECTRONIC DEVICES: WIRES AND RECTIFIERS

Charge transport mechanisms through organic molecules: a fundamental issue for the development of future electronic devices based on molecules, such as wires, rectifiers, switches, or transistors.

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[1] Operative Mechanism of Hole-Assisted Negative Charge Motion in Ground States of Radical-Anion Molecular Wires. *J. Am. Chem. Soc.*, 2017, 139 (2), 686–692

[2] Tuning the Rectification Ratio by Changing the Electronic Nature (Open-Shell and Closed-Shell) in Donor Acceptor Self-Assembled Monolayers. *J. Am. Chem. Soc.*, 2017, 139 (12), 4262–4265(2), 686–692

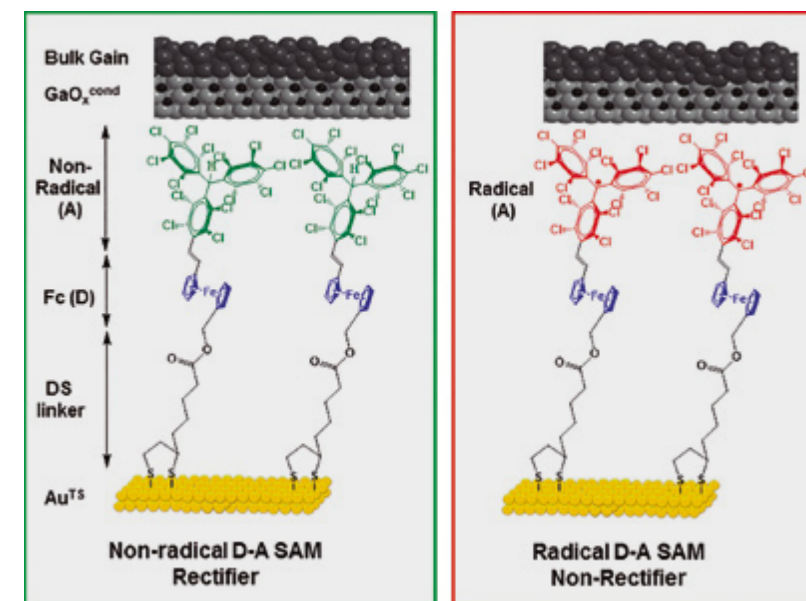


FIGURE Molecular junctions based on non-radical and radical self-assembled monolayers studied.

In the first paper [1] we report the operating mechanisms for unimolecular electron transfer/transport in the ground state of radical-anion mixed-valence derivatives occurring between their terminal perchlorotriphenylmethyl/ide groups through thiophene-vinylene oligomers that act as conjugated wires of increasing length up to 53 Å have. The unique finding was that the net transport of the electron in the larger molecular wires is initiated by an electron-hole dissociation intermediated by hole delocalization (conformationally assisted and thermally dependent) forming mobile polaronic states in the bridge that terminate by an electron-hole recombination at the other wire extreme. On the contrary, for the shorter radical-anions our results suggest that a

flickering resonance mechanism, which is intermediate between hopping and superexchange, is the operative one. We support these mechanistic interpretations by applying the pertinent biased kinetic models of the charge/spin exchange rates determined by electron paramagnetic resonance and by molecular structural level information obtained from UV-Vis and Raman spectroscopies and by quantum chemical modelling. In the second paper [2] we describe the mechanism of charge transport across self-assembled monolayers (SAMs) of two donor-acceptor systems consisting of a polychlorotriphenylmethyl/methane (PTM) electron-acceptor moiety linked to an electron-donor ferrocene (Fc) unit supported on ultraflat template-stripped Au and contacted by a eutectic alloy of gallium and indium top contacts (Figure). The PTM unit can be switched between the non-radical and radical forms, which influence the rectification behavior of the junction. Those junctions based on non-radical units rectify currents via the highest occupied molecular orbital (HOMO) with a rectification ratio $R = 99$, but junctions with radical units have a new accessible state, a single-unoccupied molecular orbital (SUMO), which turns rectification off and drops R to 6.

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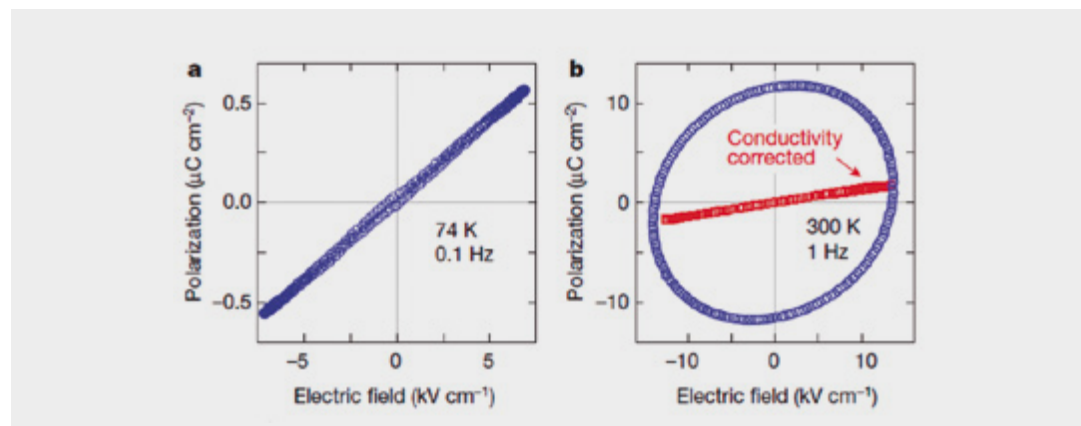
REVISITING ROOM-TEMPERATURE FERROELECTRICITY CLAIMED FOR ORGANIC CHARGE-TRANSFER CRYSTALS FORMED BY AN ELECTRON ACCEPTOR AND THREE DIFFERENT DONORS

The presence of ferroelectricity at room temperature in organic charge transfer crystals, generated by the LASO supramolecular technique, previously published by a team led by J.F. Stoddart (Nobel Prize for Chemistry 2016) and S.I. Stupp (Northwestern U.) is disputed

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[1] Conflicting evidence for ferroelectricity. **Nature**, 2017, 547, E9-E10

FIGURE
Dielectric measurements for A LASO D-A compound. Electric-field-dependent polarization at 74 K (a) and at 300 K (b). The red squares in (b) show the conductivity-corrected result at 300 K. A neat paraelectric response is obtained for temperatures in the range 7–400 K.



