INSTITUT DE CIÈNCIA DE MATERIALS DE BARCELONA - ICMAB-CSIC ANNUAL REPORT 2018

ANNUAL REPORT 2018

ICMAB
INSTITUT DE CIÈNCIA DE MATERIALS DE BARCELONA
EXCELENCIA SEVERO OCHOA

CSIC
CONSEJO SUPERIOR DE INVESTIGACIONES CIENTÍFICAS

ANNUAL REPORT

2018

ICMAB INSTITUT DE CIÈNCIA DE MATERIALS DE BARCELONA
EXCELENCIA SEVERO OCHOA

CSIC CONSEJO SUPERIOR DE INVESTIGACIONES CIENTÍFICAS

Institut de Ciència de Materials de Barcelona (ICMAB)
Consell Superior d'Investigacions Científiques (CSIC)
Campus de la UAB 08193 Bellaterra (Barcelona)
Catalunya, Spain
Phone: +34 935 801 853
Fax: +34 935 805 729

www.icmab.es · info@icmab.es
Annual Report 2018 website: https//resources.icmab.es/annualreport2018

@icmabCSIC @icmab @icmab @icmab @ICMABCSIC

Thank you to the contributors who participated in this publication:
Núria Aliaga-Alcalde, Esther Barrena, Mariano Campoy-Quiles, Enric Canadell, Nieves Casañ-Pastor, Núria Crivillers, Concepción Domingo Ignasi Fina, Josep Fontcuberta, Amparo Fuertes, Jose-Luís García-Muñoz, Juan Luis Garcia-Pomar, José Giner, Susana Garelik, Martí Gich Enikö György, Gervasi Herranz, Anna Laromaine, Ana M. López-Periago, Benjamín Martínez, Marta Mas-Torrent, Agustín Mihi, Rosario Núñez Xavier Obradors, Carmen Ocal, M. Rosa Palacín, Anna Palau, Ángel Pérez del Pino, Teresa Puig, Imma Ratera, Susagna Ricart, Anna Roig Riccardo Rurali, Florencio Sánchez, Felip Sandiumenge, Massimiliano Stengel, Francesc Teixidor, Gerard Tobias, Dino Tonti, Jaume Veciana Albert Verdaguer, Marta Vendrell, Nora Ventosa, Clara Viñas
Edition and Coordination: Anna May Masnou
Graphic design, Infographics and Webmaster: José Antonio Gómez
Cover Image: "Photonic Leaf" by Cristiano Matricardi
Printing: GAM Digital
Copies: 150 issues
Legal deposit: B-12355-2011

Contents

"ICMAB has been a very active and enthusiastic research center in advanced materials during our already long history, more than three decades"

Xavier Obradors
Director ICMAB-CSIC

ANNUAL REPORT 2018

Foreword of the Director

Welcome to the ICMAB Annual Report 2018!

This annual report corresponds to that of the third year of our Severo Ochoa "Center of Excellence" called "Smart FUNctional MATerials for social grand challenges" (FUNMAT). The Research Program includes several scientific and technological actions addressing three very timely social grand challenges: Clean and Secure Energy, Sustainable and low cost electronics and Smart Nanomedicine. The R&D activities are organized following 5 different Research Lines (RLs): RL1: Sustainable energy conversion and storage systems; RL2: Superconductors for power applications; RL3: Oxide electronics; RL4: Molecular electronics; RL5: Multifunctional nanostructured biomaterials. I'm sure you will enjoy reading the provided summaries of our research and the different activities providing evidence of the ICMAB enthusiasm and effectiveness in advancing knowledge and address the critical goals of these challenges.

One of the priorities of our FUNMAT project was the attraction of new talent. The success in this issue has been overwhelming as demonstrated by a huge increase of the total personnel at ICMAB: 80 more people since starting FUNMAT, i.e. 65 % increase of non-permanent people, reaching a total of 340 people. We had in 2018 a total of 113 PhD fellows (47 % of them from abroad, from 24 different countries), 58 postdoctoral researchers, 34 undergraduate and master students and we also assured 3 new permanent scientists reaching a total of 61. The availability of new spaces in the neighboring MATGAS building has been essential to properly accommodate this outstanding staff growth.

The R&D activities and projects where our researchers have been engaged are surely deeply diversified. For instance, we have been awarded up to 2018 with a total of 9 ERC Grants (2 more will start soon), additionally, we were also awarded with several new outstanding European research projects. Overall, during 2018 a total of 35 European or international projects were alive which have provided to ICMAB a total budget of 22.2 M€. The total budget for 2018 is similar to 2017 (14.7 M€) and consolidates a 34 % growth since starting FUNMAT thanks to a competitive funding of 64 %. The success in attracting and managing competitive funds strongly relies on the international leadership of our researchers and also on the support of the Strategic Project Managing Unit build up in the scope of FUNMAT and the general administration and maintenance staff. It is also worth to mention that FUNMAT has strongly promoted the internal synergy among research groups, for instance through the allocation of 24 Frontier Interdisciplinary Projects (FIP).

The scientific production of ICMAB researchers continues to be outstanding and of high quality, a total of 226 articles were published, reaching an average impact factor of the journals of 6.30 in 2018. As an indicator of our outstanding impact we should also mention that ICMAB reached the highest CSIC Nature Index per researcher and the second position in absolute values. We continue also to increase the total number of citations (> 145.000 at the end of 2018 from 5,223 publications). Our researchers are widely selected to lecture in international conferences as reference speakers and they receive awards and recognitions.

The scientific highlights that we selected for this report correspond to outstanding publications of the different Research Lines. I'm sure you will enjoy reading these presentations about the diverse topics investigated at ICMAB. They cover contributions at the frontiers of materials research. You will see how we envisage novel research opportunities to make synthesis and processing of materials, how we use or develop new advanced tools to characterize or simulate properties of materials and also how these materials are integrated into devices or adapted for competitive practical applications, bringing appealing opportunities for technological innovation. You will see how we tune optical properties of sustainable cellulose through plasmonics, of low cost photovoltaic cells or inorganic nanotube heterostructures, you will further understand how complex is the chemistry of batteries and supercapacitors and how we can make them more competitive. Multifunctionality of complex oxides remains a topic where ICMAB is extremely active: new magnetic, ferroelectric or superconducting epitaxial thin films with controlled nanostructures and defects show a plethora of attractive properties useful for information technologies or power applications. Understanding and controlling the electronic properties of molecular materials at the nanoscale is shown to be a very rich source of appealing properties which the ICMABers know how to design and use in electronic devices. Finally, remarkable and very promising advances on materials for nanomedicine are demonstrated, spanning from nanoparticles, nanovesicles, metalorganic frameworks and molecules which help to grow cells, deliver drugs for specific therapies or create biomarkers for improved imaging.

Overall, you will be able to realize that these advances are expected to contribute to address the three social challenges of FUNMAT.

The international evaluation of the ICMAB activities by our Scientific Advisory Board (SAB) was celebrated through a third edition which focused particularly this year on three Research Lines: RL2 "Superconductors for power applications", RL4 "Molecular electronics" and RL5 "Multifunctional nanostructured biomaterials". The members of the SAB strongly appreciated the high quality and excellence of the research being performed and they provided useful advice for the future strategies of ICMAB.

The success in increasing the ICMAB visibility is a remarkable success of our new Communication and Outreach office. A strong increase of the number of outreach activities developed by the ICMAB researchers and technicians has been registered, together with an enhanced impact in the social media, for instance the ICMAB web site reached the highest visibility of CSIC in 2018. An external evaluation of the knowledge transfer capabilities of ICMAB was performed during 2018 which is being extremely useful to focus our goals and promoting our interaction with external stakeholders, and starting to give fruit.

In conclusion, we are sure that this report will help to spread the vitality of ICMABers, to widely transmit the many new ideas and achievements that we have made and our passion for progressing towards a better future.

For more information about the ICMAB activities you can access the website version of our report (https://resources.icmab.es/annualreport2018/).

Enjoy the tour!
Xavier Obradors
ICMAB Director

ANNUAL REPORT 2018

About Us

We are a public and multidisciplinary research center dedicated to cutting-edge research in functional advanced nanomaterials, pursuing excellence in the generation and transfer of knowledge, and in the development of scientific and technical tools and methodologies.

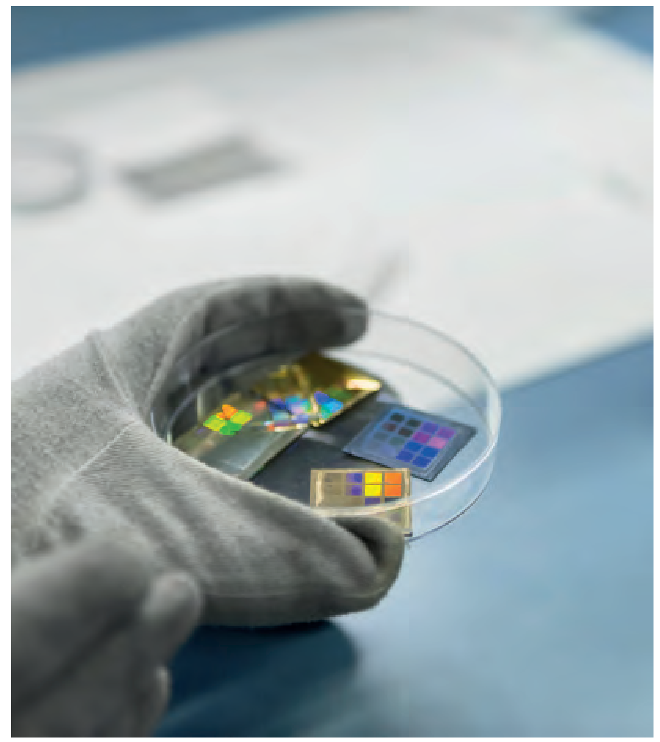
Our aim is to create new knowledge and innovative solutions in some of the biggest and more complex challenges that our society currently faces: materials for a clean and secure energy, materials for low-cost electronics, and materials for nanomedicine.

We are located at the Autonomous University of Barcelona (UAB) campus, surrounded by other research and technological centres and with access to many state-of-the art equipment and scientific facilities. With over 300 members, it is a very attractive place to work for young researchers.

Our R&D activities are strongly backed up by state-of-the-art scientific instrumentation and specialised technical staff available in our scientific services. We are ready and able to deploy R&D activities at the forefront of international knowledge.

The ICMAB is integrated within the Barcelona Nanocluster in Bellaterra (BNC-b), a research network that aims to share advanced scientific equipment and promote and disseminate nanoscience and nanotechnology to the society.

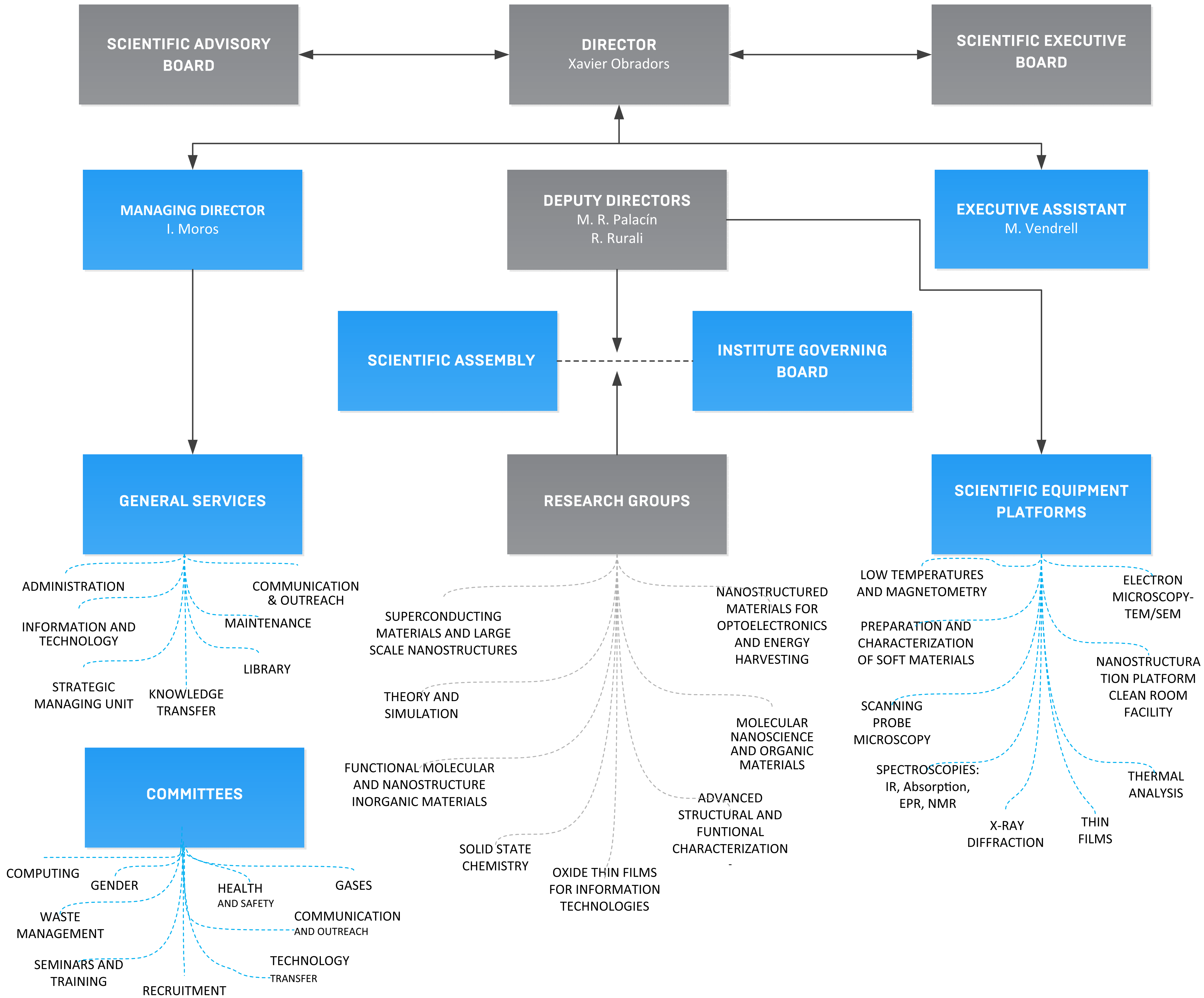
The ICMAB therefore offers a complete range of scientific services, including a 10,000 class cleanroom (the Nanoquim Platform) that are open to interested parties, whether these are academic or from industry, and it participates in all kinds of educational and promotional activities. Many ICMAB researchers teach at the UABMaster's degree in Nanotechnology and Materials Science and also on the UAB degree on Nanoscience and Nanotechnology.



- Founded in 1986
- An international leading research center in Materials Science
- We are one of the 120 research institutes of the CSIC
- Close to 119 senior and postdoc scientists and 113 pre-doctoral fellows
- Scientists are grouped in five research areas: sustainable energy conversion and storage systems, superconductors for power applications, oxide electronics, molecular electronics, and multifunctional nanostructured biomaterials
- We are located at the campus of the Autonomous University of Barcelona
- Funded by governments, international and national research projects, and private companies

CENTER OF EXCELLENCE

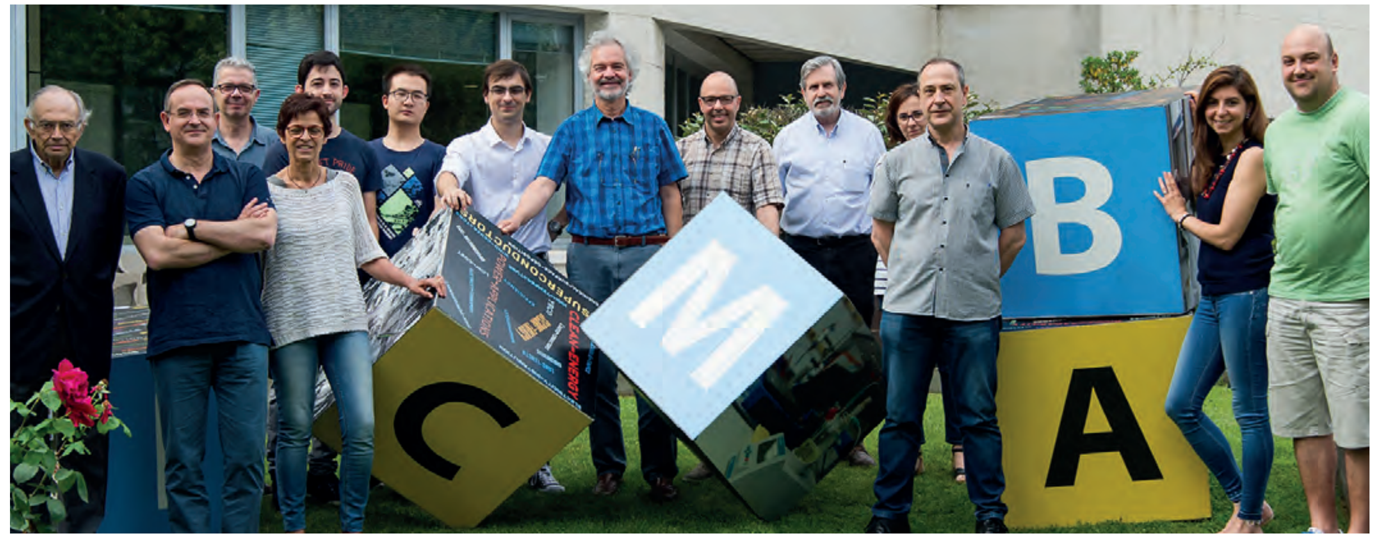
Organisation



CENTER OF EXCELLENCE

ICMAB Staff 2018

RESEARCH GROUPS



Crystallography of Magnetic and Electronic Oxides and Surfaces (CMEOS)

This group is 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.

departments.icmab.es/cmeos

Prof. José Luis García-Muñoz

He 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. Xavier Torrelles

He is graduated in Physics with a PhD in Physical Sciences. His scientific interest are focused on the design of switchable ferroelectric buffer films as support of TiO_2 catalysts for water splitting and gas-liquid-solid-molecular interfaces with oxide-metal crystals to deepen in the knowledge of fundamental surface interactions.

Crystallography Group

The aim of the group is 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.

departments.icmab.es/crystallography

Prof. Carles Miravitlles

Prof. Carles Miravitlles has always combined his research in crystallography and characterization of materials with multiple responsibilities during his career, such ad 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, Môssbauer spectroscopy and aerogels and related porous materials.

Dr. Xabier M. 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. Mónica Benito

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

Dr. Ignasi Mata

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.

Prof. Jordi Rius Palleiro

Graduated in Geology and holds a PhD in Natural Sciences from the Philipps-Univeristät (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.

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 the fields of energy, environmental science, molecular electronics and medicine.

departments.icmab.es/lmi

Prof. Francesc Teixidor

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

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

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

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. 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.

departments.icmab.es/nn

Prof. Anna Roig

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

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

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)

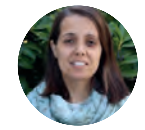
The group interests relate to the fields of nanoscience and nanotechnology, particularly the areas of molecular electronics, molecular magnetism and biology. We design molecular systems capable of providing inputs at the nano-scale and focus our efforts in the control and organization of such species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

departments.icmab.es/funnanosurf

Dr. Núria Aliaga-Alcalde

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



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.

Fluorescent Boron compounds

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

projects.icmab.es/nanomol

Prof. Jaume Veciana

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.

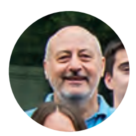
Prof. Concepció Rovira

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.

Dr. Nora Ventosa

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 reach clinical testing.