Organic ferroelectric materials operating at room temperature are in demand for advanced technological applications in the emerging field of lightweight, flexible and environmentally friendly electronics. Tayi *et al.* (Nature, 2012, 488) reported room-temperature ferroelectricity in three organic mixed-stack charge-transfer crystals, produced using a supramolecular design concept—the lock-arm supramolecular ordering (LASO), that synergistically combines intermolecular charge transfer and hydrogen bonds and organize properly electron donor and acceptor units. Here we present an independent experimental investigation using vibrational spectroscopy techniques and X-ray diffraction data together with theoretical DFT calculations. These new results demonstrate that there is no evidence for ferroelectricity in one of the LASO compounds described by Tayi *et al.* and, therefore, it demonstrates that a possible ferroelectric behavior is not of electronic origin as proposed in by such authors. In conclusion, the findings call into question the claim of room-temperature

charge-transfer ferroelectricity in LASO systems. Indeed, the measurements on one studied crystal just reveal a neat paraelectric response (Figure), instead of the hysteresis loops reported by Tayi *et al.* Thus, additional work is needed to reconcile the conflicting evidence through a rigorous protocol of sample preparation and of ferroelectricity measurements, to establish reproducibility and to exclude all possible causes of experimental artefacts. In any case, our analysis rules out the possibility that the ferroelectricity of LASO systems, if present, is electronic in nature.

(This brief communication arises from “S. A. Tayi *et al.* Nature, 2012, 488, 485–489)

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ELECTROSTIMULATION WITH IRIIDIUM OXIDE-GRAPHENE HYBRID ELECTRODES FOR NEURAL GROWTH AND REPAIR

Electrostimulation using direct current influences neural growth and repair. Recently developed iridium oxide-graphene nanostructured hybrid materials yield to neural repair in short periods of time.

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[1] Short term electrostimulation enhancing neural repair in vitro using large charge capacity intercalation electrodes. **Applied Materials Today**, 6, 2017, 29-43

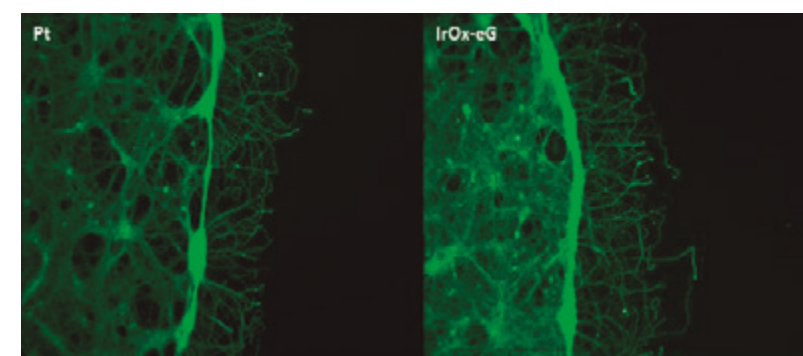
Electrostimulation in the central nervous system is being applied to treat symptoms of several conditions like Parkinson, by using alternating current protocols with near zero net charge. However, if continuous constant fields are applied for cell directioning, actual repair may be favored. The electrode materials in DC fields however have more constraints. Noble metals like platinum or its alloys are biocompatible in static form, but when used as electrode, water splitting and oxygen radical formation occur at the interface with the electrolyte. If charge is actually delivered the extent of radicals is sufficient to produce inflammation in the tissue and even burning, and the implanted electrode needs to be removed.

Alternative materials with mixed valence and intercalation possibilities create an alternative redox reaction within the material that prevents radical formation, in the range of their charge capacity. Therefore, there is a need to develop new materials that result biocompatible without and with applied electric fields, that is, with large charge capacities. A careful screening has been done of the materials in media that imitate the neural extracellular conditions, and their chemistry, compatibility and redox behavior has been evaluated. By changing the deposition conditions of iridium oxide (IrOx) we have

increased 5 times its charge capacity (from 2-5 to 20 mC/cm²), and several orders of magnitude its adhesion to the substrate, with resulting stable electrochemical cycling and optimal impedance values. Furthermore, the combination of IrOx with carbon nanotubes and graphene has yielded nanostructured hybrids resembling reinforced concrete or mil-feuille structures with one order of magnitude larger charge capacity (140 mC/cm²) and largely improved redox cyclability (1000 cycles tested). IrOx-nanocarbons large capacity is retained over the cycles. Exfoliated graphene by electrochemical methods renders a IrOx-graphene with the same charge capacity that any other combination, but stable over cycling and with much less carbon and low roughness.

New methods were also explored to mimic in vitro the environment of neural lesions. Electrostimulation using a scratch method was developed without fields and later with fields to assess the viability of new electrodes. During 40 min electrostimulation, those materials are the best electrode found. New hybrid materials based on electrochemically exfoliated materials are being developed, as well as new protocols for electric field application. Some stages of new electric field protocols are the subject of a patent filed in 2015.

FIGURE
Neural cells response at the cathode, after a scratch wound for Platinum and IrOx-graphene electrodes. The neurites extend more in the last case during a 40 min electrostimulation.



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SYNTHESIS OF DESERT-ROSE COORDINATION POLYMERS NANOSHEETS IN SUPERCRITICAL CO₂

In this work we used supercritical CO₂ for the synthesis of Cu, Ni and Mn diethyloxaloacetate based 1D coordination polymers crystallized in the form of nanosheets, formed by layers of 15-40 nm thickness

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[1] Bottom-up approach for the preparation of hybrid nanosheets based on coordination polymers made of metal-diethyloxaloacetate complexes linked by 4,4'-bipyridine. *CrystEngComm*, 2017, 19, 4972-4982

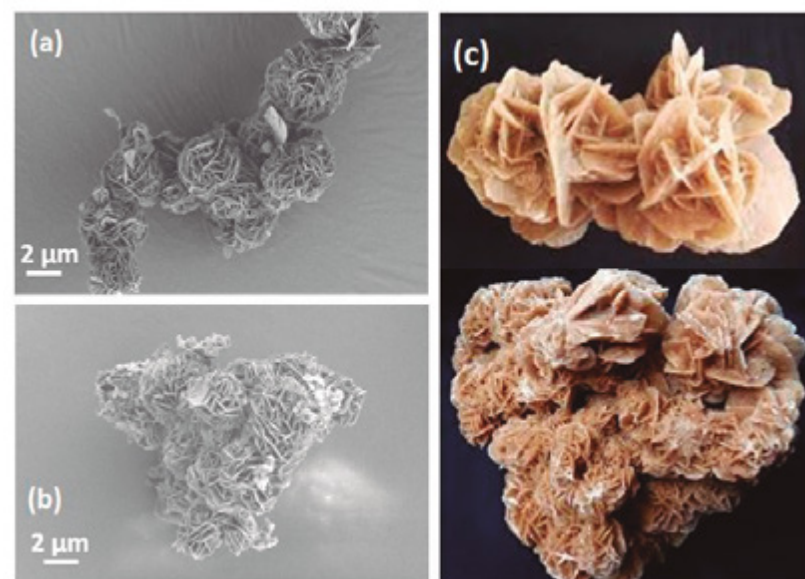


FIGURE
SEM micrographs of [M(deox)₂(bpy)]_n using scCO₂ (a) and (b). Samples show flower-like microstructures resembling a desert-rose type structure (c)

Research in coordination polymers (CPs) and metal organic frameworks (MOFs) has increased considerably in the last decade, since these materials are potential candidates for numerous applications, such as drug delivery, catalyst, gas separations, gas storage and others. To date, published reports on the use of this solvent in the field of CPs and MOFs processing are scarce. The use of supercritical carbon dioxide (scCO₂) has been generally applied for the activation or cleaning of these materials. In our research group, a method for the generation of CPs and MOFs in scCO₂ has been already developed. In this work, we proposed a supercritical route to synthesize CPs nanosheets (2D-MOFs) with formula [M(deox)₂(bpy)]_n (deox = diethyl oxaloacetate), using transition metals as Cu, Ni and Mn. Results showed that in scCO₂ it was possible to crystallize them in layers of 15-40 nm thickness, agglomerated in a desert-rose conformation [Fig 1(a, b and c)].

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EVALUATION OF INORGANIC NANOPARTICLES IN THE NEMATODE CAENORHABDITIS ELEGANS

Genetic analysis and advanced imaging techniques have been applied to evaluate inorganic nanoparticles for biomedical applications in the model organism *Caenorhabditis elegans*, revealing composition-, coating-, size- and dose-dependent effects.

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[1] In vivo screening of gold nanoparticles using the *Caenorhabditis elegans* model organism. *Acta Biomaterialia*, 2017, 53, 598-609

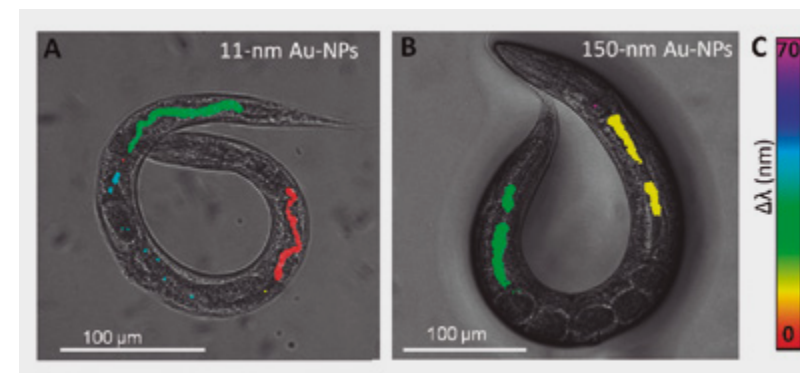
[2] Toxicogenomics of iron oxide nanoparticles in the nematode *C. elegans*. *Nanotoxicology*, 2017, 11, 5, 647-657

[3] Materials and toxicological approaches to study metal and metal-oxide nanoparticles in the model organism *Caenorhabditis elegans*. *Materials Horizons*, 2017, 4, 719-746

The simple model organism *Caenorhabditis elegans* (*C. elegans*) was used as an *in vivo* biological system to screen nanoparticles currently under revision for biomedical uses. In particular, iron oxide and gold nanoparticles were assessed. The nano-bio interactions of the two materials were studied in the *C. elegans* with special focus on their uptake, fate, biological effects and molecular mechanisms. Toxicity tests, imaging techniques and gene expression analysis were combined to also investigate the influence of nanoparticle's composition, coating and size on the worm [1]. In particular, applying two-photon luminescence microscopy and absorbance micro-spectroscopy, we concluded that gold nanoparticles ingested by *C. elegans* accumulated in the intestine but were not internalized by the intestinal cells (Figure). Translocation of nanoparticles to secondary organs, either entrance by other routes or body openings was not observed. Moreover, gold particles appeared resistant to degradation but showed some degree of aggregation inside *C. elegans*, which was reversible and depended on the specific area of the gut. In addition, molecular

mechanisms triggered in *C. elegans* by iron oxide nanoparticles exposure were investigated by genetic analysis tools (i.e. qPCR and microarrays). Nanoparticle treatment disrupted the oxidative stress and metal detoxification pathways of the worm, indicating that they might be involved in the protective response of *C. elegans* to their exposure. Furthermore, coating-dependent effects were identified: citrate-coated particles affected the processing of environmental and genetic information, while the albumin-coated ones affected metabolic mechanisms. Therefore, we confirmed that nanoparticles can trigger both general stress mechanisms and specific pathways depending on their properties, in good agreement with other investigations in the field [2]. In conclusion, we contributed to expand the range of available techniques to characterize nano-bio interactions *in vivo* and have set a systematic and comprehensive evaluation of the effects of nanoparticles in *C. elegans*. Those results and relevant publications on the field were included in a review on materials and toxicological approaches to study metal and metal-oxide nanoparticles in this *in vivo* model [3].

FIGURE
Combination of two-photon luminescence microscopy and absorbance micro-spectroscopy to characterize nematodes treated with gold nanoparticles of A) 11 nm and B) 150 nm.



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CORE-CANOPY QUANTUM DOTS: TRAPPED IONS IN VOIDS INDUCE KINETIC FLUORESCENCE SWITCHING

The object of the study was to incorporate hollow spherical carboranes as capping agent for quantum dots instead of linear chains of carbon using colloidal synthetic route and this led us to get the unique property of Kinetic Fluorescence Switching

ARPITA SAHA, ELENA OLESHKEVICH, CLARA VIÑAS AND FRANCESC TEIXIDOR

[1] Biomimetic Inspired Core-Canopy Quantum Dots: Ions Trapped in Voids Induce Kinetic Fluorescence Switching. *Adv. Mater.*, 2017, 29, 1704238.

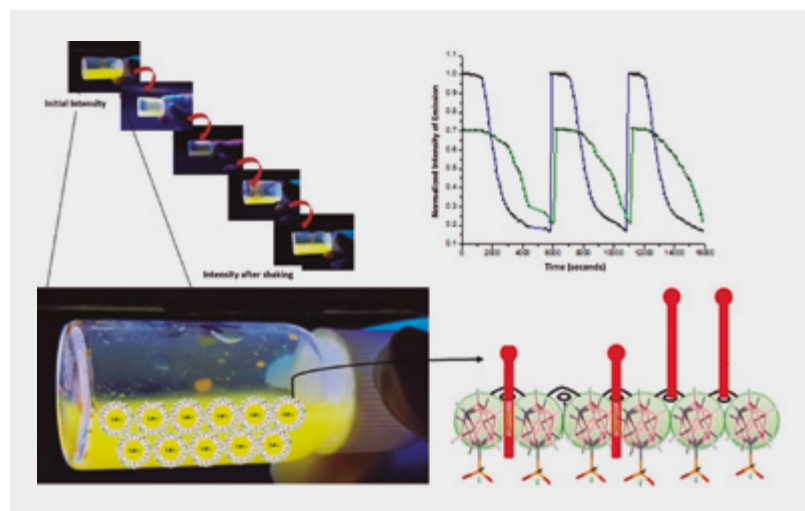


FIGURE The naked eye evolution of the intermittent behavior of the fluorescence is visible here. And the graphical representation of the KFS is shown on the right hand side. The blue one is of a freshly made [CdSe@CarbOPH(O)]@Cl/[N(Caprylyl)₃Me₃]⁺ and the green one is of a 5 months old [CdSe@CarbOPH(O)]@Cl/[N(Caprylyl)₃Me₃]⁺. The enlarged image of the vial shows the representation of the proposed model for the Core Canopy Quantum dots which lead to this KFS phenomena. The pictographic model on the right of the enlarged vial show the gates created by the core canopy quantum dots. The canopy created by the carborane spheres when closely packed generate openings which are converted to gates due to the presence of the alkyl ammoniums.