Dr. José Vidal-Gancedo



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 & Dr. Judith Guasch

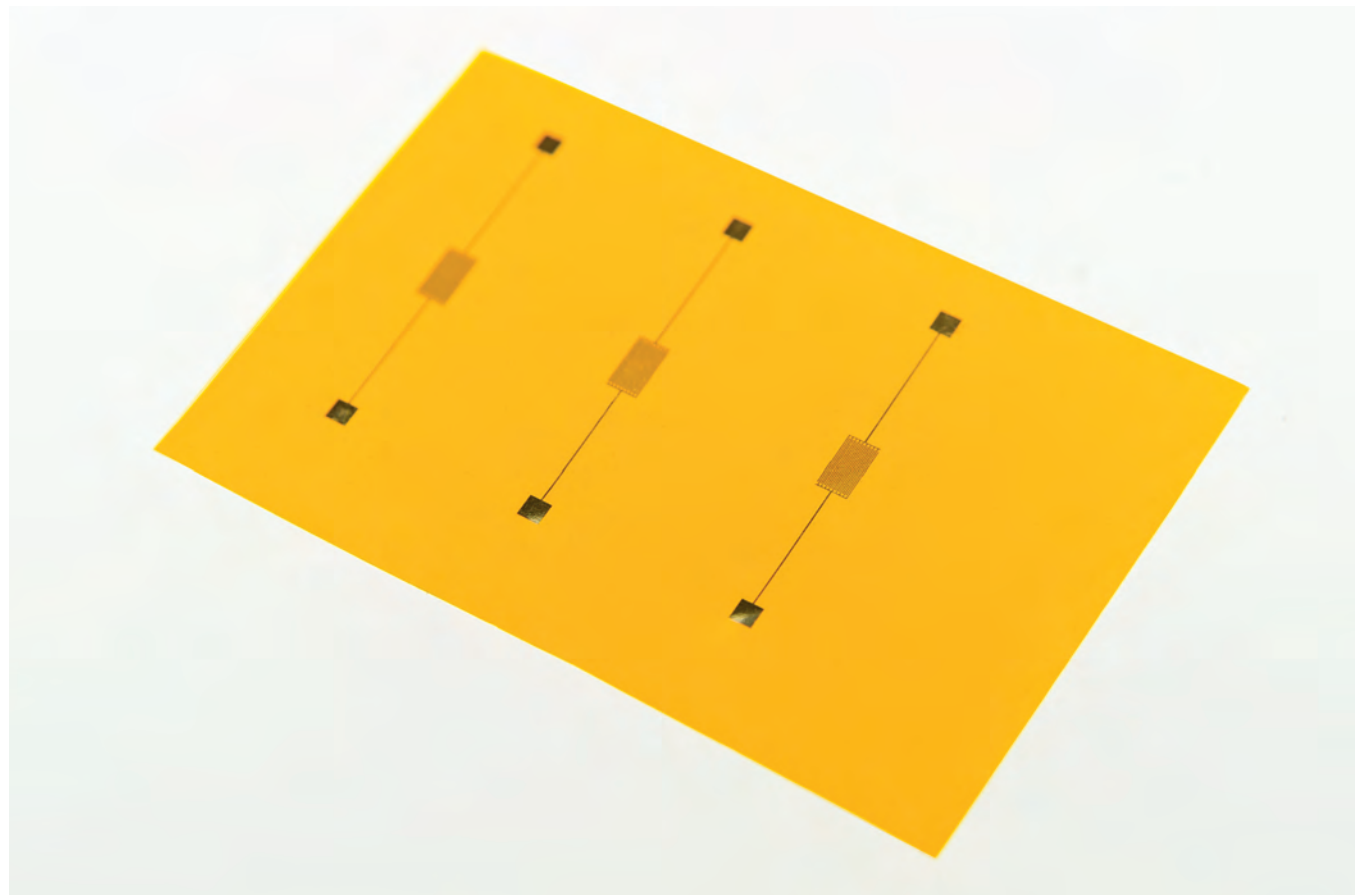
Dr. Imma Ratera's Lab interests are focused on the design and synthesis of novel multifunctional organic electroactive and radical molecules and their molecular and supramolecular chemistry. The group is interested in the properties of these molecules once nanostructured as self-assembled monolayer, 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 & Dr. Núria Crivillers

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

Dr. Elena Laukhina

Dr. Elena Laukhina is a CIBER researcher specialized in molecular electronics. Her research is focused on flexible films with responsive properties, such as hydroresistive, conducting, piezoresistive, etc. that can be used as sensors, such as for sensing pressure or temperature



Flexible and organic support for electronic circuits

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 1.- the search for disruptive approaches to materials and methods in photovoltaic conversion, 2.- 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 3.- explore data storage and data manipulation alternatives to current methods, by using non-dissipative currents or efficient plasmonic signals

departments.icmab.es/mulfox

Prof. Josep Fontcuberta

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.

Dr. Lourdes Fàbrega

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

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.

Dr. Gervasi Herranz

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.

Dr. Ferran Macià

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.

Dr. Ignasi Fina

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 Nanostructued 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

departments.icmab.es/acnm

Prof. Benjamín Martínez

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

Dr. Lluís Balcells interests are focused on magnetic materials, including thin films and nanoparticles, for applications in electronics and spintronics.

Dr. Felip Sandiumenge

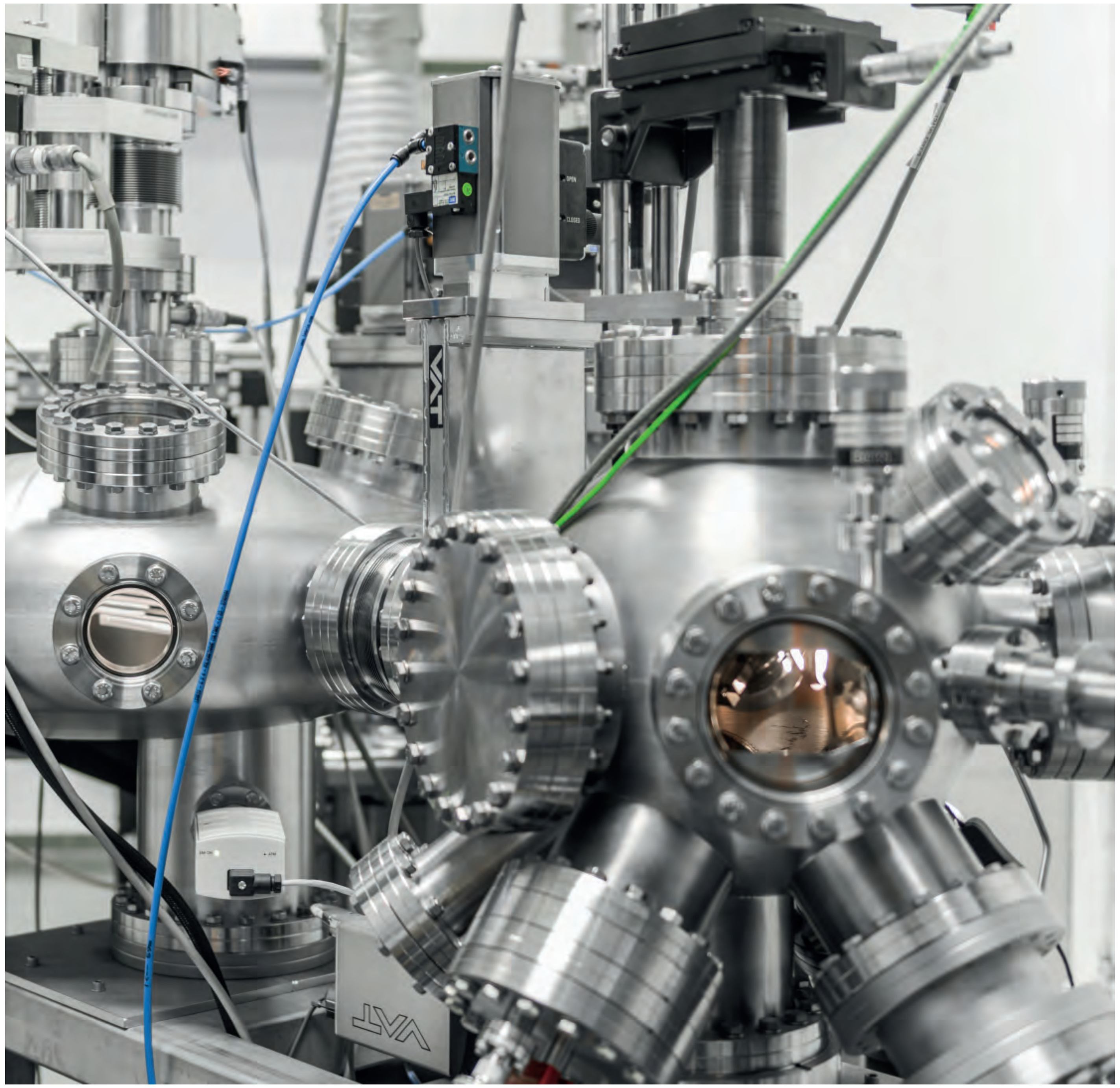
Dr. Felip Sandiumenge scientific interest is focused on the correlation between structure and function in oxide epitaxial films, with emphasis on the atomic structure and defect chemistry of crystalline defects such as dislocations and domain walls.

Dr. Carlos Frontera

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

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.



Pulsed Laser Deposition equipment

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

departments.icmab.es/surfaces

Prof. Carmen Ocal

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

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 organic-field transistors and photovoltaics). Her expertise includes real-time x-ray diffraction, organic growth, self-assembly and scanning probe microscopies.

Dr. Albert Verdaguer

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.

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

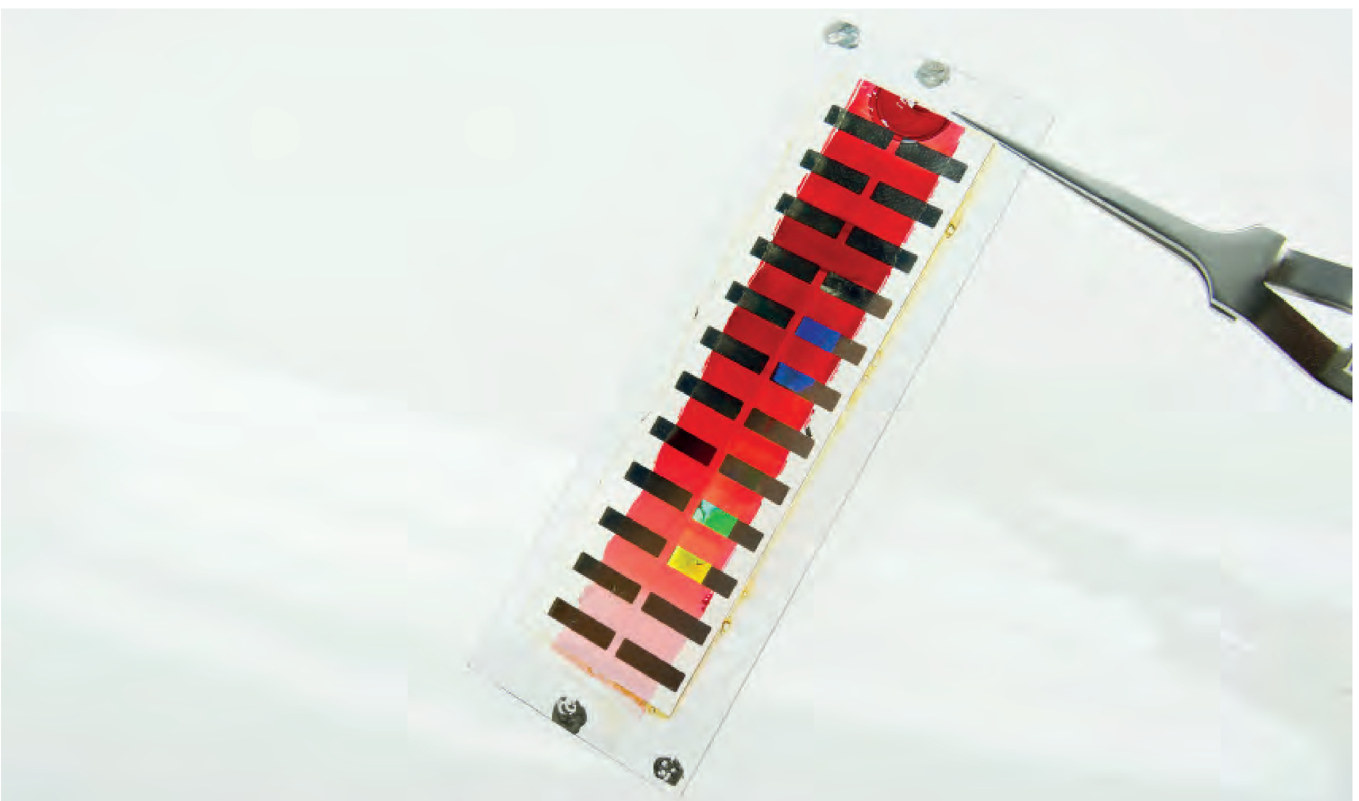
icmab.es/laserprocessing

Dr. Ángel Pérez del Pino

Dr. Enikö György

Dr. Angel Perez del Pino and Dr. Enikö György are the managers of the group. They are specialists in

- 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)
- Study of laser-matter interactions, and
- Advanced characterization of nanomaterials.



Organic solar cell with gradients

Nanostructured 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

departments.icmab.es/nanopto

Dr. M. Isabel Alonso

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.

Dr. Mariano Campoy-Quiles

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 Goñi

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.

Dr. Miquel Garriga

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 hight critical temperature superconductors.

Dr. Agustín Mihi

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 mater interaction applied to emerging optoelectronic devices.

Dr. Sebastián Reparaz

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.

Solid State Chemistry (SSC)

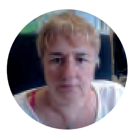
The research interests of the Solid State Chemistry group are centered in the areas of battery materials, inorganic and carbon nanomaterials, hybrid materials, biomaterials and nitride-based materials. The design of new inorganic phases, basing on crystal chemical criteria, mixed-valence character and 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

departments.icmab.es/ssc

Prof. Nieves Casañ-Pastor

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



Prof. Concha Domingo is an expert in the use of supercritical CO_2 technology for materials processing. Her current research focuses on the construction of graphene oxide aerogels with multiple applications ranging from CO_2 capture to batteries.

Prof. Amparo Fuertes

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

Dr. Ana M. López-Periago research involves the design and synthesis of metal-organic frameworks using supercritical CO_2, with applications in the area of gas separation and sustained drug release.

Prof. M. Rosa Palacín

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

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.

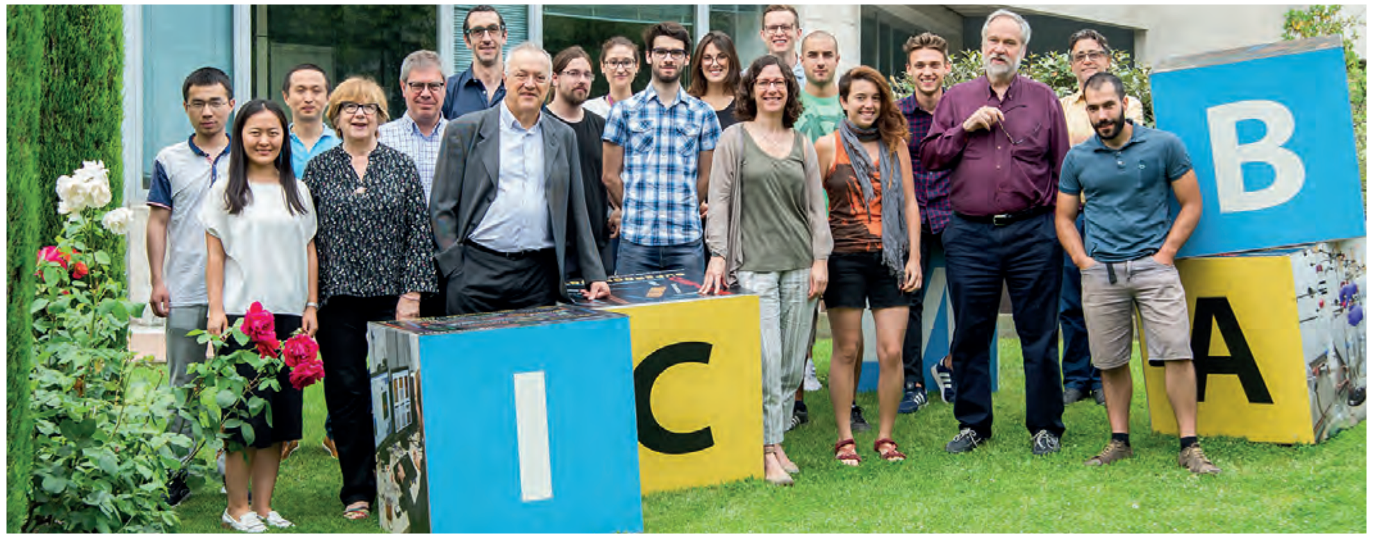
Dr. Gerard Tobias

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

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.

Porous and ultralightweight reduced Graphene Oxide foam



SUMAN Research Group (SUMAN)

The 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 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.

departments.icmab.es/suman

Prof. Teresa Puig

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

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

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

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

Dra. 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

Dra. 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.

Dra. Mariona Coll

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

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

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.

Levitation of a magnet using superconducting YBCO and liquid nitrogen

Materials Simulation and Theory group (MST)

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

departments.icmab.es/mst

Prof. Enric Canadell

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

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

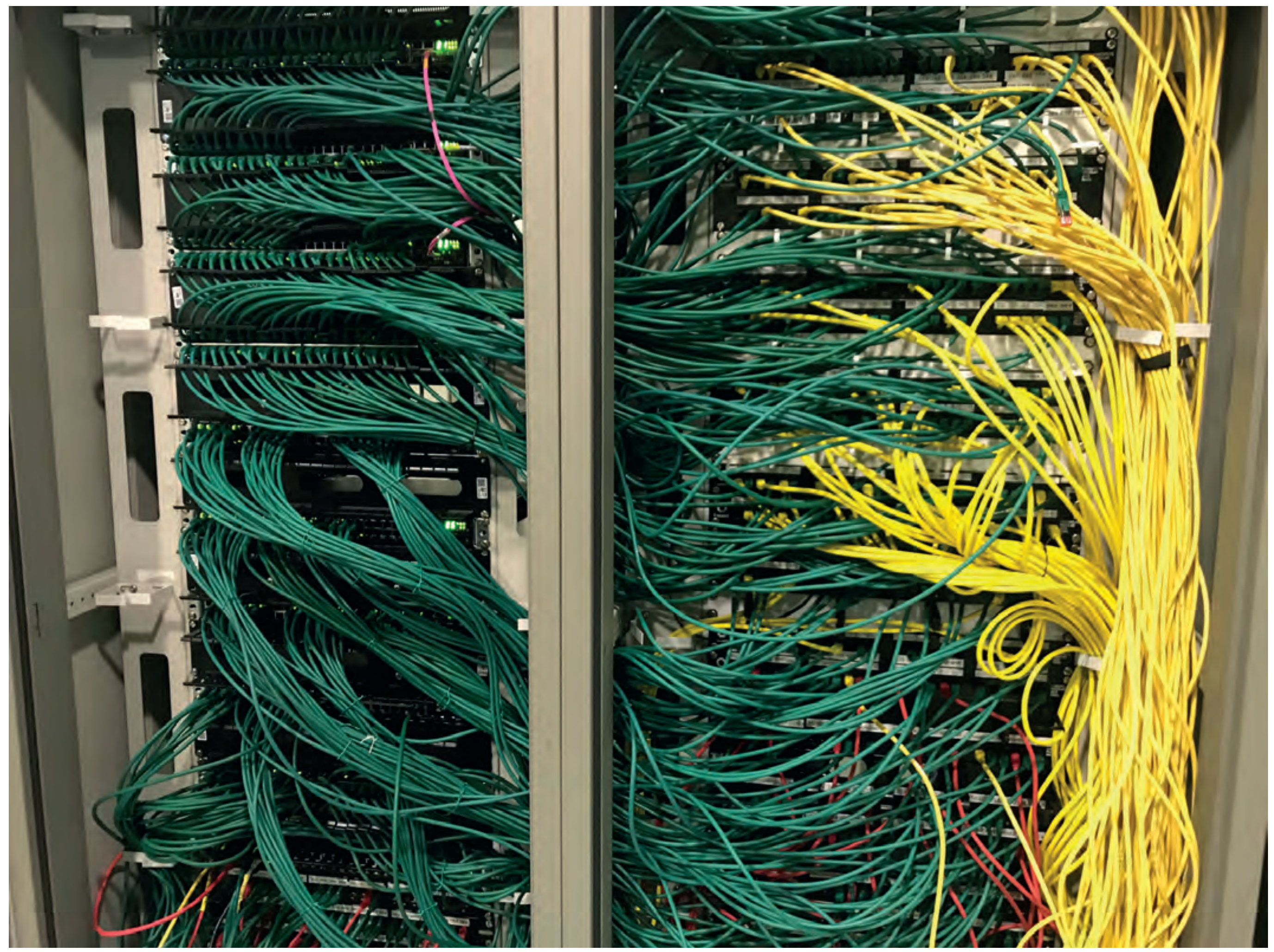
Dr. Massimiliano Stengel's research focuses on the development of frontier electronic-structure methods, and their application at tackling key fundamental and technological questions in ferroelectricity, magnetism, surface science and metal/oxide interfaces. In the past few years he has been particularly 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

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). (STEM- EELS).