Quantum Dots (QDs) are nanoparticles with dimensions between 1 to 20 nm. Their various fascinating properties have made them ideal for a vast array of commercial applications such as solar light harvesting, LEDs, or LASERS.

Here we report an unprecedented phenomenon, namely Kinetic Fluorescence Switching (KFS), which is observed due to a synergism created by preparing Cadmium Selenide (CdSe) QDs capped with hollow spherical carborane ligands. Carboranes, which are aromatic and highly stable species, having the ability to sustain high temperatures and extremely harsh chemical conditions, can be visualized as hollow spheres. Very few carbon based molecules are hollow spheres and they are quite difficult to obtain, hence needing the use of carboranes for this purpose. This is the first time that hollow spheres have been linked to the QDs through their binding sites and this has led to the introduction of new concepts and distinct properties that arise from the development

of this novel architecture in QDs, named core-canopy QDs. The foremost property is the aforementioned KFS: the QDs, which are initially fluorescent, lose their fluorescence when left to aggregate, but upon being provided mild kinetic energy (by shaking them) they shine back again to their maximum fluorescent intensity. This sequential process of luminescence and fading out can be continuously run for several months. Water soluble m-carboranylphosphinate Na[1-OPH(O)-1,7-closo-C₂B₁₀H₁₁] is the carborane ligand used for the capping of the QDs, which leads to this fascinating and unprecedented property. Also notable is the fact that the intensity of these QDs is around 100 times higher than of those QDs prepared by traditional methods. In addition, these QDs show minimal loss of intensity even after a period of 5 months.

The spherical carboranyl entities are arranged in either a square or hexagonal close packing to produce maximum coverage of the CdSe surface, leaving openings and generating voids/channels that trap anions that, in this case Cl⁻, increase the negative charge of the core-canopy QDs. Through the openings, the methyl groups from alkylammonium surfactants can be appended. The surfactant, in this case [N(Caprylyl)₃Me₃]⁺, is the plug that converts the openings into gates. The KFS property is the result of a core-canopy QDs architecture and the adequate choice of the targeted property ingredients. We are working on discovering new properties by keeping the same architecture and choosing new components for other addressed properties

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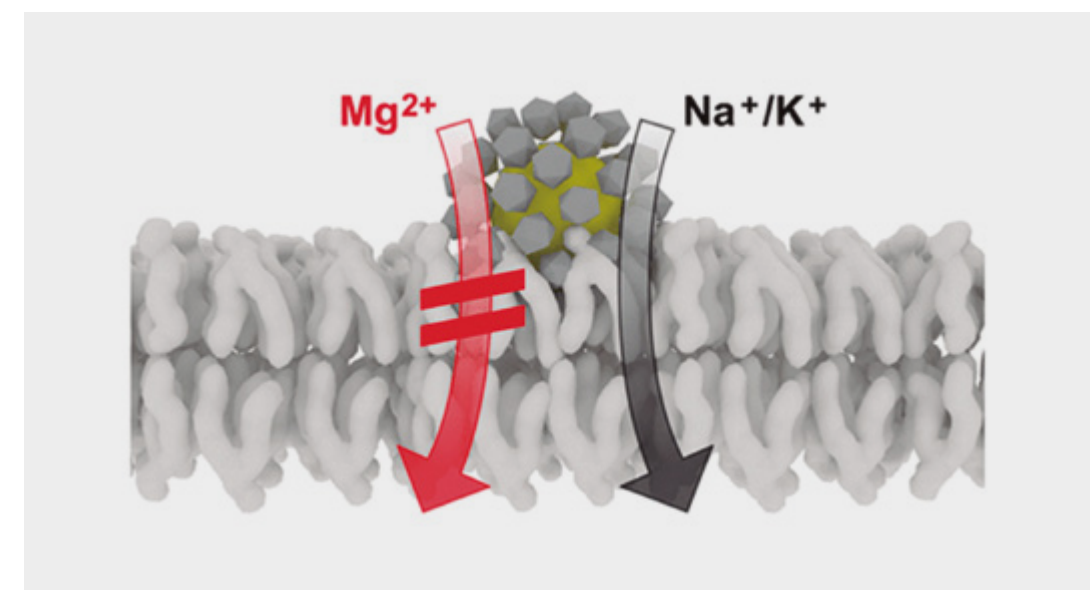
MERCAPTOCARBORANYL-CAPPED GOLD NANOPARTICLES AS ARTIFICIAL ION TRANSPORTER ACROSS BIOLOGICAL MEMBRANES

We report that gold nanoparticles protected by hollow sphere carborane-based molecules can penetrate phospholipid bilayer membranes and act as alkali-ion specific transporters

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Ion Transport across Biological Membranes by Carborane-Capped Gold Nanoparticles. *ACS Nano* 2017, 11 (12), 12492-12499

FIGURE Schematic representation of alkali-ion specific transporters after addition of anionic Au/carborane NPs to the aqueous medium outside the phospholipid bilayer vesicles.



Ion transport across biological membranes is a fundamental phenomenon ubiquitous in nature. Photosynthesis, the respiratory chain, ATP production, muscle contraction, neuronal signaling, and many other key biological processes depend on it. Numerous active and passive transport mechanisms exist ranging from simple ion channels to highly complex processes. Substances that affect ion transport or its regulation play important roles in both basic research and drug development. Very few carbon based molecules are hollow spheres and they are quite difficult to obtain, hence carboranes are ideal for this purpose. Gold nanoparticles capped with mercaptocarborane ligands, which are hollow spheres ready to link to gold, lead to monolayer protected clusters that exhibit the uniqueness to store and release cationic charge that is counterbalanced by electrons in the metal core. This is possible due to the

inevitable voids in the ligand shell, which are caused by the hollow spheres of the carborane ligand. We reported that 2-3 nm gold nanoparticles protected by hollow sphere mercaptocarborane ligands (a) readily penetrate phospholipid bilayer membranes and establish a membrane potential as partitioning anions and (b) effect the transport of alkali cations across the membrane and hence represent a class of membrane alkali-ion specific transporters. The gold nanoparticles act as alkali-ion-specific transporters across free-standing membranes under potentiostatic control. Magnesium ions are not transported.