Dr. Jordi Faraudo

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.



Connection cables from computers and phones at the ICMAB Server Room

Severo Ochoa Project

2018 is the third year of the Severo Ochoa Project of our Institute "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

EXCELENCIA SEVERO OCHOA

Objectives

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.

Research Lines

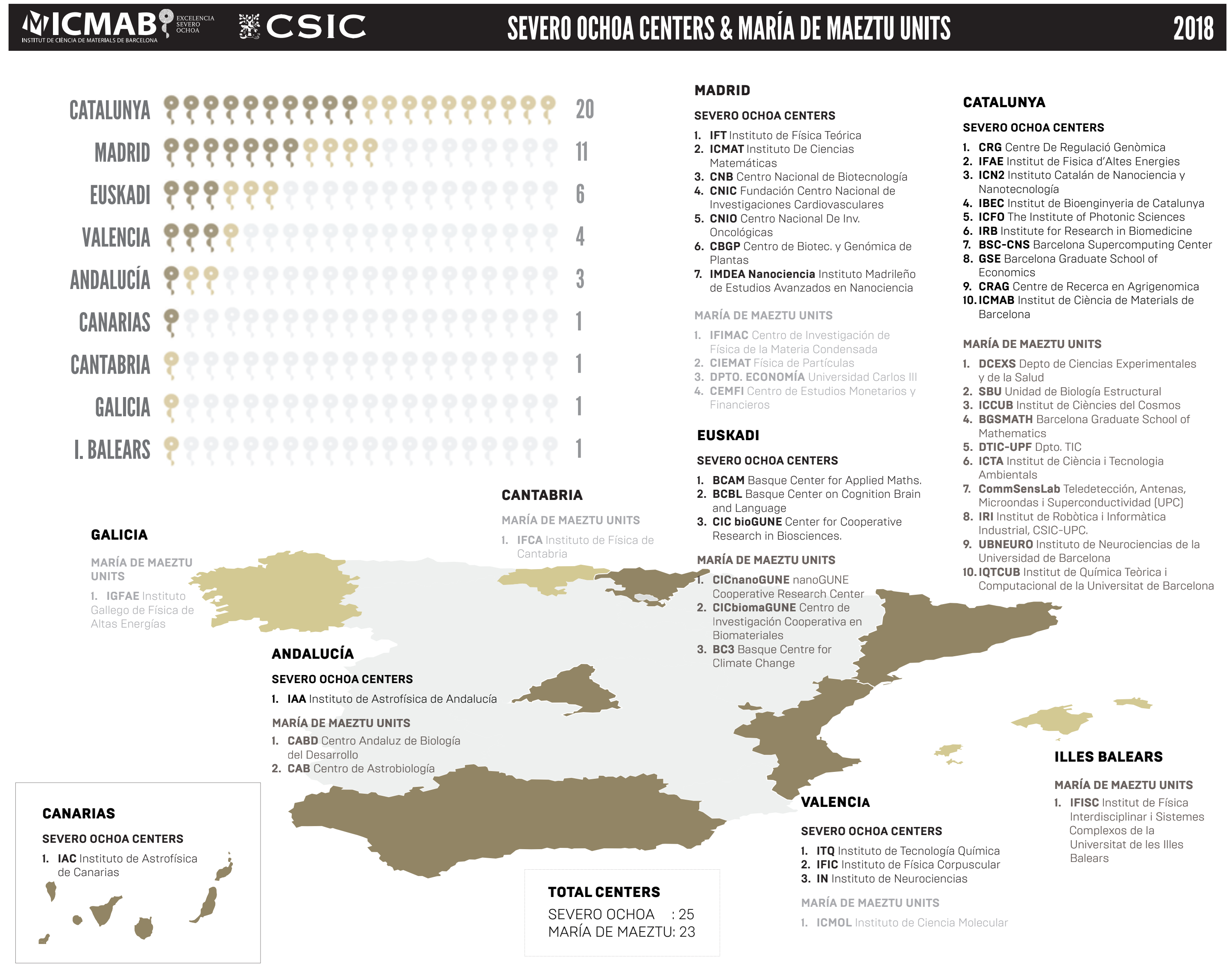
2018 is the third year of the Severo Ochoa Project of our Institute "Smart Functional Materials for Social Grand Challenges" (FUNMAT). The ICMAB became a Severo Ochoa Centre of Excellence in 2016, becoming one of the top research centers in Spain in Materials Science.

The associated strategic research programme brings together the institute's eight research units 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 three social grand challenges of the 21st Century, aligned with the main European Social Challenges in H2020:

CLEAN AND SECURE ENERGY
SUSTAINABLE AND LOW COST ELECTRONICS
SMART NANOMEDICINE



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.

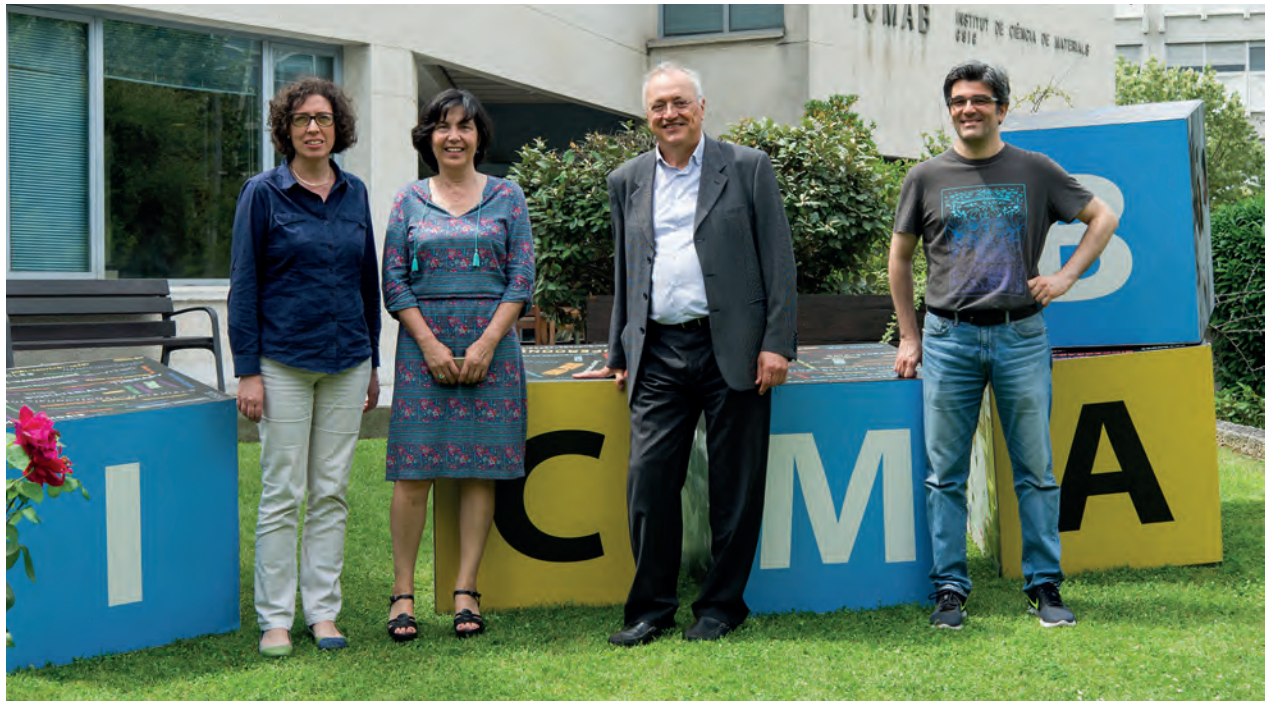
SMART NANOMEDICINE

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 contribution to Nanomedecine, 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.

CENTER OF EXCELLENCE

Governing Bodies

Along with the restructuration of the research, the governance and strategic actions have been updated with the Severo Ochoa mention of Excellence. They include:



Left to right: M. Rosa Palacín, Imma Moros, Xavier Obradors and Riccardo Rurali

Direction Team

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

Governing Bodies

Scientific Advisory Board (SAB)

The Scientific Advisoy Board (SAB) is an international committee in charge of the evaluation of the Severo Ochoa Project implementation. It is formed by 12 international members, 11 of which are non-Spanish, and 5 of which are women (42 %). The members are:

Silke CHRISTIANSEN
Max Planck Institute for Science of Light Erlangen (Gemany)

Patrick COUVREUR
Laboratoire de Physico-Chimie, Pharmacotechnie et Biopharmacie (France)

Rudolf GROSS
Technische Universität München, Physik Department (Germany)

David LARBALESTIER
Florida State University; High Magnetic Field Laboratory, Tallahassee (USA)

Luis LIZ-MARZAN
CIC biomaGUNE (Spain)

Judith MacMANUS-DRISCOLL
University of Cambridge, Department of Materials Science & Metallurgy (UK)

Jean-Marie TARASCON
Collège de France, Chimie du solide et de l'énergie (France)

Erio TOSATTI
Scuola Internazionale Superiore di Studi Avanzati (SISSA) (Italy)

Susan TROLIER-McKINSTRY
W. M. Keck Smart Materials Integration Laboratory (USA)

Maurizio PRATO
Università di Triste (Italy) and CIC biomaGUNE (Spain)

Elsa REICHMANIS
School of Chemical & Biomolecular Engineering at Georgia Institute of Technology (USA)

Natalie STINGELIN
School of Materials Science in Engineering at Georgia Institute of Technology (USA)

Governing Bodies

Institute Board

The Institute Board is formed by the Director, the Vicedirectors, the Managing Director, the Heads of the Department, the Staff representatives and the Graduate researchers' representative. The meetings of the Institue Board are held twice a year.

Governing Bodies

Scientific Executive Board (SEB)

Direction team

- Xavier Obradors - Director
- M. Rosa Palacín - Vicedirector
- Riccardo Rurali - Vicedirector

Strategic Managing Unit

- Jorge Pérez / Laura Cabana
- Montse Salas

Research Line coordinators:

- Mariano Campoy-Quiles
  RL1, Sustainable Energy Conversion and Storage Systems
- Teresa Puig
  RL2, Superconductors for Power Applications
- Josep Fontcuberta
  RL3, Oxide Electronics
- Marta Mas-Torrent
  RL4, Molecular Electronics
- Immaculada Ratera
  RL5, Multifunctional Nanostructured Biomaterials

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: excellent Spanish research 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 interconnedted 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.

100xCiencia meetings

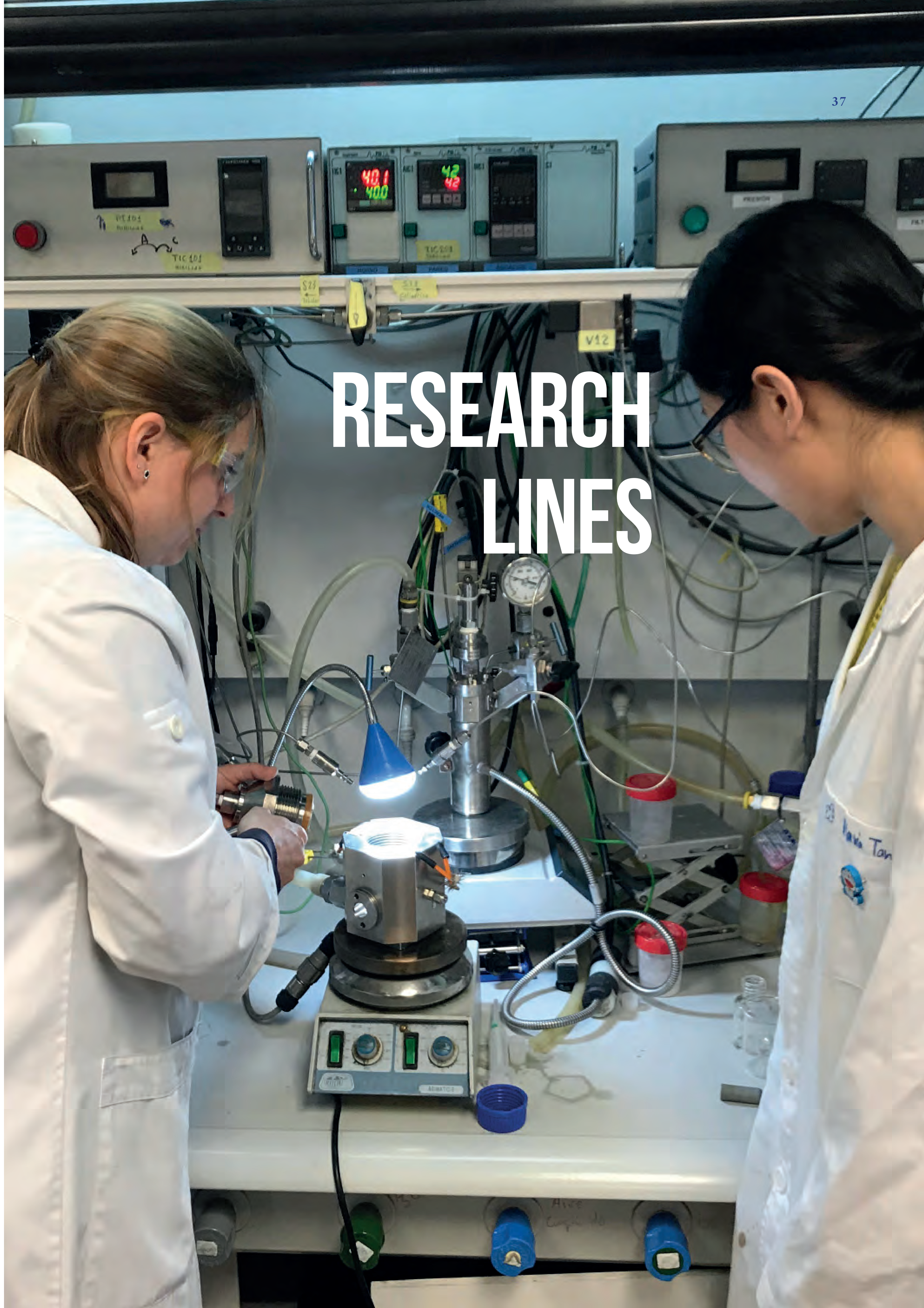
The alliance's starting activities comprised the establishment of its own governance, the launching of the website (somma.es) and the organisation of task forces to address the different objectives.

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.

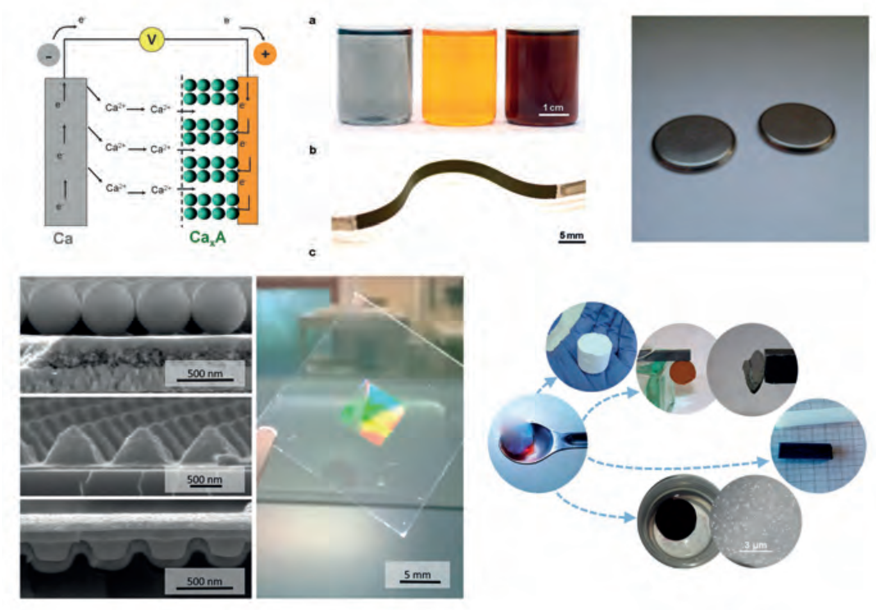
In 2017, the meeting was held in Alicante, and its topic was "Co-creating value in scientific research" and was focused on technology transfer success stories. In 2018, the meeting was held in Madrid, and the topic was "Bridging science and society" and was more devoted to outreach and educational activities.

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.



RL1: Sustainable energy conversion and storage system

Mission: contribute in the global energy challenge by advancing in the next generation materials for energy conversion and storage



Strategic fields

- **Advance in the next generation materials for renewable energy generation:**
  - From the sun (photovoltaics): organics, perovskites, boron-based, oxides, nanostructured inorganics, hybrid systems, photonic structures
  - From waste heat (emerging thermoelectrics): organics, nanocarbon (polymer/carbon strategies).
- **Advance in the next generation materials for storage technologies** (post-Li-ion battery technologies): hard carbon anodes for Na-ion batteries; electrolytes, anodes and cathodes for Mg- and Ca-based batteries, Zn-air batteires
- **Develop innovative sustainable technologies**, replacing critical or toxic materials by others, in the field of metal organic frameworks (MOFs), oxide-nitride layers, carbons and polymeric materials.
- **Advance characterization and theoretical tools that help the understanding of materials for energy** (e.g. XRD, AFM/SPM, TEM, IR, UV and Raman spectroscopies, ALBA's synchrotron lines, theoretical simulations).

Highlights 2018

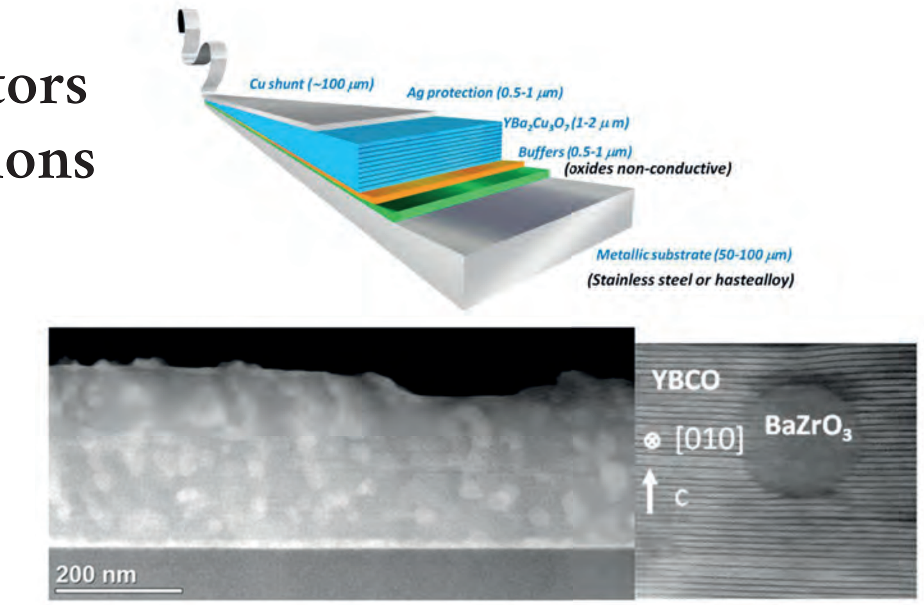
Publications: 72
Books: 7
PhD defenses: 1
Technology transfer: 3 patents filed and contracts (Repsol, Toyota, Eurecat…)

EU Projects (since 2012)

- MSCA-IF TELIOTES (2018)MSCA-IF BATCA (2017)
- FET-OPEN CARBAT (2017)
- ERC-StG CAMBAT (2017)
- MSCA-ITN SEPOMO (2016)
- ERC-CoG FOREMAT (2015)
- ERC-CoG ENLIGHTMENT (2015)
- SOCIETAL-CHALLENGES NAIADES (2015)

RL2: Superconductors for power applications

Create knowledge on material science and physics of high temperature superconductors to promote their use in energy efficient applications and large scale infrastructures



Strategic fields

- **Low cost and high throughput processing of nanostructured Superconducting Coated Conductors** by chemical solution processing and ink jet printing techniques
- **Boost the superconducting state** by controlling the strain and electronic states of high temperature superconducting films
- **New functionalities for energy-efficient cuprate superconducting electronic devices** based on the metal-insulator transition and superconducting-ferromagnetic interactions
- **Superconducting materials customization** for their integration in large scale infrastructures (energy, fusion and accelerators)

Highlights 2018

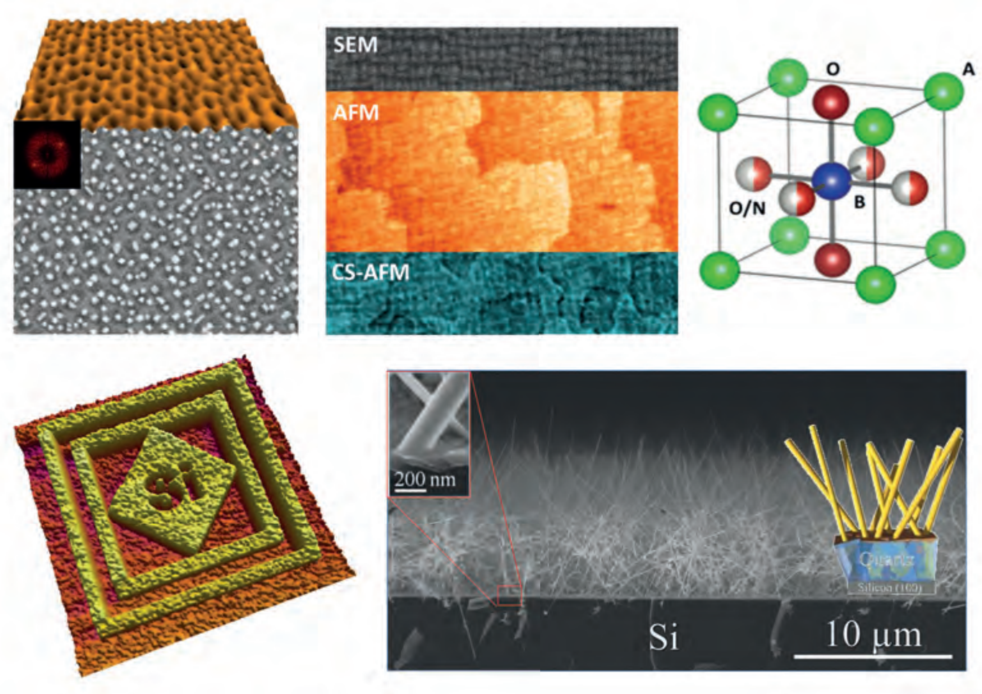
Publications: 20
Books: 1
PhD defenses: 5
Technology transfer: 1 patent filed and contracts (Oxolutia, CEA…)

EU Projects (since 2012)

- EU Projects (since 2012)
- LEIT-NMBP FASTGRID (2017)
- CERN HTS-FCCbs (2017)
- COST NANOCOHYBRI (2017)
- ERC-AdG ULTRASUPERTAPE (2015)
- EURATOM EUROFUSION (2014)
- COOP-ICT FORTISSIMO (2013)
- COOP-NMP EUROTAPES (2012)

RL3: Oxide electronics

Mission: the study of transition metal oxides, considered to be the building blocks for efficient and energy friendly data storage, advanced computing and energy harvesting devices.



Strategic fields

- **Contribute in exploiting orbital physics and interface engineering** to induce emerging properties, using oxides for data storage, communications and light harvesting.
- **Engineering magnetic properties**, searching and understanding multiferroic materials, integrating ferroelectric and ferromagnetic oxides on silicon, tailoring electronic properties with nitrides and designing and making artificial polar materials.
- **Development of thin films of these materials with subnanometric precision.**
- **Use the most advanced tools of lithography for device microfabrication**, prior to electrical, magnetic and optical characterization.
- **Structural, morphological and microstructural analysis** are done by a combination of in-house techniques (e.g. PLD) and extensive use of large scale facilities (ALBA synchrotron radiation, neutron beams, most advances electron microscopes, etc.).
- **Theory and simulation of the properties** and behavior of the materials (flexoelectricity, thermal transport…).

Highlights 2018

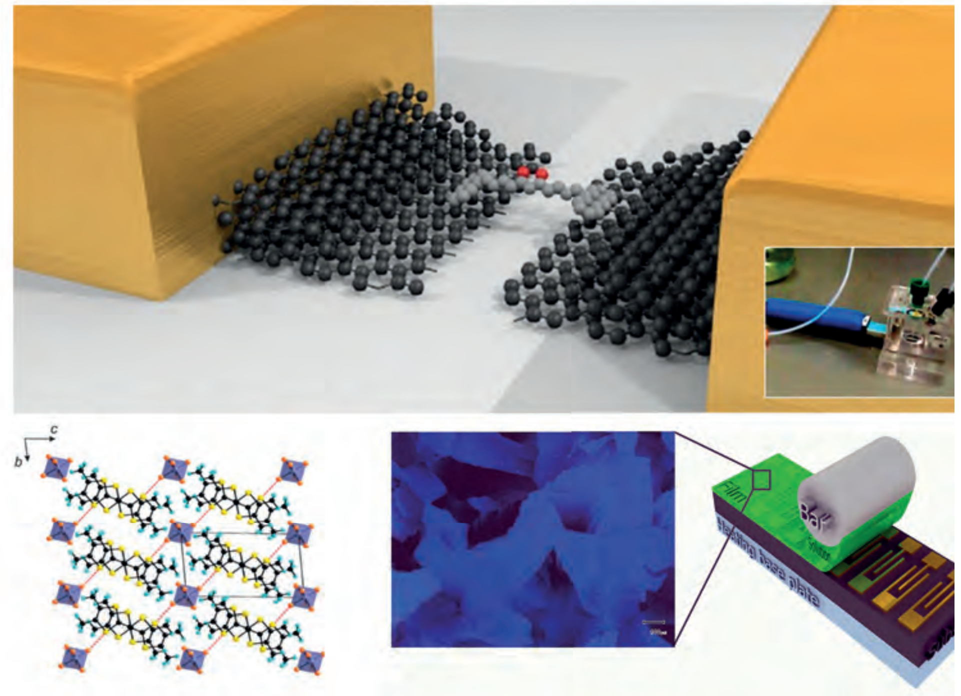
Publications: 45
PhD defenses: 3

EU Projects (since 2012)

- MSCA-IF EMPHASIS (2018)
- INFRAEDI Max (2018)
- ERC-CoG MULTIFLEXO (2017)
- EIT-RAW MATERIALS MAGNET (2017)
- MSCA-RISE DAFNEOX (2015)
- INFRAIA AHEAD (2015)
- INTERREG V-A TNSI (2014)
- COOP-ENVIRONMENT COMMON-SENSE (2013)

RL4: Molecular electronics

Mission: the fabrication of organic semiconductors for molecular and flexible electronics, which have a strong impact on the wellbeing of society, especially in the technological advances and health areas.



Strategic fields

- **Use or organic molecules in electronic devices.**
- **Design novel molecular switches**, memory electronic and spintronic devices, low-cost organic field-effect transistors and (bio) chemical and temperature sensor devices.
- **The devices are developed considering a holistic perspective including:** design and synthesis of the molecules, structural, morphological and electronic characterization, device fabrication and integration, and theory prediction and rationalization.
- **From fundamental studies** (molecule/surface interactions, structure/property correlations) and proof-of-concept devices.
- **Nanoscale behavior, structure and geometry of the molecular systems**, organic devices and engineered surface are characterized by STM, AFM, Kelvin probe, among others.

Highlights 2018

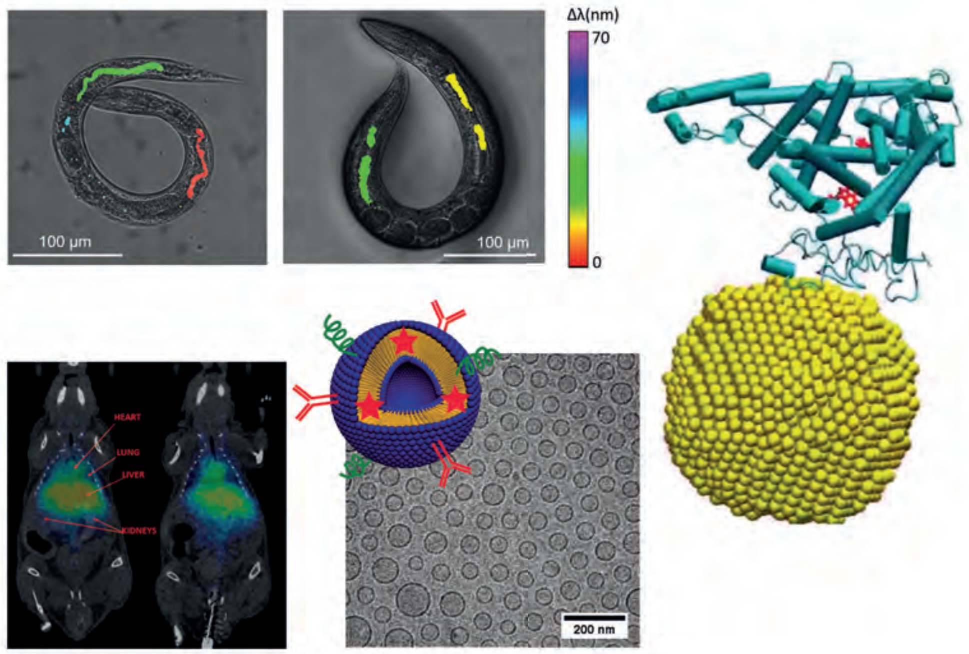
Publications: 57
PhD defenses: 7
Technology transfer: 2 patents filed

EU Projects (since 2012)

- ERC-CoG Tmol4TRANS (2017)
- MSCA-ITN SEPOMO (2016)
- MSCA-ITN iSWITCH (2015)
- ERC-PoC LAB-TECH (2014)
- FET Young Explorers ACMOL (2014)
- MSCA-ITN nano2fun (2013)
- COOP ENVIRONMENT COMMON-SENSE (2013)
- ERC-StG E-GAMES (2012)

RL5: Multifunctional nanostructured biomaterials

Mission: provide key inputs in the current nanomedicine challenges with strong impact on health: therapy, diagnosis and tissue repair.



Strategic fields

- **Synthesis of nanomaterials for therapy and diagnosis** obtained by new manufacturing schemes and able to cross biological barriers (nanovesicles, nanocapsules, nanoparticles, dendrimers, nanotubes, containing bioactive molecules…),
- **Synthesis of nanomaterials for multimodal diagnosis** enabling to obtain images of the different tissues and metabolites distribution based on contrast agents magnetic nanoparticles and organic free radicals, X-ray absorbers or radionuclei.
- **Synthesis of nanostructured materials for tissue repair** to understand and control signals directing cell behavior towards vascular or neural reparation therapies (biocompatible nanostructured electrodes based on graphene; endothelial cells and magnetic nanoparticles, and surfaces that trigger the organization of growth factors…)
- **Simulation of the behavior and self-assembly of soft and biomaterials.**

Highlights 2018

Publications: 51
Books: 3
PhD defenses: 1
Technology transfer: 3 patents filed and contracts (Grifols, Nanomol Technologies…)

EU Projects (since 2012)

- EURONANOMED MAGBBRIS (2017)
- ERC-CoG NEST (2017)
- MSCA-IF TUNING COPs (2017)
- LEIT-NMBP SMART-4-FABRY (2017)
- LEIT-NMBP KARDIATOOL (2017)
- MSCA-IF NANOTER (2016)
- MSCA-IF 3D-PRINTGRAPH (2016)
- COOP-FOOD SEA-ON-A-CHIP (2013)
- COOP-HEALTH BERENICE (2012)
- MSCA-ITN RADDEL (2012)
- MSCA-CIG 3DINVITRONPC (2012)

CENTER OF EXCELLENCE

Timeline

- Science in the press
- Outreach
- Workshops and conferences
- Projects
- Press release

JANUARY FEBRUARY MARCH

16 Jan | 23 Jan | 5 Feb | 11 Feb | 20 Feb | 12Mar

16 Jan — Next generation graphene-based biosensor for the fast detection of xanthine

ICMAB researchers have prepared a novel hybrid graphene-based electrochemical biosensor for the fast and 100 times more sensitive detection of xanthine, with respect to previously reported sensors

23 Jan — ICMAB offers a course on "Essential Documentation Tools" for young researchers

5 Feb — The revolution of nanomaterials: superabsorbers that trap sunlight

Researchers from ICMAB, led by Dr. Agustín Mihi, have created materials that largely absorb a wide range of the solar spectrum, between 400 and 1500 nm, using an ultrathin layer of less than 100 nm thick of material

11 Feb — The initiative "I became a scientist" and posters on the role of women in science for the International Day of Women and Girls in Science 2018 organized by the Gender and Equality Committee researchers

20 Feb — ICMAB and IMB-CNM participate in the European project KardiaTool, developing a portable device to detect heart failure from saliva samples

Prof. Francesc Teixidor and his team (LMI-ICMAB) are working on the synthesis and functionalization of the magnetic nanoparticles, which are the support of the specific antibodies for each biomarker.

12 Mar — Presentation of the Severo Ochoa Excellence Centres and Maria de Maeztu Excellence Units Alliance (#SOMMa). The Alliance aims at promoting Spanish excellence science, and preserving its competitiveness

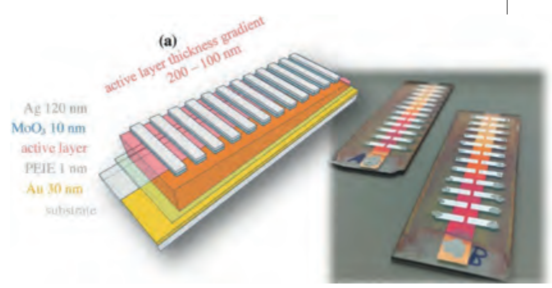
APRIL MAY

16 Mar | 3 Apr | 9 Apr | 10 Apr | 19-20 Apr | 3 May

16 Mar — The ICMAB organizes a workshop on Ethics and Responsible Research & Innovation in Research in the framework of the MSCA-ITN i-Switch

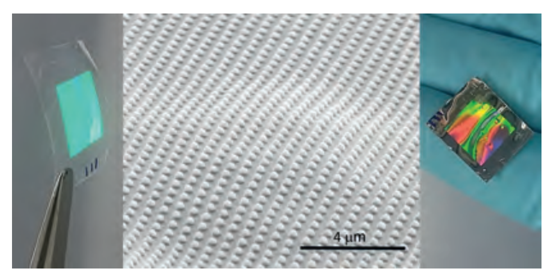
3 Apr — New organic and miniaturized photodetectors that absorb light beyond the visible range

A study led by the Technische Universität Dresden, in which the group of Dr. Mariano Campoy-Quiles of the Institute of Materials Science of Barcelona (ICMAB-CSIC) participated, has developed organic photodetectors that detect light below its absorption band, with high efficiency, in a tunable way and in a very precise wavelength of the electromagnetic spectrum.



9 Apr — Iridescent photonic cellulose, mimicking the structural color of insects, with optical applications

The study published today in Nature Photonics, led by Dr. Agustín Mihi (NANOPTO-ICMAB) creates for the first time photonic crystals and plasmonic structures of a cellulose derivative through its nanostructuring with the soft lithography technique.

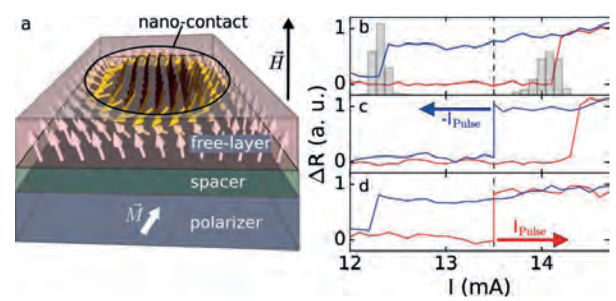


10 Apr — The 10alamenos9 Festival arrives to its 3rd edition with great success!

19-20 Apr — The Knowledge Transfer Unit organizes a workshop to assess the technology transfer potentials at ICMAB in collaboration with the Fraunhofer Institute in Germany

3 May — Physicists uncover properties of a magnetic soliton of interest for brain-inspired computing

"Solitons are solitary waves, like a tsunami or a tidal bore, are very interesting because they can be used to propagate energy or information, in a similar way as our neurons work. This is why they have promising applications in neuromorphic computing applications, for example" explains researcher Ferran Macià, one of the leaders of this study



MAY

JUNE

JULY

AUGUST

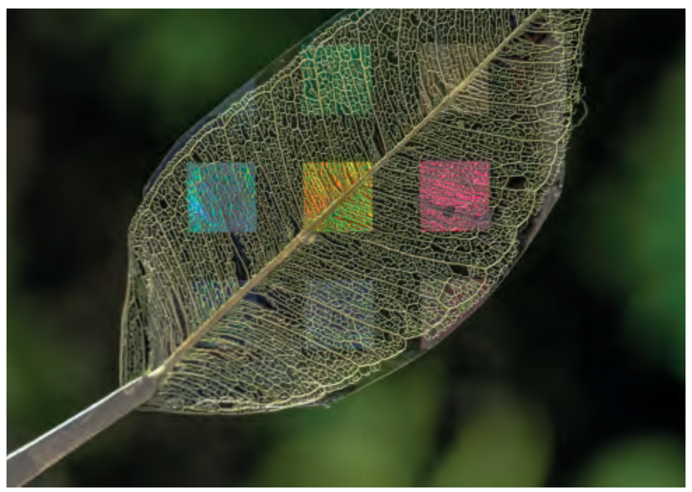
16 May

Disentangling the origin of magnetic proximity effects at the magnetic/non-magnetic interface

Researchers from ICMAB-CSIC and ALBA have analyzed the microscopic origin of the so-called "magnetic proximity effect" occurring at the interface between a magnetic material ($CoFe_2O_4$) and a nonmagnetic metal (Pt), which may induce a magnetic moment in the latter. The results are published in ACS Applied Materials & Interfaces.

17 May

"Photonic leaf" the winning picture of FOTICMAB 2018, our photo contest



30 May

ICMAB researchers develop flexible materials that switch from nano-porous 3D to 2D structures in a reversible way

"The spherical shape of the ligands is the key factor that enables the structures to go back to their original shape, allowing for the rearrangement of the different parts, and without collapsing the whole structure" – describes Jose Giner (LMI-ICMAB)

9-10 Jun

The Barcelona Science Festival counts with ICMAB researchers for microtalks, photonic contest and nanotechnology activities

14 Jun

Minimalist Biostructures Designed to Create Nanomaterials

The study, published in ACS Nano included the collaboration of Isabel Fuentes and Francesc Teixidor from the ICMAB-CSIC

26 Jun

Four students from the UAB Argó Program spend 10 days at the ICMAB this summer

12 Jul

Kick-off of the interactive exhibition "Matheroes: Supermaterials, heroes of the future"

17 Jul

New boost to future calcium batteries - A possible cathode?

This breakthrough demonstrates that this oxide could be used as cathode (positive electrode) in future rechargeable calcium batteries. This finding can help solve one of the main problems to produce rechargeable calcium batteries, which consists in finding cathodes that can extract and incorporate calcium ions in a reversible way, explains the ICMAB researcher M. Rosa Palacín, leader of the study

25 Jul

Nine Frontier Interdisciplinary Projects (FIP) granted in the third internal call within the Severo Ochoa FUNMAT programme

22 Aug

"The materials that will change the world" featured in La Vanguardia

Some of our researchers and their research were featured in the article "Los materiales que cambiarán el mundo" written by the journalist Elsa Velasco, in La Vanguardia (Big Vang)

30 Aug

Marta Mas-Torrent and Teresa Puig, ERC researchers, in #LasCientíficasCuentan, a project to visibilize ERC women

31 Aug

Extremely sensitive radiation detectors to explore the universe in the forthcoming ESA space missions

Dr. Lourdes Fàbrega (MULFOX-ICMAB), leads the development in Spain of a special type of sensors that can detect very small changes in temperature and that will be used in the forthcoming European space missions. These sensors are extremely sensitive and miniaturized microcalorimeters, like small thermometers, that can detect even the energy of one single photon.