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NANOCAPSULES FOR TARGETED RADIOTHERAPY: PAVING THE WAY FOR AN OPTIMAL PRODUCTION

An environmentally friendly protocol has been engineered for the production of nanocapsules (filled carbon nanotubes), which immunological profile after antibody-functionalization reveals their suitability for future testing in the field of targeted radiotherapy

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[1] Evaluation of the immunological profile of antibody-functionalized metal-filled single-walled carbon nanocapsules for targeted radiotherapy. **Scientific Reports**, 2017, 7, 42605

[2] Filling Single-Walled Carbon Nanotubes with Lutetium Chloride:

A Sustainable Production of Nanocapsules Free of Nonencapsulated Material. **ACS Sustainable Chem. Eng.** 2017, 5 (3), 2501-2508

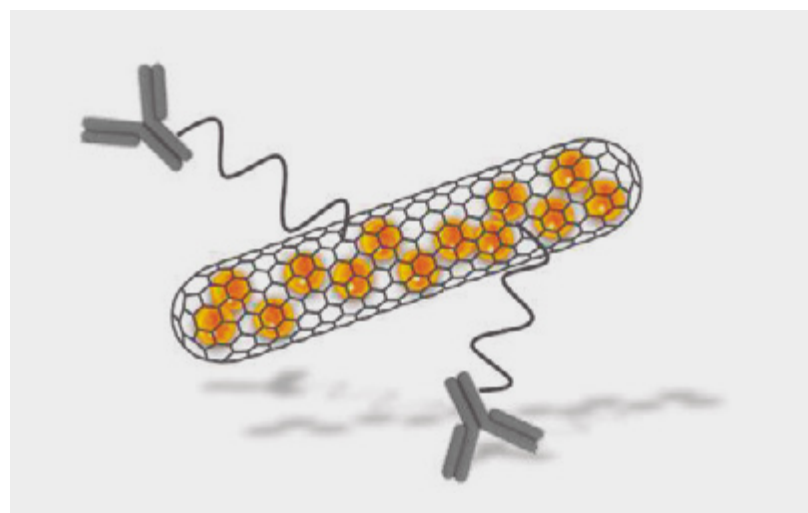


FIGURE
Schematic representation of a filled carbon nanotube (carbon nanocapsule) externally functionalized with monoclonal antibodies

We have explored the effect of differently functionalized single-walled carbon nanotube (SWCNT) conjugates on the immune system activation. These nanotubes correspond to empty amino-functionalized CNTs, samarium chloride-filled amino-functionalized CNTs, and filled CNTs further functionalized with the targeting antibody Cetuximab (Figure). Overall, biocompatibility of the conjugates is observed. In addition, our experiments have shown the importance of the functionalization of the CNTs, particularly in terms of dispersibility and possible interactions through dangling bonds. Therefore, these results remind us of the need for inclusion of relevant cytotoxicity assays for a particular biomedical

application of CNTs. Altogether, the information obtained in this investigation encourage us to perform further studies for tumor targeting with the carbon nanocapsules functionalized with the antibody Cetuximab. Given the short half-life times of common clinically used radionuclides, rapidity is a must [1]. With the aim to develop such antibody-functionalized nanocapsules with radionuclides for targeted radiotherapeutic applications, we have developed a sustainable system to process samples of filled carbon nanotubes. The green protocol allows a 95 % reduction in water waste, which gets contaminated with hazardous heavy (radioactive) elements. The developed methodology benefits from a synergistic combination of both Soxhlet and dialysis. We foresee the use of such optimized purification protocol as a path towards high-quality filled SWCNTs, exclusively endohedral, to be employed not only in the biomedical field but also in other applications where the presence of non-encapsulated material can be detrimental [2].

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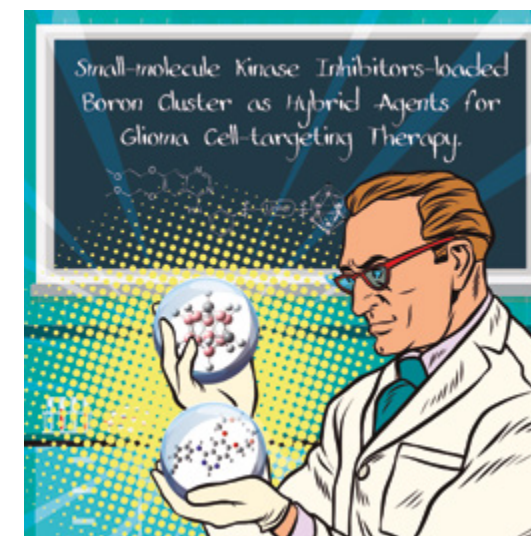
GLIOMA-CELL-TARGETING THERAPY APPROACH BY USING SMALL-MOLECULE KINASE-INHIBITORS-LOADED BORON CLUSTER AS HYBRID DRUGS

The aim of the study was the synthesis of anilinoquinazoline-icosahedral borane hybrids to be used as boron carriers to enrich glioma cancer cells with boron atoms for BNCT cancer therapy

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[1] Small-Molecule Kinase-Inhibitors-Loaded Boron Cluster as Hybrid Agents for Glioma-Cell-Targeting Therapy. **Chem. Eur. J.** 2017, 23 (39), 9233 – 9238

FIGURE
The two components, boron-rich carboranyl clusters and erlotinib, that were hybridized to achieve a series of possible anticancer compounds for BNCT.



Glioblastoma multiforme (GBM) is the most common primary central nervous system tumor in USA and Europe: WHO reported that more than 50 % of all gliomas being a grade IV glioma, the most malignant one. Despite GBM is a genetically heterogeneous tumor, common molecular characteristics have been described such as the amplification of the epidermal growth factor receptor (EGFR) gene on chromosome 7. EGFR is a member of ErbB family of transmembrane tyrosine kinase receptor (TKR) involved in enhancing growth, proliferation, migration, tumor neovascularization, and resistance to chemotherapies.

The GBM standard treatment is surgical tumor resection followed by a combination of radiation and chemotherapy in order to kill any remaining tumor cells infiltrated in the brain parenchyma. As the current therapeutic success is still limited, new chemotherapies are under investigation. EGFR and other TKRs are among the most

studied pathways for the development of new targeted molecular agents. The 4-anilinoquinazoline framework has been described as TKRs-inhibitors pharmacophore that competitively binds to the ATP binding site of the protein kinases intracellularly located in the transmembrane receptor. On the other hand, Boron Neutron Capture Therapy (BNCT) is a cancer dual treatment modality based on the high cross-section of ¹⁰B atoms when interact with thermal neutrons. After capture of thermal neutrons by a non-radioactive ¹⁰B containing drug, high linear energy transfer particles (⁴He and ⁷Li) that have a linear path trajectory similar to the diameter of a cell are formed; the BNCT damage is selectively confined in the tumor tissue when the drug is selectively delivered in its cells.

We reported on the synthesis of new anilinoquinazoline-icosahedral borane hybrids with the aim to be evaluated as glioma-targeting for their potential use in BNCT cancer therapy. Anti-glioma activity depends on hybrids' lipophilicity; the most powerful compound against glioma cells, a 1,7-closo-derivative, displays at least 3.3-times higher activity than the parent erlotinib. According to the cytotoxic effects on normal glia cells, the hybrids were selective for EGFR-overexpressed tumoral cells. These hybrids could be used as boron carriers to enrich glioma cancer cells with boron atoms for BNCT application. These results were chosen as frontispiece (Figure) by Wiley VCH & ChemPubSoc Europe and highlighted at the ChemistryViews website by Joseph D. Unsay.

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NANOSTRUCTURED MOLECULAR LIQUIDS WITH APPLICATION IN NANOMEDICINE, PREPARED USING COMPRESSED CO₂

We use compresses CO₂ to prepare compressible and pressure responsive nanostructured fluids and fluorescent organic nanoparticles for bioimaging applications

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[1] Pressure-Responsive, Surfactant-Free CO₂-Based Nanostructured Fluids.

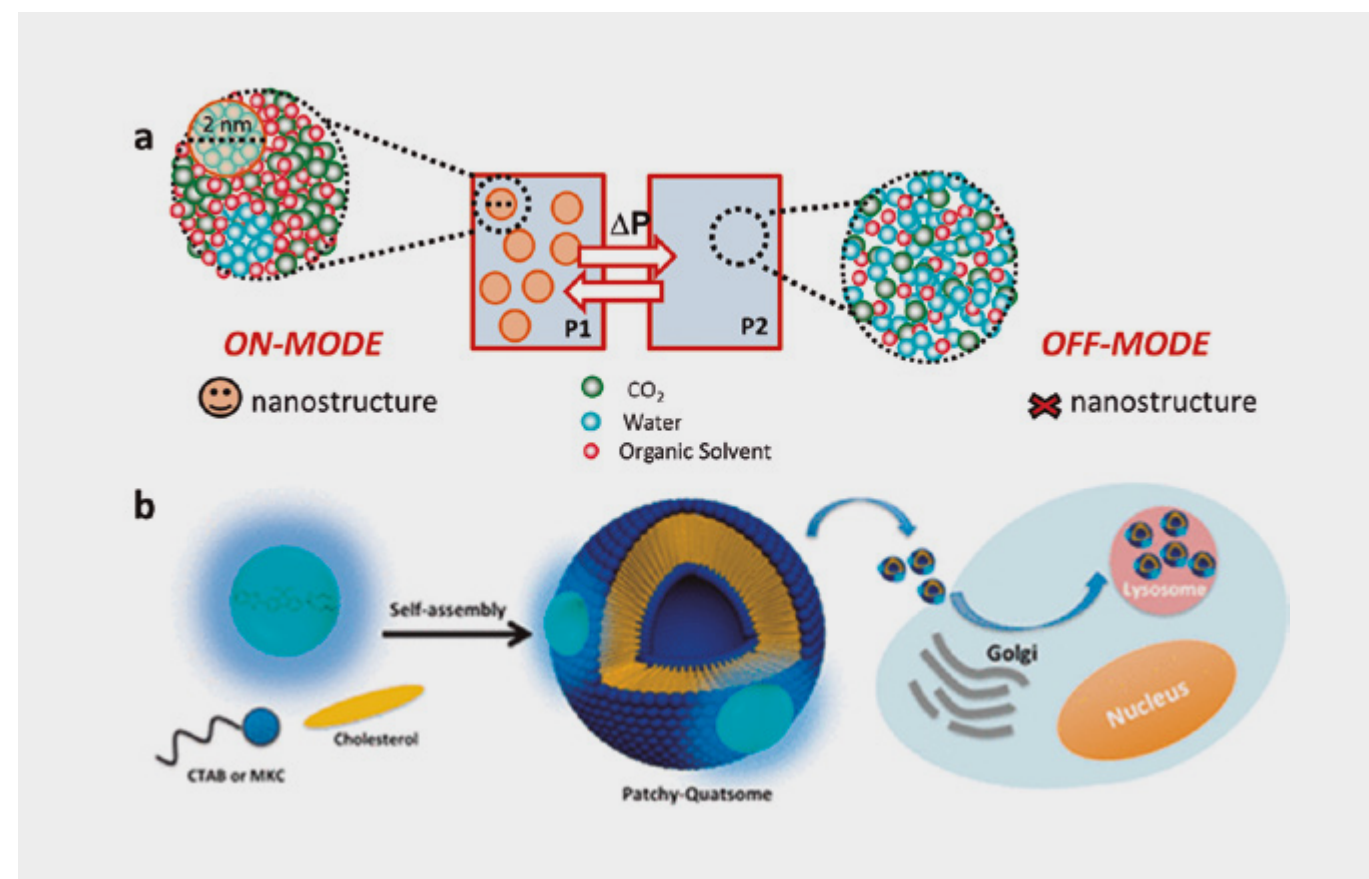
ACS Nano, 2017 11 (11), 10774-10784

[2] Highly Fluorescent Silicon Nanocrystals Stabilized in Water Using Quatsomes.

Langmuir, 2017, 33 (50), pp 14366-14377

[3] Fluorenyl-Loaded Quatsome Nanostructured Fluorescent Probes.

ACS Omega 2017 2 (8), 4112-4122.



FIGURE

(a) Pressurized mixtures of "water/organic solvent/CO₂" can be nanostructured, providing water-rich nanodomains that coexist with water-lean ones. These fluids are compressible and pressure responsive, showing a reversible, pressure-triggered ON/OFF nanostructure: when "ON" at pressure P_1 the fluid is macroscopically homogeneous, but structured at the nano-scale; conversely, when "OFF" at pressure P_2 ($P_2 > P_1$), the medium remains macroscopically homogeneous, but does not show any nm-scale structure. (b) Highly bright fluorescent nanovesicles, named quatsomes, for cellular bioimaging

Understanding of molecular assembling in the formation of liquid materials is crucial for the development of new medicines and contrast agents for diagnosis, with high efficacy, selectivity and safety. Moreover, the arrival of these nanomedicines to the clinical practice is strongly dependent on the existence of scalable productive technologies, which allow a high control of molecular assembling and permit to reproducibly synthesize batches with identical properties and in enough quantities for clinical applications.

Nanomol group has a long trajectory on the use of compressed CO₂, considered green/eco-friendly solvent, for the development of production platforms and multifunctional nanostructured molecular materials of interest for the biotech and pharmaceutical sector.

In the frame of an interdisciplinary collaboration, we have recently discovered and deeply characterized a novel class of surfactant-free pressurized nanostructured fluids, composed of an organic solvent, CO₂ and water, able to dissolve highly hydrophobic compounds, in the presence of excess water, without the aid of any surfactant [1]. Crucially, the breakthrough potential is in the fact that these fluids are compressible and pressure responsive, showing a reversible, pressure-triggered ON/OFF nanostructure (see Figure-a). These fluids have huge possibilities as media for the scale-independent, controlled crystallization of high added-value particulate materials for the pharmaceutical and fine chemicals industry.