SEPTEMBER

OCTOBER

5 Sep | 17-20 Sep | 24 Sep | 11 Oct | 30 Oct | 31 Oct

The Severo Ochoa Summer School on Materials for Energy (MATENER 2018) takes place at ICMAB and receives more than 40 participants

Superconducting materials and levitation of magnets with Teresa Puig in "Els Matins de TV3"

Little scientists for a day: great Kids' Day at ICMAB 2018!

On Wednesday, 5 September, the ICMAB staff could bring their children, their grandchildren, and even their nephews and nieces to spend a morning at our centre full of scientific activities for another edition of the Kids Day!
In the end, more than 75 kids of ages between 1 and 17 joined us! Many volunteers from the ICMAB helped out during the day, organizing the activities and taking care of the kids. Thank you all for your great collaboration and participation!

"El reto de ser científicas y madres" by Valentina Raffio in El Periódico

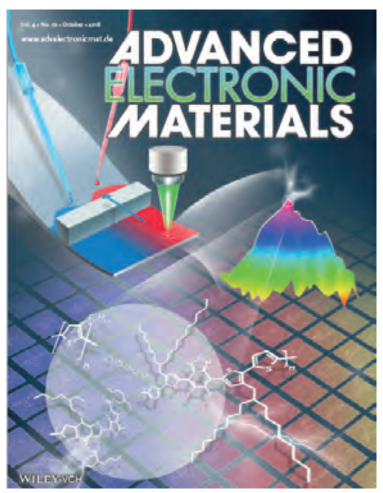
The article is written by the journalist Valentina Raffio, and features two ICMAB researchers, Teresa Puig and Marta Mas-Torrent, in the framework of the project #LasCientíficasCuentan, an initiative by CSIC-Brussels and funded by the FECYT.

Finding a needle in the haystack: 50 times faster evaluation of organic materials for solar cells

Researchers from the Institute of Materials Science of Barcelona (ICMAB-CSIC) have successfully demonstrated a combinatorial platform that evaluates how good an organic material is for photovoltaic applications

A project to prevent infectious diseases with functionalized catheters led by Imma Ratera awarded by La Marató de TV3

The project, about prevention of infections related with vascular catheters, is "Prevenció d'infeccions relacionades amb els CATèters vasculars mitjançant la FUNcionalització de catèters impregnats d'hidrogels activables tèrmicament amb antimicrobians d'ampli espectre (FUNCATH)"



NOVEMBER

DECEMBER

9-11 Nov | 15-16 Nov | 21 Nov | 3 Dec | 19 Dec | 21 Dec

Third visit of the Scientific Advisory Board (SAB) at the ICMAB

The new IEC members, including Nora Ventosa, invited to "El matí de Catalunya Ràdio"

The ICMAB at the Expominer, with talks, workshops and the Matheroes

The ICMAB participated with some outreach talks given by five of our researchers, workshops in our stand about superconducting materials, minerals, diffraction and photonic materials, and with the exhibition "Matheroes: Supermaterials, heroes of the future"

Soft organic materials that change color and charge transfer with the application of an electric field

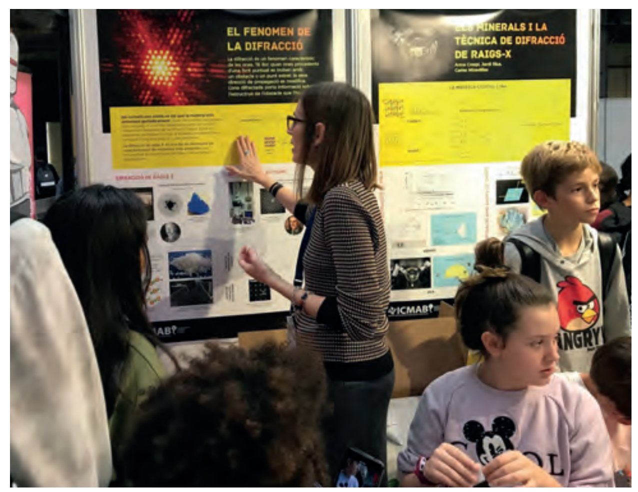
A group of researchers from the ICMAB-CSIC, led by Prof. Jaume Veciana, has proven the ability of an organic molecular metal $[(\text{BEDO-TTF})_{2,4}I_3]$ to reversibly change its color (electrochromic properties) and its degree of charge transfer (rectifying properties) upon the application of an electric field and have explained its mechanism.

A new iron oxide polymorph found at high pressures

A team of researchers with the participation of ICMAB-CSIC has conducted a study, published in Nature Communications, which reveals that the epsilon phase of iron oxide (until now considered rare) can be found in the inner layers of the Earth.

Celebrating Christmas 2018 at ICMAB

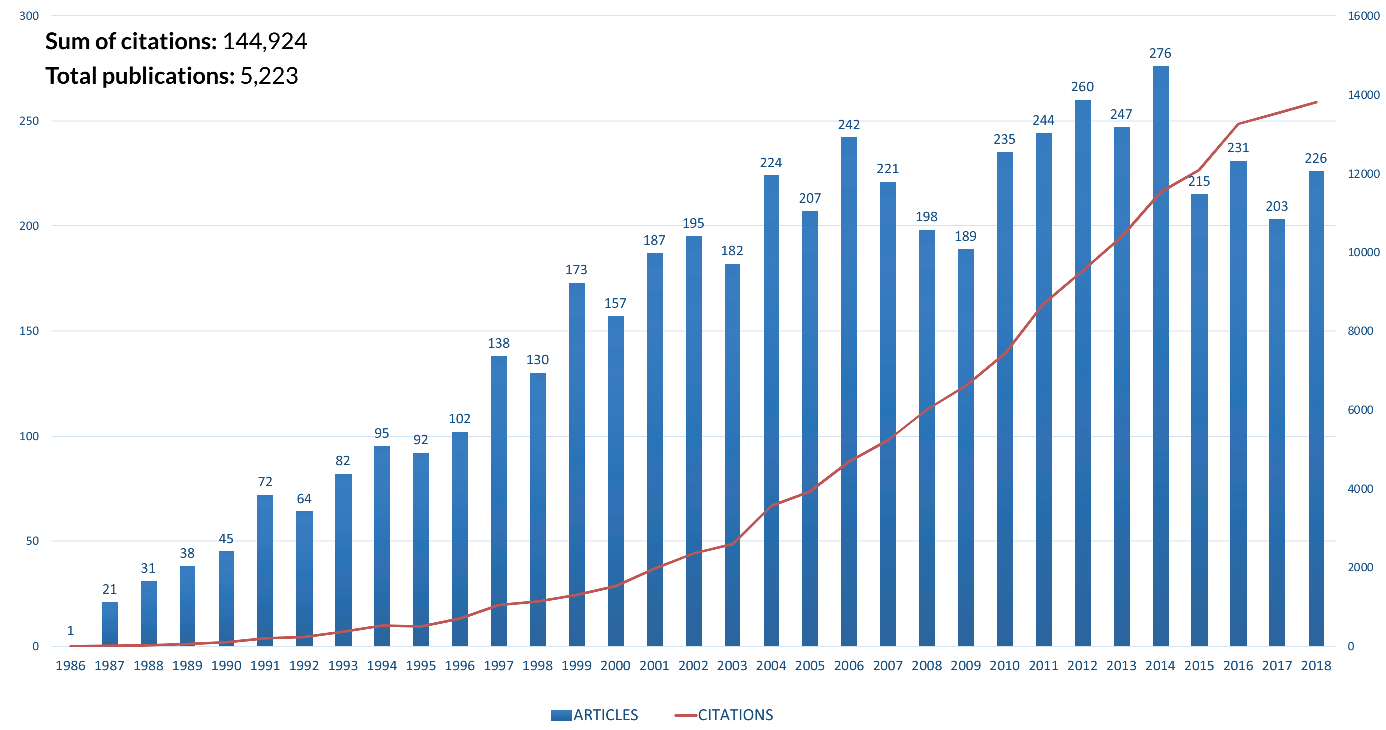
Xavier Lasauca, from the Direcció General de Recerca (GenCat), gave some insights in the use of twitter and blogs for researchers, and gave us a lot of information and resources about the use of social media for researchers, to increase the impact and networking of the research.