For bioimaging purposes, non-cytotoxic fluorescent labels are in demand, stable in biological media and capable of site-specific labelling. In the frame of Nano2Fun Marie Curie ITN project, we have engineered a new class of fluorescent organic nanoparticles (FONs) using thermodynamically stable nanovesicles named quatsomes (see Figure-b). These fluorescent nanostructures, patent protected, are obtained by the self-assembly of organic or inorganic fluorophores with sterols and quaternary ammonium

surfactants. They show excellent colloidal stability and structural homogeneity along with superior optical properties, in comparison with the fluorophores in solution [2,3]. When these new FONs are prepared by a CO₂-based process, named DELOS-SUSP, homogeneous supramolecular arrangement is guaranteed, leading to higher optical performances.

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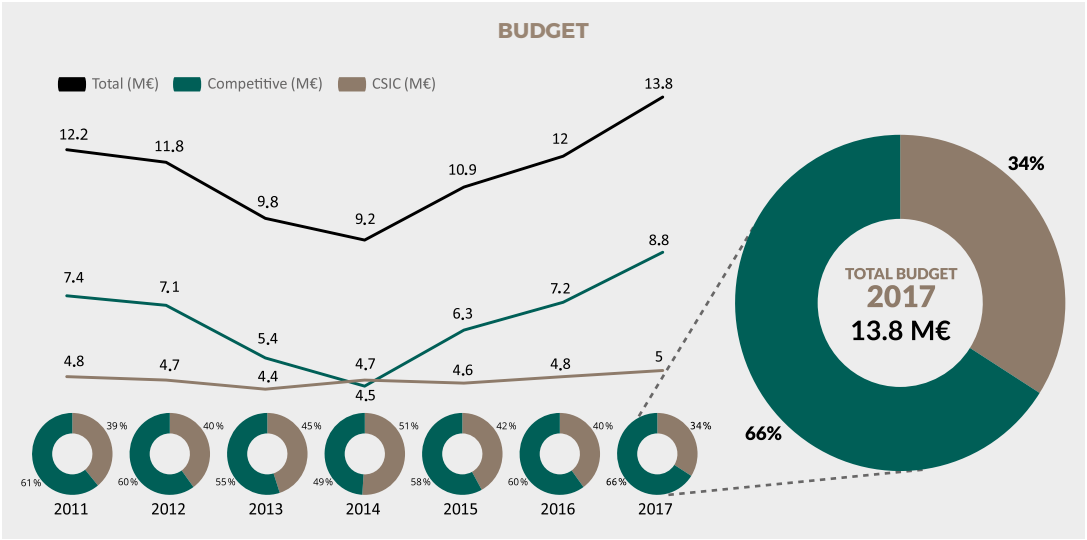
⁷McKetta Department of Chemical Engineering and Texas Materials Institute, The University of Texas at Austin, USA

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INSTITUTIONAL HIGHLIGHTS



EXTERNAL FUNDING

The Institute secured a total budget of 13.8 M€ in 2017, the largest budget ever achieved for the ICMAB. This increase is mainly associated to the increase of the competitive contribution, which was of 64 %, also the highest value ever achieved. The total budget associated to the ongoing EU projects amounted 25.5 M€, and in 2017, 31 % of the total budget (4.2 M€) were of EU origin. A 22 % of the total budget came from national projects (MINEICO) and a 36 % from the CSIC. The main CSIC contribution is for personnel expenses (~ 90 %). The rest of the budget came from the Generalitat de Catalunya (1 %) and from contracts with the Industry (1 %) and from different PhD or postdoc fellowships (8 %).





AWARDS

• **Anna Laromaine**, top 100 influential women talents in Spain

• **Anna Roig** receives the Albus Grifols Award for her project on "Albumin iron-oxide nanocages"

• **Enric Canadell**, Doctor Honoris Causa by the University of Rennes 1. Member of the Royal Academy of Science and Arts of Barcelona.

• **Ignasi Fina**, Young Researchers First Prize at the Biennial Meeting of the RSEF

• **Imma Moros**, CSIC award for the Managing Program of the Institute

• **Jaume Veciana** received a Mention of Honor for his dedication in the creation of NANBIOSIS

• IEEE Magnetism recognizes the dissemination activity of **Josep Fontcuberta** as Distinguished Lecturer 2016 at the Award Ceremony of INTERMAG 2017

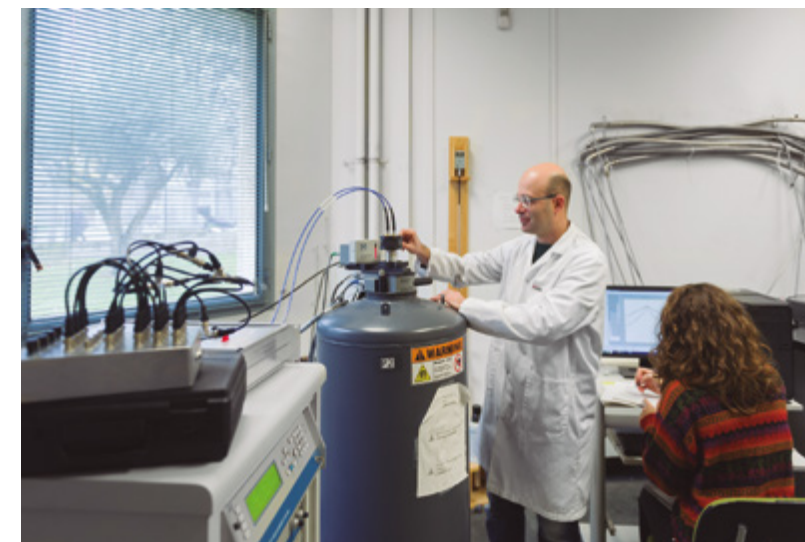
• **Judith Guasch**, awarded with a leader position of a Max Planck Partner Group

• **Mariona Coll**, Research Award L'Oréal-Unesco "For Women in Science" 2017

• **Xavier Obradors** honored with the Ambassador Regió 7 Award

• **Four ICMAB researchers** acknowledged by the CSIC for their Scientific Merits during 2016

• **Miquel Torras** awarded with the Premi Sant Jordi 2017 for his Undergraduate Project



NEW EQUIPMENT AND COLLABORATIONS WITHIN THE SCIENTIFIC EQUIPMENT PLATFORMS

Low Temperatures and Magnetometry Service

During 2017 a new PPMS was installed, and the helium recovering and liquefaction system was installed. Liquid helium is used at the Low Temperatures and Magnetometry Service in all the magnetometry measures, which are carried out at extremely low temperatures (approximately at $-269\text{ }^{\circ}\text{C}$ (about 4 K)). Once the liquid helium is used, it is lost in the atmosphere in its gaseous form, since it evaporates really quickly. The new equipment acquired, the ATL 160 (Quantum Design), is used to recover the helium used in the experiments and to liquify it. Therefore, the liquid helium is available for its reuse in subsequent magnetometry measures. A total of 9,692 hours have been devoted to measures, divided into the different equipment: 4,847 on the PPMS and 4,845 on the SQUID. A total of 602 internal and 23 external services have been carried out.