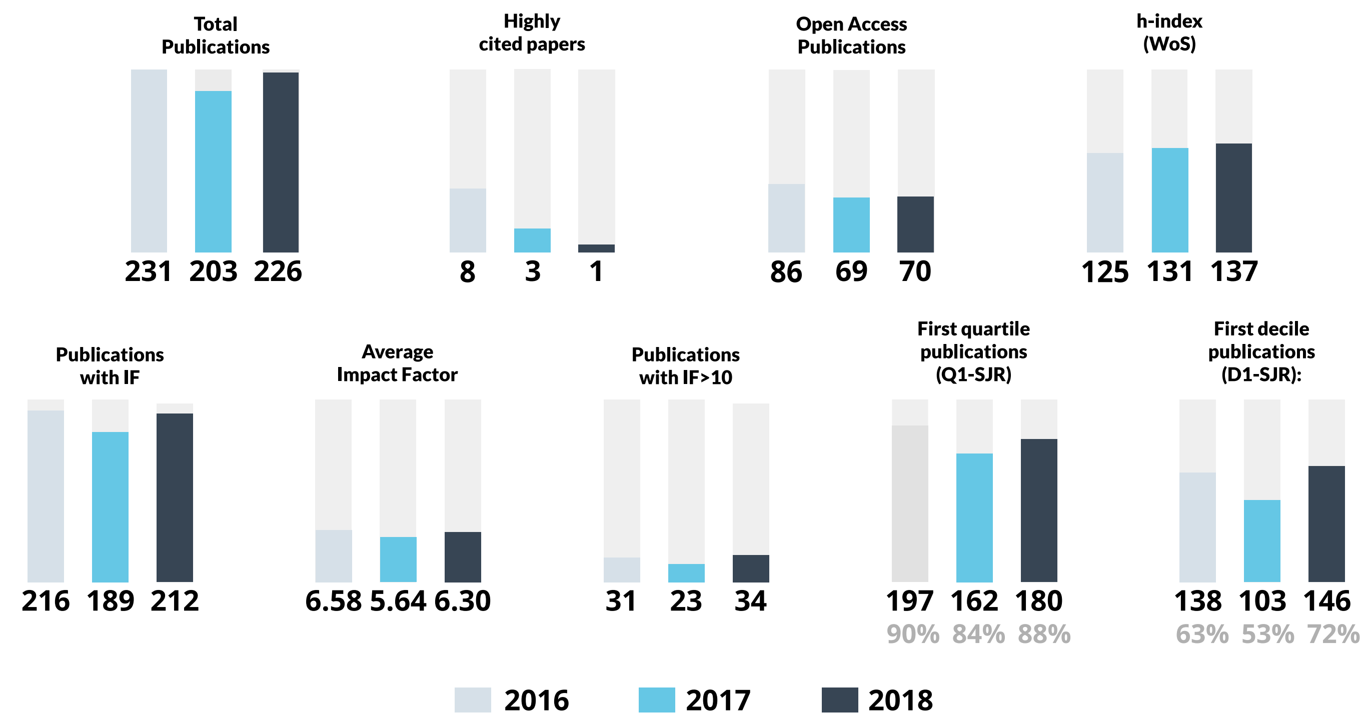
FACTS AND FIGURES

Publications

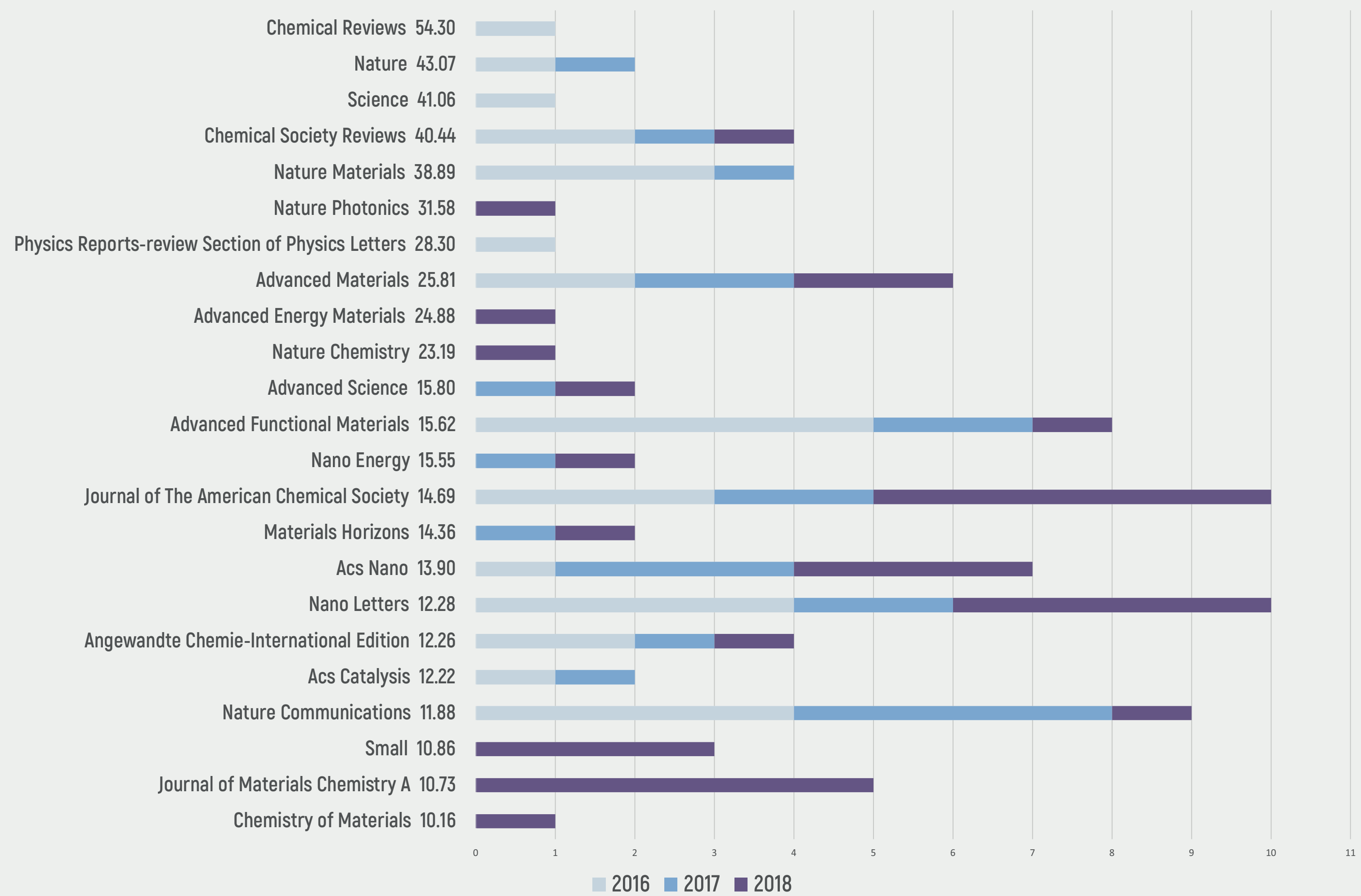
1986-2018



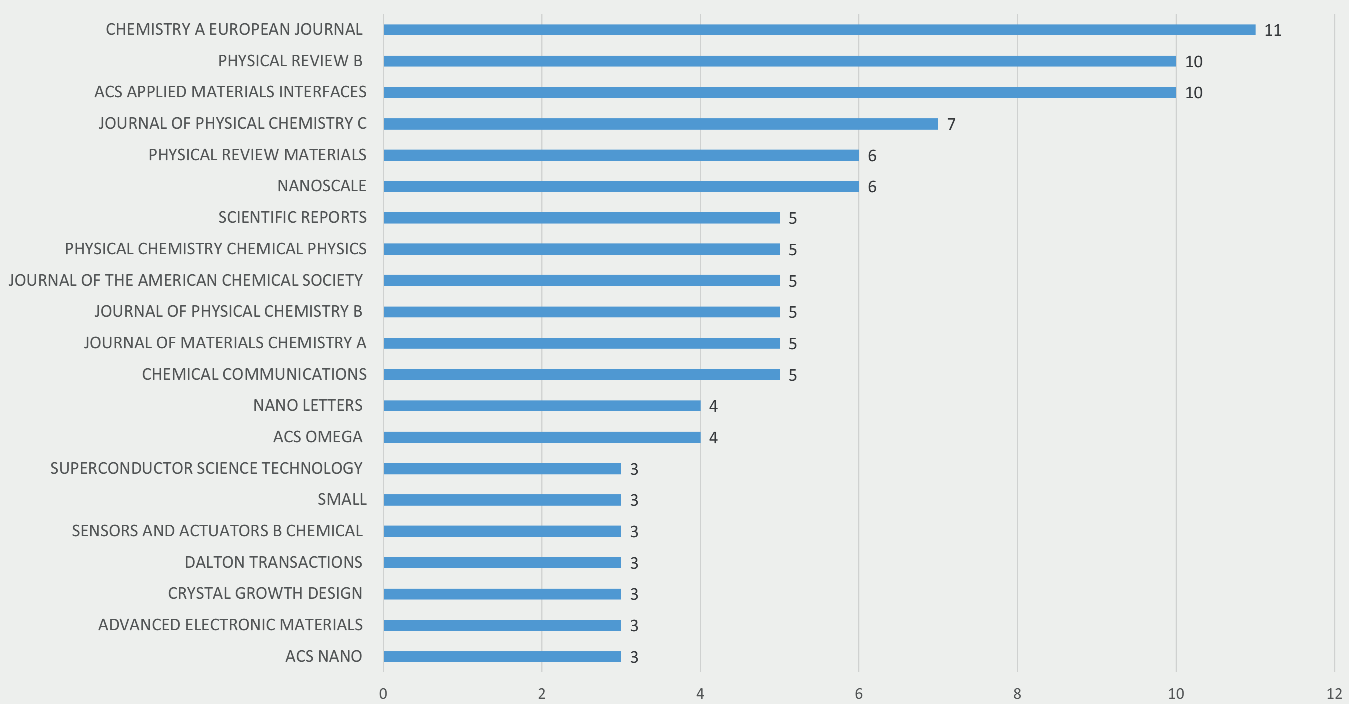
2016-2018



Top journals with IF > 10 2016-2018

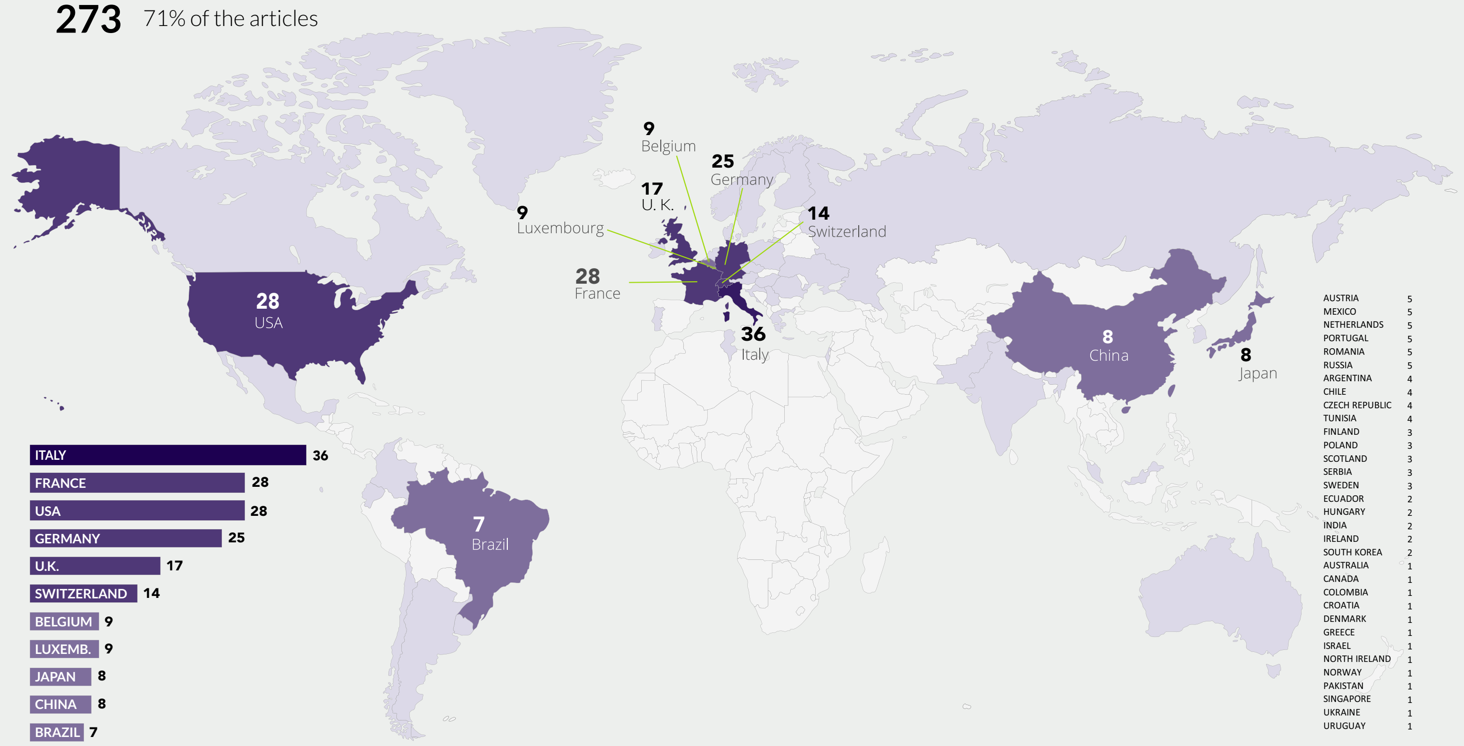


Most published journals in 2018

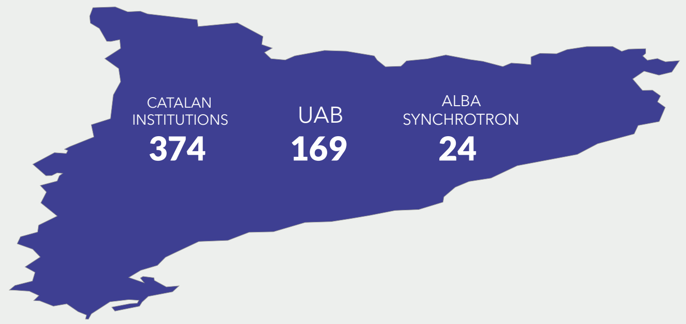


PUBLICATIONS: Collaborations worlwide

TOTAL COLLABORATIONS
273 71% of the articles

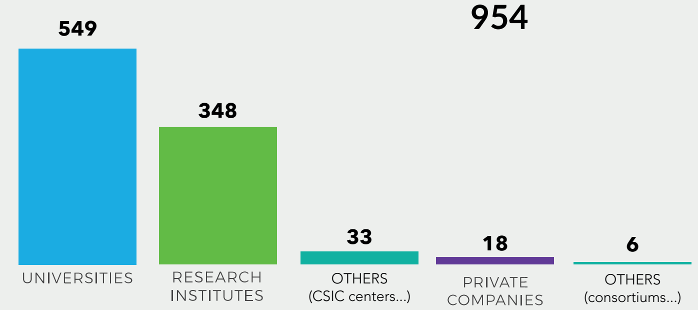


Collaborations with neighboring institutions



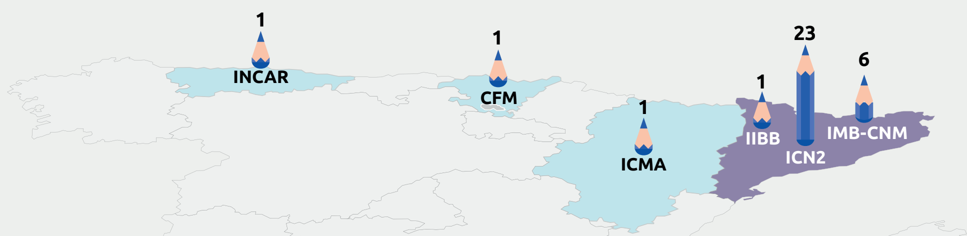
Collaborations with institutions

TOTAL COLLABORATIONS
954



Collaborations within the CSIC

TOTAL COLLABORATIONS
33 *(30 articles)*

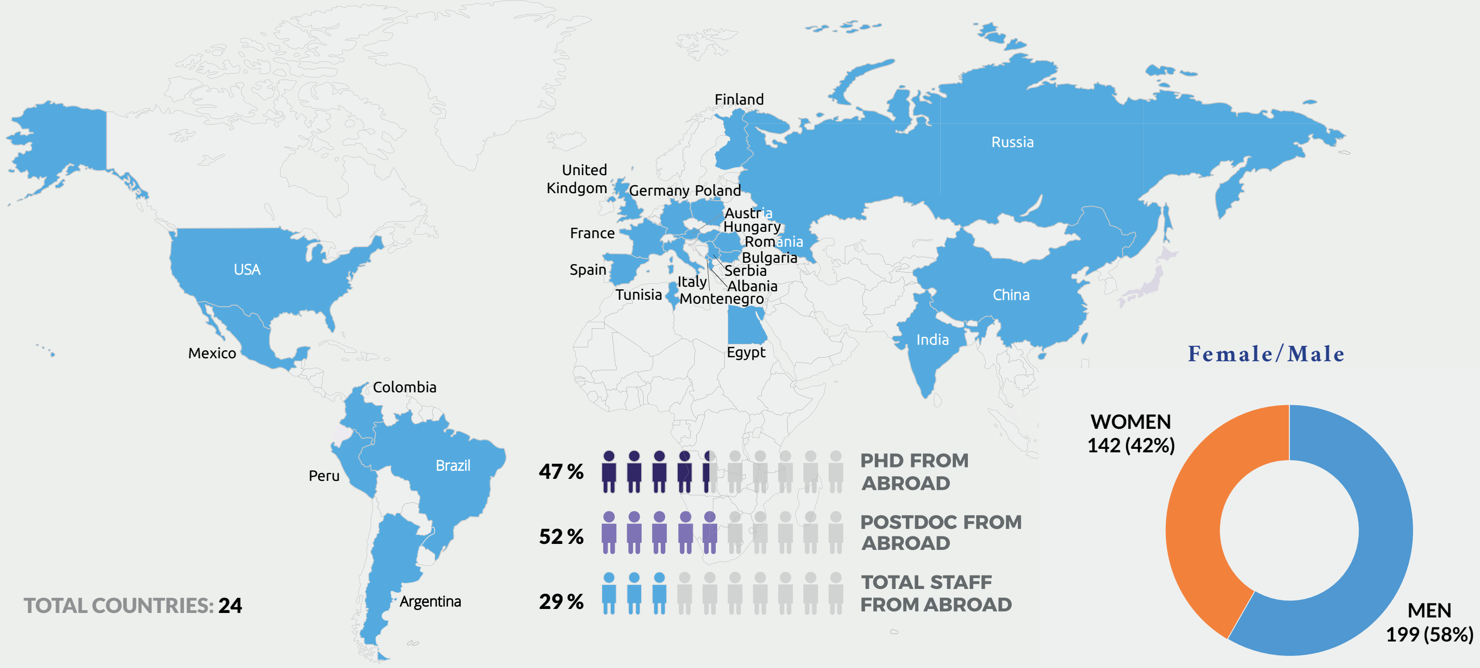


ICN2 CATALAN INSTITUTE OF NANOSCIENCE AND NANOTECHNOLOGY
ICMA ARAGÓN MATERIALS SCIENCE INSTITUTE
CFM MATERIALS PHYSICS CENTER
IMB-CNM INSTITUTE OF MICROELECTRONICS OF BARCELONA
IIBB INSTITUTO DE INVESTIGACIONES BIOMÉDICAS DE BARCELONA
INCAR INSTITUTO NACIONAL DEL CARBÓN DE OVIEDO

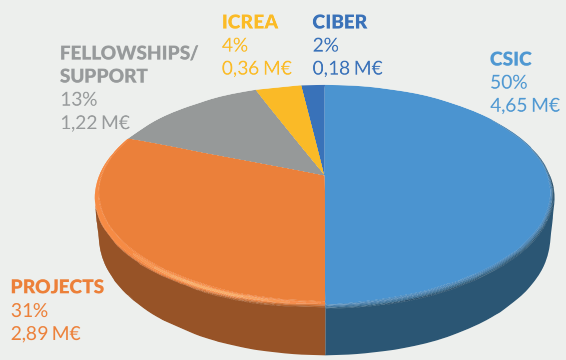
Personnel

Internationality

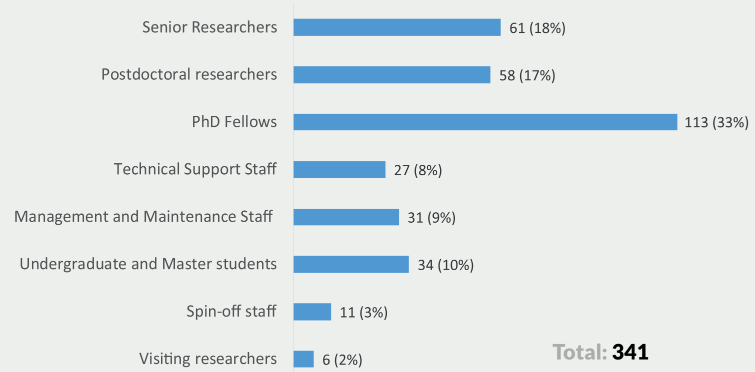
Female/Male



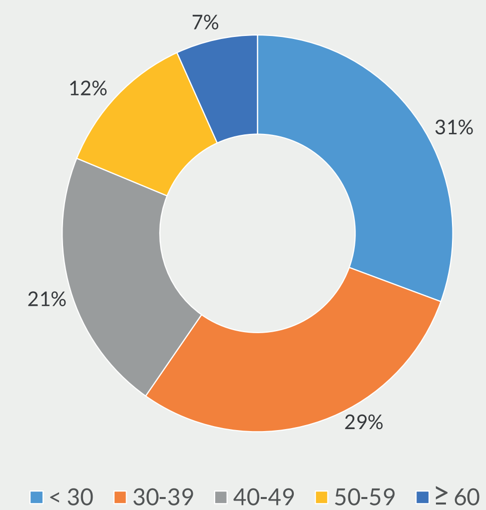
Personnel funded by



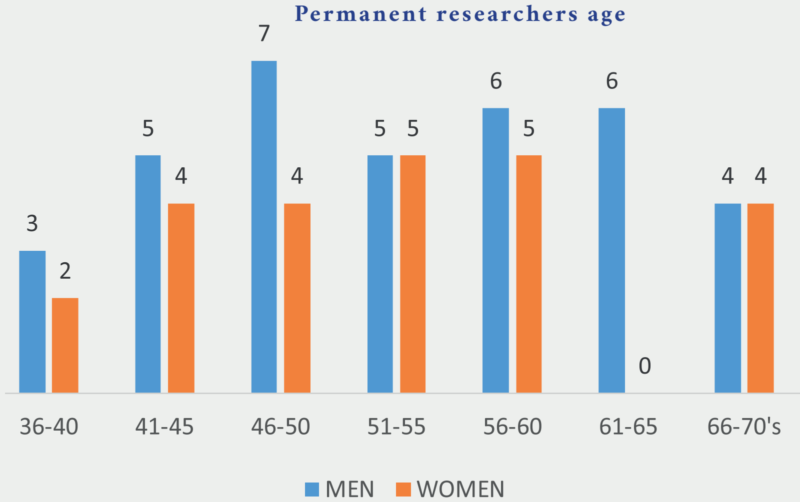
Personnel by categories



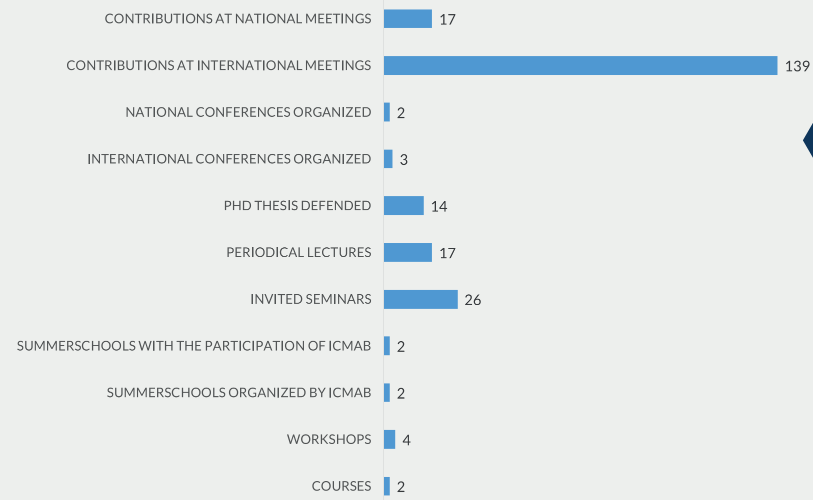
Personnel age



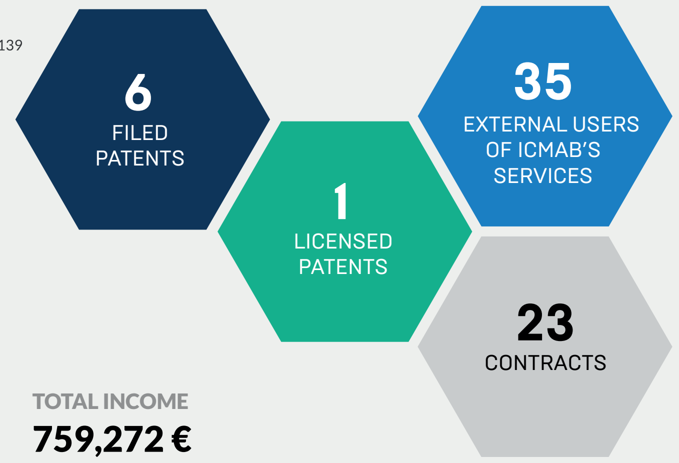
Permanent researchers age



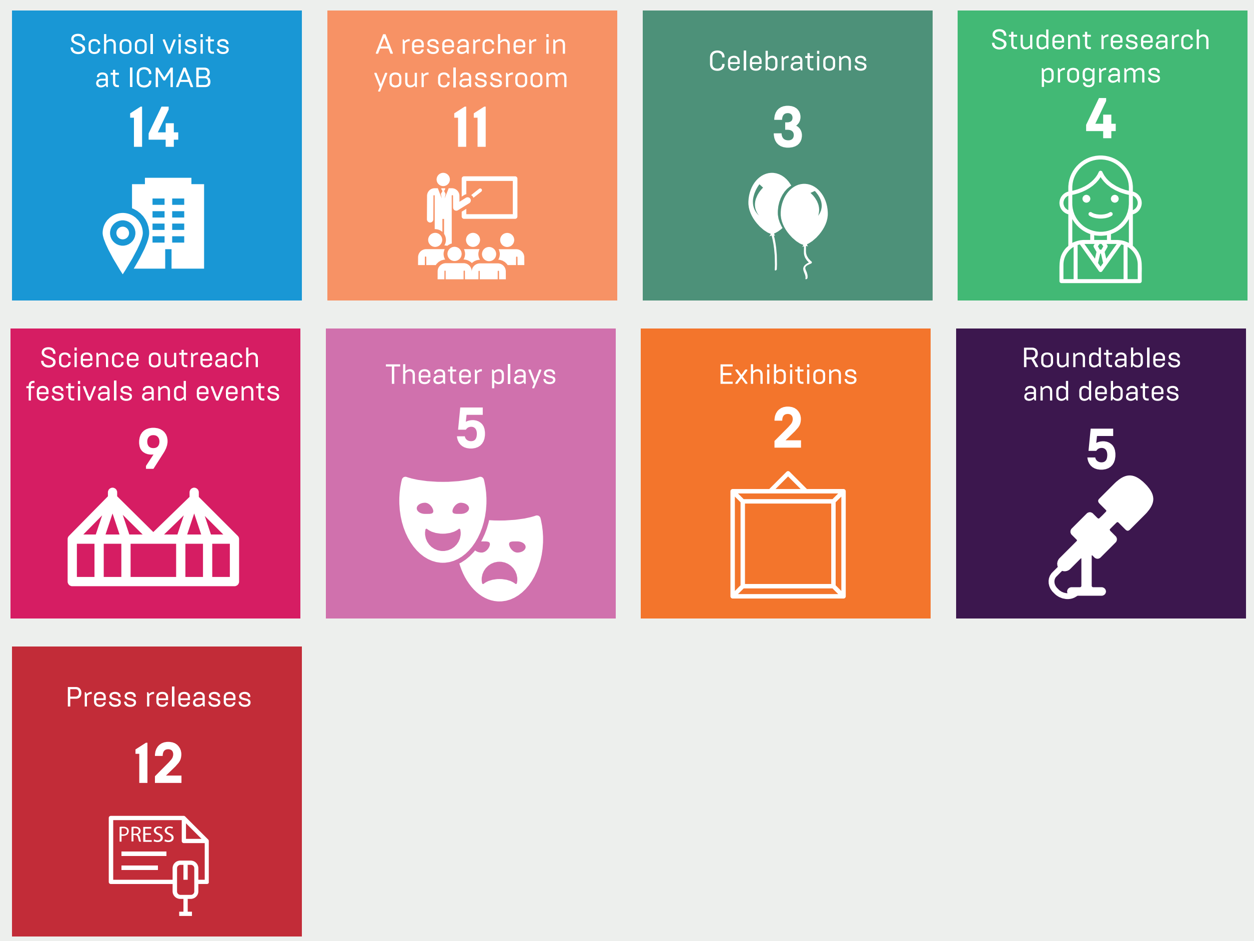
Meetings and advanced training



Technology transfer and business development



Communication & Outreach



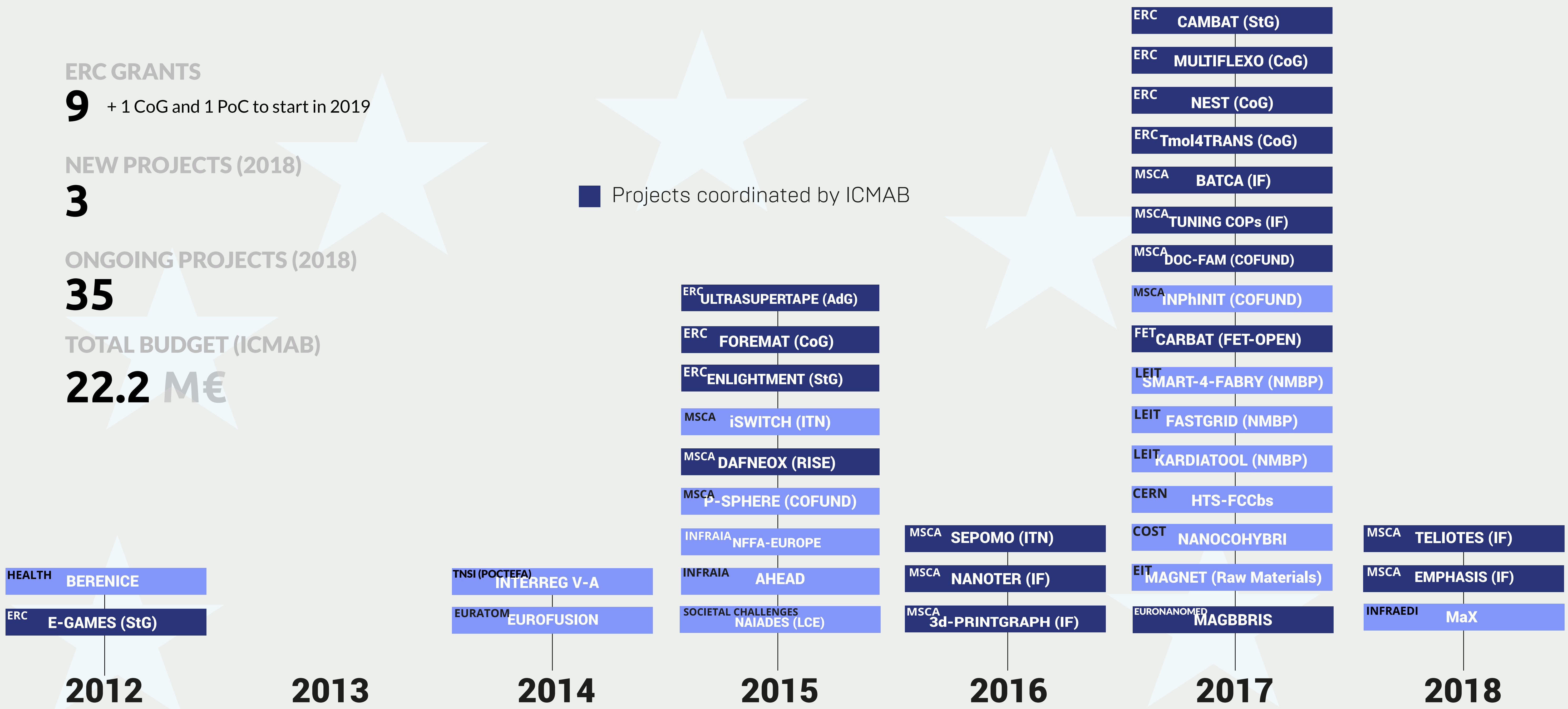
EU Funded Projects

ERC GRANTS
9 + 1 CoG and 1 PoC to start in 2019

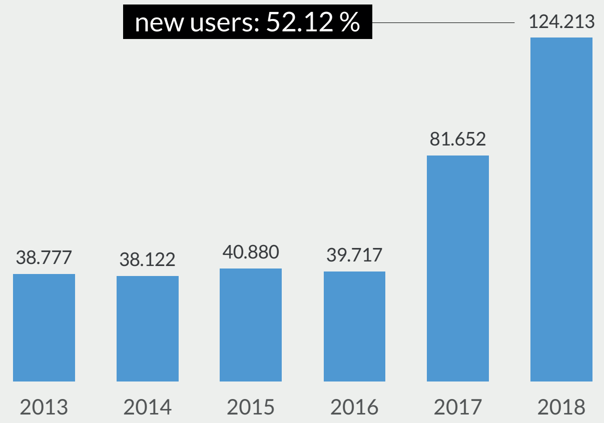
NEW PROJECTS (2018)
3

ONGOING PROJECTS (2018)
35

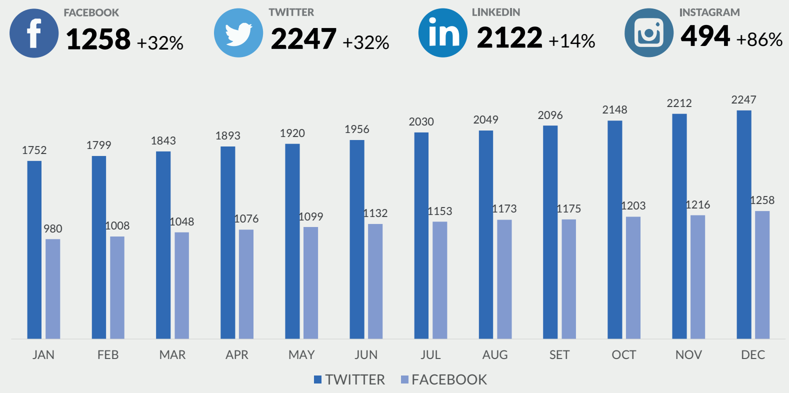
TOTAL BUDGET (ICMAB)
22.2 M€



Website Visitors

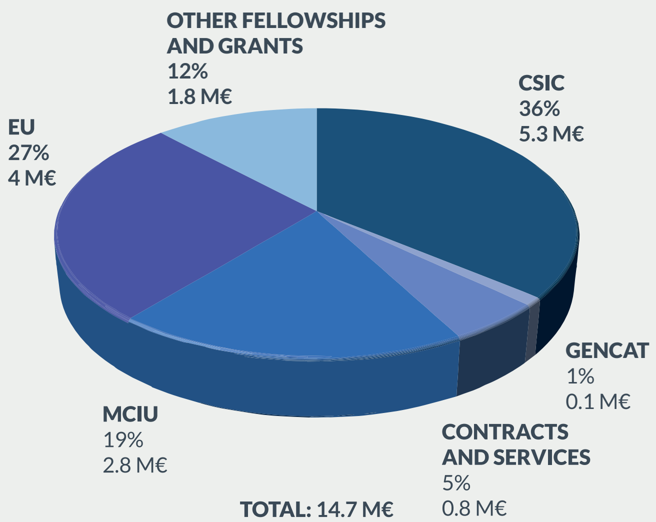


Followers

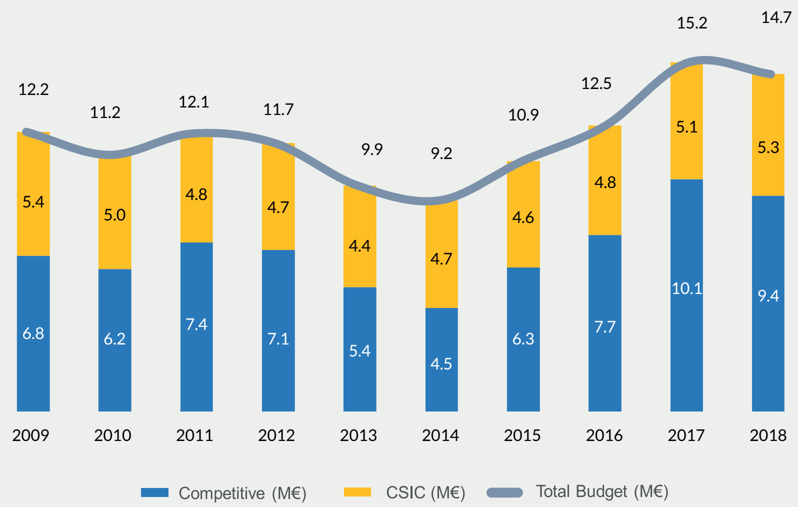


Budget

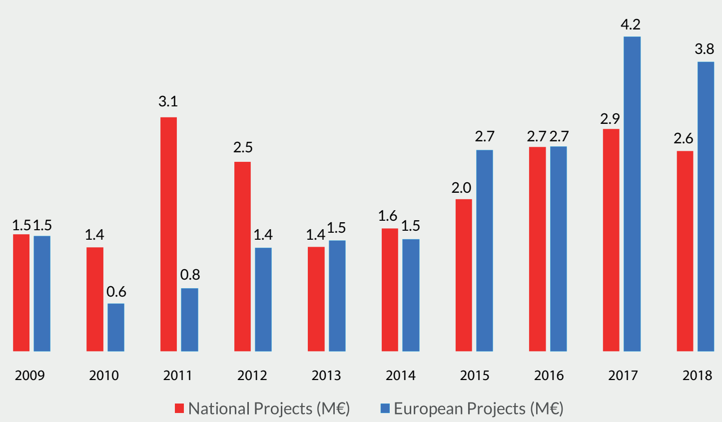
Budget by source



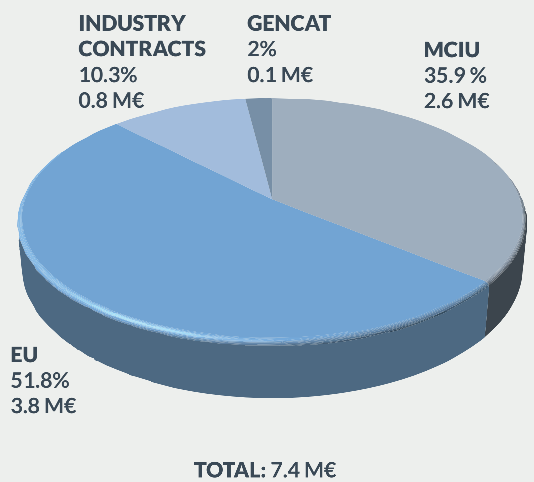
Budget Evolution



Projects evolution



Distribution of projects



SCIENTIFIC HIGHLIGHTS

M. Rosa Palacín

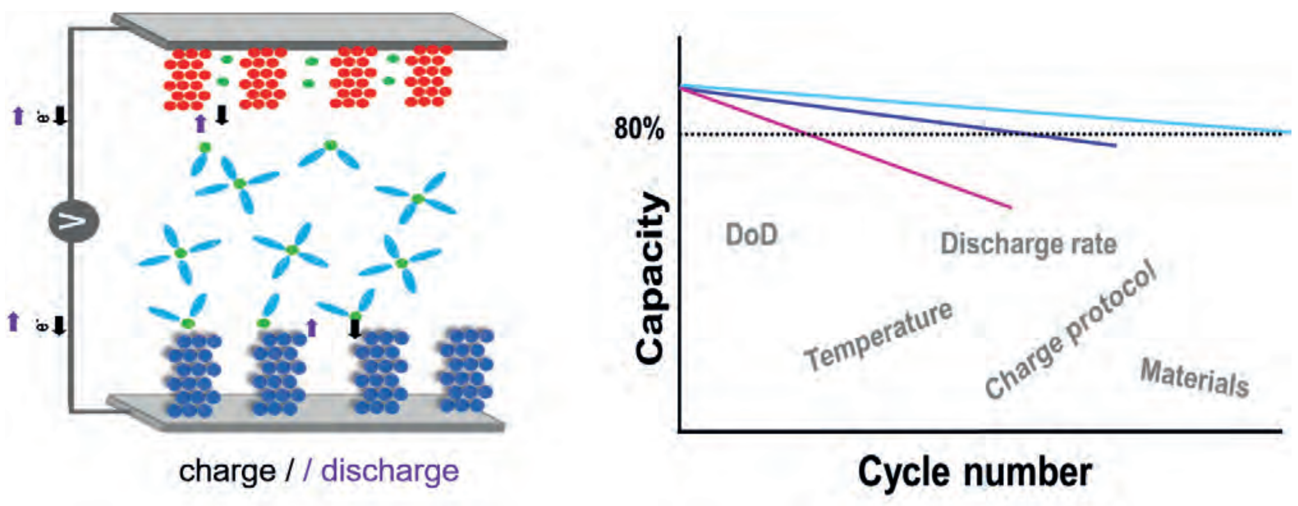
Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Spain

Understanding ageing in Li-ion batteries: a chemical issue.
Chem. Soc. Rev., 47, 4924-4933 (2018)

RL1 SCIENTIFIC HIGHLIGHTS

Battery ageing

Performance degradation upon Li-ion battery lifetime is rooted in chemical processes mostly determined by battery material components and operation conditions.



Schematics of a Li-ion battery and different possible evolutions of capacity vs. cycle number for Li-ion cells as a result of differences in operation conditions

Performance degradation upon Li-ion battery lifetime is rooted in chemical processes mostly determined by battery material components and operation conditions.

Batteries start to degrade as soon as they are assembled, just as human beings start to age from the moment they are born. The process depends on biological/genetic factors (which can be assimilated to battery materials and design), environmental/behavioral aspects (battery operation conditions) and access to medical care (optimized Battery Management System).

Performance degradation upon Li-ion battery lifetime is ultimately rooted in chemical processes the extent of which is mostly determined by battery material components and operation conditions (charge/discharge rates, voltage operation limits and temperature) and can also be influenced by battery design. The two major factors contributing to loss of negative electrode performance are the instability of the passivation layers formed at the electrode/electrolyte interface (enhanced at higher temperatures) and lithium metal plating (intensified at low temperatures). In contrast, capacity fading at the positive electrode mostly result from partial dissolution of the active material during cycling/storage or electrolyte solvent oxidation, which is promoted by temperature and high potential. While it would be most useful to be able to monitor degradation at all levels while the cell is being cycled, the feasibility of this approach remains limited, and most approaches involve accelerated testing with ante/post mortem characterization. Yet, the use of suitable protocols for battery opening and disassembling is crucial to avoid biased interpretation.

Understanding such issues is crucial to extend cycle life of Li-ion batteries to successfully embrace larger scale applications such as transportation or grid. Overall, battery ageing is a very complex and challenging research topic with a too broader scope to be addressed by conventional research approaches and one which will clearly benefit from synergies between academia (model systems, fundamental research with cross cutting characterization techniques available) and industry (real commercial systems, large empiric know how and cumulated knowledge about battery response in real operation).

Tomoko K. Shimizu,[1] Sabine Maier,[2] Albert Verdaguer,[3] Juan-Jesus Velasco-Velez,[4] Miquel Salmeron[5]

[1]Faculty of Science and Technology, Keio University, Japan.
[2]Department of Physics, Friedrich-Alexander-University Erlangen-Nürnberg, Germany.
[3]Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Spain.
[4]Department of Inorganic Chemistry, Fritz-Haber-Institute der Max-Planck-Gesellschaft, Germany.
[5]Lawrence Berkeley National Laboratory, and Materials Science and Engineering Dept., University of California, Berkeley, USA.

Water at surfaces and interfaces: From molecules to ice and bulk liquid
Progress in Surface Science 93(4), 87-107 (2018)

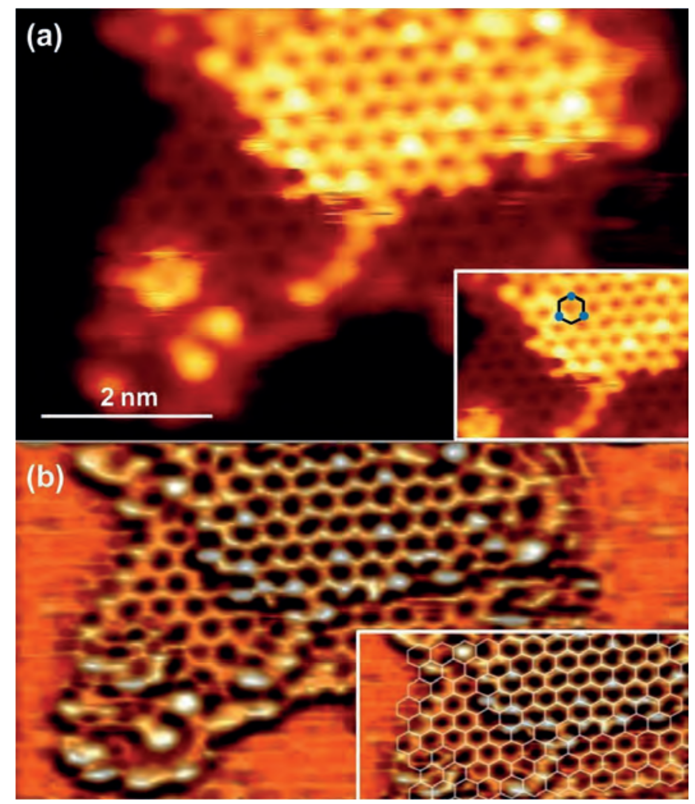
RL1 SCIENTIFIC HIGHLIGHTS

"Water everywhere…" what do we know about water molecules coating all the surfaces?

The structure and growth of water films on surfaces is reviewed, from single molecules to wetting layers, from cryogenic and high-vacuum conditions to ambient conditions

Water/solid interfaces are of fundamental interest in various fields including geology, metrology, biology, and chemistry. Despite its simple molecular structure the structure and interactions of water with surfaces, which determines wetting and reactivity remain unsolved. The knowledge of this structure at the nanoscale is crucial to understand key properties that determine corrosion, dissolution, and electrochemical processes. This review focuses mainly in the use of Scanning probe Microscopy (SPM) to study water/solid interfaces. One of the differences of SPM from other techniques is the locality of the information. SPM uses a probe tip to scan over the surface, and obtain structural information together with, e.g., electronic, mechanical, and vibrational properties. Because it is not an averaged information over a wide area, as in the case of all the other techniques listed above, detailed investigations of how atomic steps, kinks, and defects residing on the surface influence on the adsorption of molecules are possible.

The review first discusses adsorption configurations, diffusion, aggregation, and dissociation of water molecules on very well defined surfaces such as metals and the formation of larger clusters up to the water monolayer. The discussion moves then to the structure of water monolayers and the formation of ice-like layers induced by the substrate, even at ambient conditions, on relevant samples such as salts and oxides and finally ending by reviewing the formation of thin liquid water films that define wetting properties of the surface. In the last section, we also review recent studies of liquid water near a solid, electrified surface. Here the knowledge obtained from X-ray absorption spectroscopy (XAS) has proved useful for better understanding of atomistic pictures of electrochemical processes, which is challenging by real-space observations using SPM.



Atomic structure of ice-clusters on Ru(0001)

Ana M. López-Periago, Concepción Domingo

Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Spain

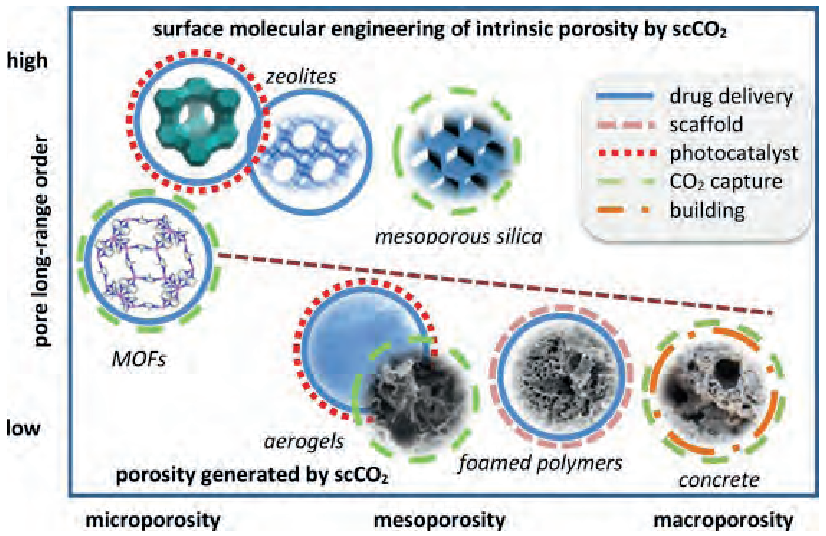
Features of supercritical CO_2 in the delicate world of the nanopores
The Journal of Supercritical Fluids, 134 204-213 (2018)

RL1 SCIENTIFIC HIGHLIGHTS

An overview of porous materials preparation under supercritical CO_2

This contribution highlights the main characteristics that make supercritical CO_2 an extraordinary solvent for performing physical processing and chemical reactions to create or modify porous nanostructures

The field of porous materials is currently at an exciting stage in its technological evolution. The research on ordered –including zeolites, zeotypes, metal-organic frameworks and mesoporous silica- and disordered –including ceramics, sintered metals and foamed polymers-porous solids [1] is among the most creative, fascinating and attractive fields of materials science. The supercritical fluid technology addressed the processing of porous matter for many differed types of materials. The basis of the developments of supercritical carbon dioxide ($scCO_2$) methodologies in porous materials is two-fold: first, the solubility of $scCO_2$ in polymers, with a pressure-dependent behaviour, is substantial in comparison with conventional solvents; and second, the adsorptive behaviour of $scCO_2$ in inorganic porous systems is insignificant when compared to liquid fluids, which allows the one-step design of surface grafting and impregnation processes.[2]



Classification of described porous materials along the text in regard of pore long-range order, interaction with $scCO_2$, and tested applications.

$scCO_2$ technology applied to nanopores takes profit of the compressed CO_2 gas-like viscosity, high diffusivity and null surface tension, so capillary stresses are suppressed, converting this fluid in a non-damaging solvent for those structures, facilitating their synthesis and modification. Most importantly, pore collapse can be avoided because the expansion of $scCO_2$ directly as a gas does not give rise to a liquid-vapour interface.

When the process is carried out from a liquid solution, the possibility of competition between solvent and solute molecules for the substrate adsorption sites often leads to the incorporation of both components into the internal surface of the porous system. Competition between the solvent and the solute for the substrate adsorption sites is reduced in $scCO_2$ with respect to liquid solvents, since supercritical fluids are essentially not absorbed.

This review, explores particular cases of the use of $scCO_2$ on polymer foaming, aerogel preparation, porous concrete densification, supercritical impregnation of zeolites and modification of mesoporous ordered silica or MOFs preparation

[1] A.G. Slater, A.I. Cooper, Function-led design of new porous materials, Science 348 (2015) aaa8075.
[2] P. Subra-Paternault, C. Domingo (Eds.), Supercritical fluid nanotechnology: Advances and applications in composites and hybrid nanomaterials, Pan Stanford Publishing, Singapore, 2015.