X-ray diffraction lab

A new versatile installation was acquired for the X-ray diffraction lab: D8 Advance A25. This equipment is funded by the ERC project from Dr. Alexander Ponrouch, "Calcium and Magnesium metal anode based batteries (CAMBAT)" project. The diffractometer has the following characteristics: it combines two configurations, the Bragg-Brentano geometry with copper radiation, which has the possibility to carry out measures of powder diffraction in an electrochemical cell to perform in situ measurements; and a the Debye-Scherrer geometry, with molybdenum radiation, Johansson monochromator focused on the detector to carry out powder diffraction measures in a capillary. Both configurations work with a high efficiency linear detector. The second geometry, allowing the measurements inside a capillary, is very useful when only a small amount of powder is available, such as for those performing research

in materials for new cathodes or anodes for batteries. In total, in 2017 the service ran a total of 3,898 hours (taking into account the Siemens D-5000, GADDS and D8 Discover diffractometers). A total of 4,200 samples were analyzed.

Spectroscopic Techniques Laboratory

In 2017 a new FT-IR was purchased at the Spectroscopic Techniques Lab, the JASCO 4700 LE, which has a higher acquisition range than the previous one, from 200 to 7800 cm⁻¹ (instead of 400-400 cm⁻¹), a higher resolution and the incorporation of a database KnowItAll to determine the spectrum bands. During 2017, the users of the FT-IR have been mainly students and researchers from 22 project IPs, the users of the UVVisNIR were students from 21 project IPs, the EPR users from 5 project IPs, and the optical microscopy users from 16 project IPs. The service counts with external institutions users, from other research centers, hospitals, spinoffs or other companies: ICN2, IMB-CNM-CSIC, Hospital Universitari Vall d'Hebron-Institut de Recerca (VHIR), Nanomol Technologies, Bioiberica S. A., and NFFA project users, who have mostly used the EPR and the UVVisNIR.

Nanoquim Platform

During 2017 two new equipment were acquired at the NANOQUIM platform: a microwave for chemical synthesis and digestion (FlexiWAVE, Milestone), and a mini tubular furnace to work with an oxygen flow at a maximum temperature of 450 °C.

Preparation and Characterization of Soft Materials

Many public institutions and private companies used the SoftLab service during 2017. Public

centers: Universitat Autònoma de Barcelona (UAB), Institut de Biotecnologia i Biomedicina (IBB), Centro Nacional de Microelectrónica (IMB-CNM), Institut Català de Nanociència i Nanotecnologia (ICN2), Institut de Recerca i Tecnologia Agroalimentàries (IRTA), Vall d'Hebron Research Institute (VHIR), Instituto de Biomedicina de Sevilla, Institut de Química Avançada de Catalunya (IQAC), Institut d'investigacions Biomèdiques August Pi i Sunyer (IDIBAPS), Centro Investigación Cáncer, Hospital de Salamanca, Centro de Cirugía de Mínima Invasión Jesús Usón, Universidad de Salamanca, Hospital de Sant Joan de Déu and Institut Químic de Sarrià (IQS). Private companies: Aidimme, Nanomol Technologies, Thermal Spray Center, Tecnia, Spherium Biomed, Peñoles, BCN-Peptide and Carbueros Metálicos.

Scanning Probe Microscopy (SPM)

Thanks to a collaboration with the CNRS, the service has incorporated an amplifier (Zurich Instruments HF2LI) that will be available for four years. A new atomic force microscopy technique, named "Direct Piezoelectric Force Microscopy" has been developed for the study of ferroelectric and piezoelectric materials, which has resulted in a European patent. In 2017 a total of 9,664 images were taken, in 1,600 hours of equipment used, and four NFFA users used the service (45 AFM Unit of Actions).

The Cell growth Laboratory, a shared facility between the ICN2 and the ICMAB, was still under construction, and the **HRTEM facility**, to be built at ALBA Synchrotron, and shared between ALBA Synchrotron, BIST, CSIC, ICN2 and ICMAB is still pending of confirmation.



ADMINISTRATION

The ICMAB Administration is responsible for all of the administrative processes at the Institute, mainly general accounting, charging and payments, and also the accounting of the different research projects. It is also responsible for the inventory, purchasing and public tenders.

In 2017, the Managing Director of the ICMAB was awarded by the CSIC for the Managing Program Implementation in the center.



LIBRARY & DOCUMENTATION

The library of the Institute is specialized in Materials Science. It is part of the global CSIC Library Network, which includes a total of 60 specialized libraries distributed among 21 cities. The library collection covers subject areas related to Materials Science such as Physics, Chemistry and Crystallography. It has over 2,000 monographs and 105 periodic publications. The library is open to all ICMAB staff and other CSIC personnel and also to other Research or Academic Centers who would like to make use of it.

2017 Activities

The library has 2,329 registered titles in the collective catalog of the institution, 6 acquired in 2017, and 77 subscriptions to scientific journals. It has registered 29 loans and 262 renewals of monographs, of 53 active readers, during the year. The online service for sharing documents counted with 174 requests to other libraries (165 of

articles and 9 of monographs) and received 37 requests (32 of articles and 5 of monographs), and 38 internal requests. The total scientific production of Professor Vladimir Laukhin, on the occasion of the tribute for his retirement, was compiled in two monographs. The bibliometric calculations for researchers and for the whole center, such as the ones needed for the evaluation of the Severo Ochoa by the SAB, are done by our librarian & documentalist, Alejandro Santos. In November 2017, the library hosted an advanced level Web of Science training course, organized in collaboration with the FECYT and Clarivate Analytics. The library contributed with a collaboration in the section "En directo" of the electronic magazine of the Network of Libraries and Archives of the CSIC Enredadera (num 30) and with an interview about the fulfillment of the Open Access mandates of the CSIC Abierto magazine (num 16).



MAINTENANCE

The Maintenance Service is in charge of the maintenance and conservation of the building, of all its facilities and of the equipment. It works from the year 1991, when the Institute moved to the new building. It is also responsible for all the equipment, materials and tools (mechanic, electronic and electric) available to all the ICMAB personnel. During 2017 the Maintenance staff was increased by 2.



NEW LABORATORIES AND OFFICES

During 2017, three new laboratories were under construction in the MATGAS building, a Cleanroom and a Chemistry Lab, which were completed by the end of 2017, corresponding to the ERC-Ultrasupertapes, and a Chemistry Lab, corresponding to the ERC-Nest, and a Chemistry and a Physics Lab, corresponding to the ERC-Tmol4Trans, which will be completed in 2018.

Moreover, during 2017 a total of 13 offices and tables were installed in the MATGAS building, giving space to nearly 50 researchers (PhD and postdoc fellows and senior researchers). At the ICMAB building, some space has been relocated and made available for more tables. Moreover, the kitchen was remodeled and a new terrace with tables for the lunch time was created.

ACKNOWLEDGEMENTS



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