Andre Espinha, Camilla Dore, Cristiano Matricardi, Maria Isabel Alonso, Alejandro R. Goñi, Agustín Mihi

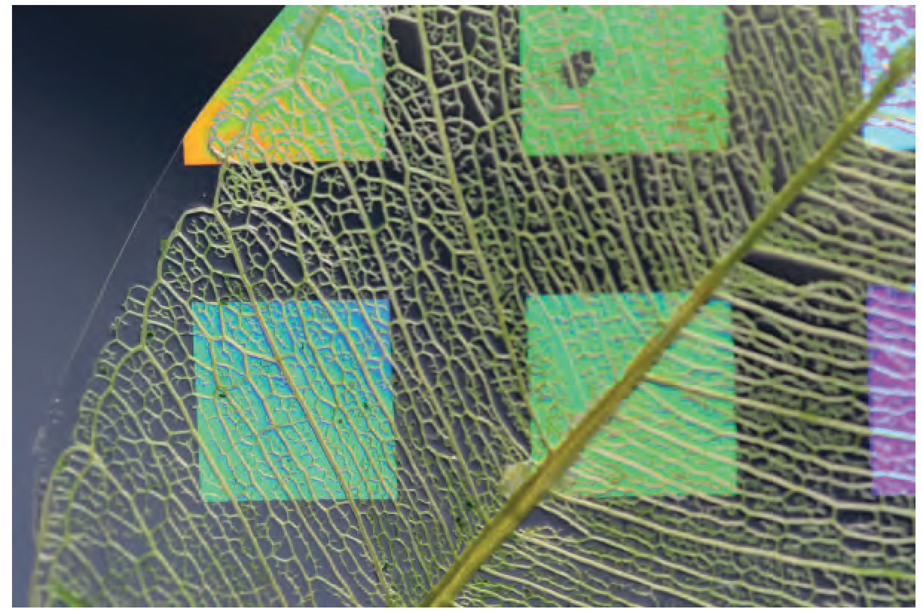
Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Spain

Hydroxypropyl cellulose photonic architectures by soft nanoimprinting lithography
Nature Photonics 12, 343–348 (2018)

RL1 SCIENTIFIC HIGHLIGHTS

Colorful cellulose Photonic Crystals

Cellulose photonic membranes featuring optical properties in addition to the biocompatibility and biodegradability of the cellulose material.



Photograph of a dried leaf covered with a hydroxypropyl cellulose membrane patterned with different photonic motifs illustrating the structural color possibilities offered by the technology.

Cellulose is the most abundant polymer on earth and for centuries has had a wide technological impact in areas such as textile, packaging or knowledge storage. It is biodegradable, biocompatible and possesses excellent mechanical characteristics that have raised the interest of many engineering fields. The only limit to this potential are the poor optical properties of the cellulose and its derivatives. Typically, cellulose exhibits a white color derived from the light scattering from micron size fibers but can become transparent if its nanometric components are separated and pressed into a thin film. In this work, we revolutionize the field of transient photonics by fabricating for the first time a variety of cellulose based photonic and plasmonic architectures via soft nanoimprinting lithography and illustrate their outstanding performance in several applications such as structural color, photoluminescence enhancement and as disposable surface enhanced raman scattering substrates.

The structural color exhibited by these architectures is produced by arrays of nanoscale pillar-like metallic or dielectric hybrid structures that reflect visible light at different wavelengths. Such structures are also found in nature, for example, in green-winged teal feathers and in some butterfly wings. While traditional colors produced by dyes or pigments fade away with time, structural color can persist longer while also being environmentally friendly. The photonic crystals made with cellulose derivatives can be dissolved in water within seconds, having potential application as a new generation of transient photonic labels.

Society needs to reduce its production of plastics, estimated at around 320 million tonnes each year, of which only 10 % is recycled. The sooner the better given the enormous amount of waste being generated that is damaging our planet's ecosystems – both aquatic and terrestrial. Biopolymers such as cellulose could come into their own here. Nanocellulose is a promising candidate for making photonics components for use in chiral electronics, photonics electrodes, anti-reflection coatings in solar cells, flexible substrates for plasmonic sensing and many more.

RL1 SCIENTIFIC HIGHLIGHTS

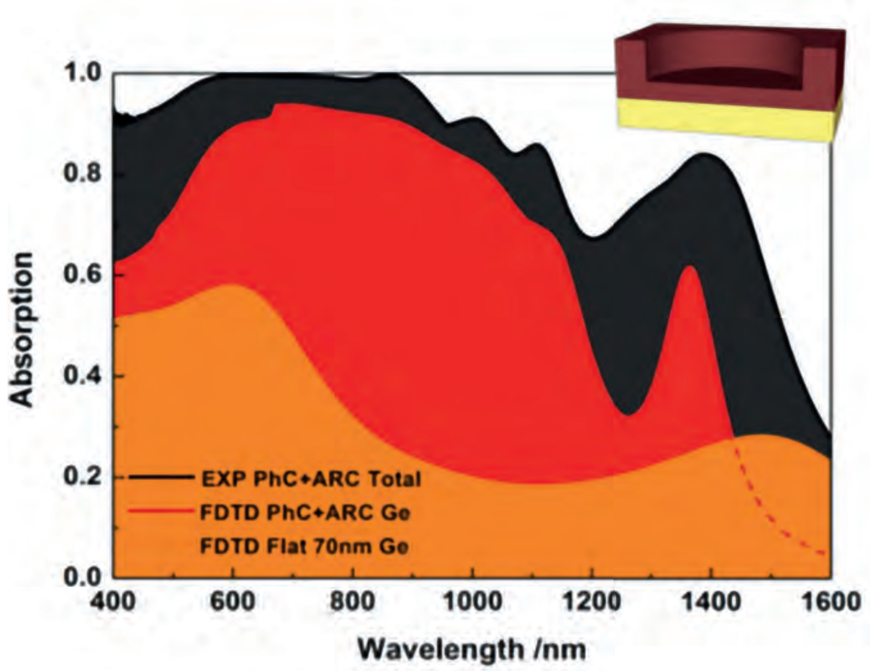
High dielectric metasurfaces exhibiting strong light absorption

Pau Molet, Juan Luis Garcia-Pomar, Cristiano Matricardi, Miquel Garriga, Maria Isabel Alonso and Agustín Mihi

Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Spain

Ultrathin Semiconductor Superabsorbers from the Visible to the Near Infrared.
Advanced Materials 30 (9), 1705876 (2018)

In this work, we transform an ultrathin slab of Germanium of less than 70 nanometers into a photonic architecture exhibiting an impressive 81 % total absorption from the visible to the near infrared



The fraction of light absorbed by a Germanium thin film on top of a mirror is compared to the absorption obtained by the same amount of Ge nanostructured as a metasurface (with and without antireflection coatings)

A more efficient interaction with light is of central importance for applications such as sensing, energy harvesting and biological research among others. Materials and strategies to guide, confine, manipulate and absorb light are being continuously sought for. One of those new strategies is looking for novel materials to absorb the maximum amount of light with the smaller amount of material, the so-called light trapping scheme, a photonic design in which the light can be confined in nanometric thin films, achieving absorptions comparable to those of thicker layers. In this line of work, the challenge resides in the optical design and molding the original material into a nanostructure where light is confined and eventually absorbed in the active layer.

In this work, we transform an ultrathin slab of Germanium of less than 70 nanometers into a photonic architecture exhibiting an impressive 81 % total absorption from the visible to the near infrared. The strong absorption in such a thin film of Ge enables novel sensing and energy harvesting devices in flexible and portable substrates. Playing with a thin metallic substrate acting as a reflector and a system of a two height hole array in the semiconductor, the light finds several ways to resonate and remain within the structure. The photonic system shows almost full absorption in a broad frequency range, vastly exceeding the absorption of a flat film design. Interestingly, as the light confinement is given by the structural parameters of the architecture, by changing parameters such as height or pitch between holes, the absorption can be tuned spectrally, opening a wide range of engineering possibilities. Moreover, the whole nanometric structure is fabricated with a simple and scalable technique termed nanoimprinting lithography, which is similar to conventional pressure or temperature printing, allowing an easy implementation in large area surfaces.

This research provides the key design guidelines for super absorptive portable surfaces readily implementable in many optoelectronic devices.

RL1 SCIENTIFIC HIGHLIGHTS

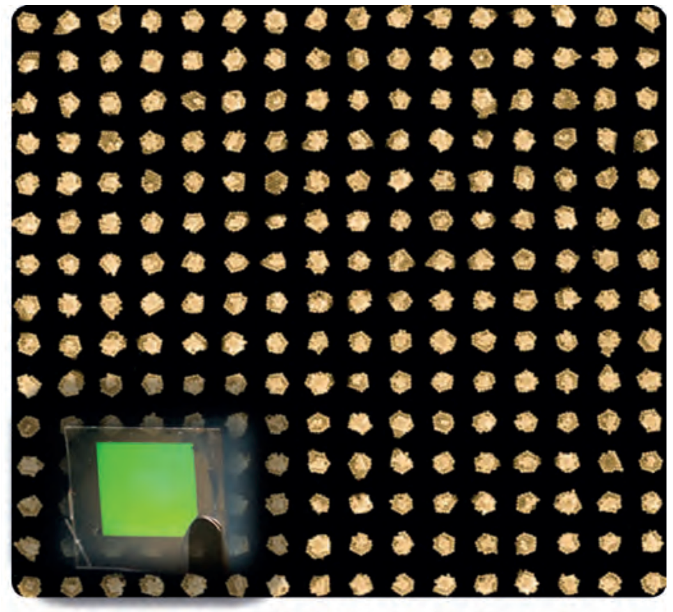
Plasmonic supercrystals made with gold colloids

Cristiano Matricardi,[1] Christoph Hanske,[2] Juan Luis Garcia-Pomar,[1] Judith Langer,[2] Agustín Mihi and Luis M Liz-Marzan[2,3]

[1] Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Spain
[2] CIC biomaGUNE and Ciber-BBN, Paseo de Miramón 182, 20014 Donostia –San Sebastián, Spain
[3] Ikerbasque, Basque Foundation for Science, 48013 Bilbao, Spain

Gold Nanoparticle Plasmonic Superlattices as Surface-Enhanced Raman Spectroscopy Substrates
ACS nano 12 (8), 8531-8539 (2018)

Plasmonic supercrystals composed of 50 nm gold colloids exhibiting enhanced SERS sensing performance



Scanning electron micrograph of a square superlattice made of 52 nm gold colloids. The inset corresponds to a photograph of the sample where the colours diffracted by the large supercrystal area of 1 x 1 cm^2 can be appreciated

Metal colloids have revolutionized the field of plasmonics due to their morphology-dependent exciting optical properties but also, because they constitute building blocks of more rich and complex plasmonic architectures. These colloids can be assembled into ordered arrays whose engineered optical response can be tailored to specific applications. These supercrystals serve as the ideal platform in which study coupling of different plasmonic resonances sustained by the structure. Precise ordering of these colloids is a challenging task typically achieved using complex lithographic techniques. However, great efforts are being placed to develop colloidal assembly routes that yield high resolution while being inexpensive and producing large area films.

In this work, we employ an inexpensive and scalable template-assisted assembly technique capable of arranging 52 nm gold nanospheres into regular, periodic arrays of well-defined plasmonic clusters over areas as large as 8 mm^2 with features as small as 300 nm. The resulting supercrystal films exhibit tunable optical properties from the visible to the NIR range. We used patterned elastomeric molds with lattice parameters ranging from 400 nm until 1700 nm. The resulting supercrystal films exhibited both strong near-field coupling and an optical response that can be tuned from the visible through the near-infrared (NIR) range. The hierarchical order present in the supercrystals enables the coupling of the different plasmonic resonances sustained by the architecture and enables us to produce films tailored to specific wavelengths.

Furthermore, we investigated the application of these superlattices as surface enhanced Raman spectroscopy substrates. We studied the correlation between the plasmon resonances sustained by the different geometrical assemblies and their performance as SERS substrates under 785 nm excitation of the Raman probe 4-acetamidothiophenol (4-AMTP). This laser line fits the first biological optical transparency window, thus providing enhanced light penetration in tissues, and is particularly interesting for biomolecular detection in complex media.

RL1 SCIENTIFIC HIGHLIGHTS

Stimuli-responsive flexible materials: the role of spherical icosahedral boron clusters

This work demonstrates the role of icosahedral boron clusters to stabilize flexible Metal-Organic Frameworks (MOFs) and thus providing a new generation of porous "stimuli-responsive" or "smart" materials

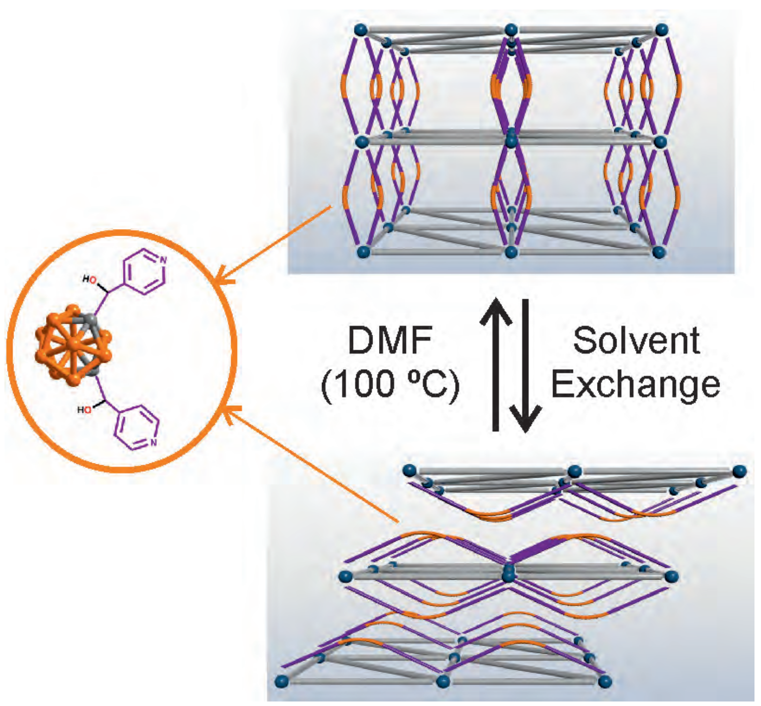
Fangchang Tan,[1] Ana M. López-Periago,[1] Mark E. Light,[2] Jordi Cirera,[3] Eliseo Ruiz,[3] Alejandro Borrás,[1] Francesc Teixidor,[1] Clara Viñas,[1] Concepción Domingo,[1] José Giner Planas[1]

[1] Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Spain

[2] Department of Chemistry, University of Southampton, Highfield, UK

[3] Departament de Química Inorgànica i Orgànica and Institut de Recerca de Química Teòrica i Computacional, Universitat de Barcelona, Spain.

An Unprecedented Stimuli Controlled Single-crystal Reversible Phase Transition of a Metal-Organic Framework and its Application to a Novel Method of Guest Encapsulation.
Advanced Materials, 30, 1800726 (2018)



3D nano-porous materials go through conformational changes and transform into a 2D non-porous structure as a result of an external stimuli

The so-called "stimuli-responsive" or "smart" materials have the ability to go through conformational changes or phase transitions as a result of external chemical or physical stimuli. Such responsiveness to specific stimuli or local environment is typical for biomolecules in nature but it is particularly difficult to achieve artificially. Such materials form the corner stone of developing intelligent technologies and are at the forefront of strategies addressing a number of global challenges.

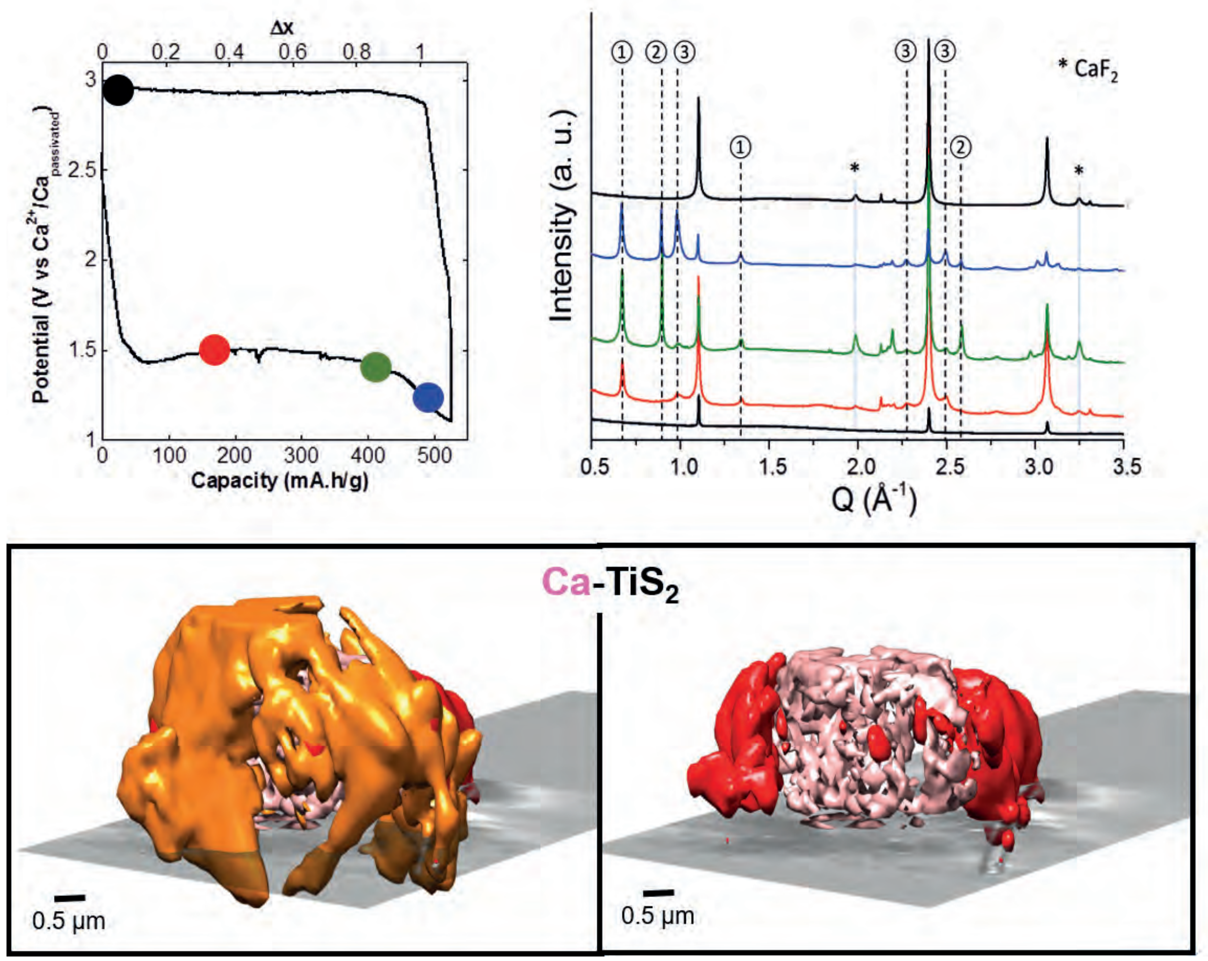
We have now developed novel 3D nano-porous materials that go through conformational changes and transform into a 2D non-porous structure as a result of an external stimuli, and then can shift to the original 3D nano-porous structure when the stimuli is reversed. This flexibility is introduced in a new Metal-Organic Frameworks (MOFs), which incorporates a flexible carborane based linker. Icosahedral carborane clusters are three-dimensional molecules with electron delocalization, highly polarizable σ-aromaticity, thermal and chemical stability and geometrical diversity. The use of spherical shaped icosahedral boron-based molecules as linkers instead of planar ones help in stabilizing the flexible structures. The spherical shape of the ligands is the key factor that enables the structures to go back to their original shape, allowing for the rearrangement of the different parts, and without collapsing the whole structure. The idea of spherically shaped linkers avoiding collapse of the structure can also be understood like this: two layers will roll over each other if separated by spheres; whereas they will collapse if non-spherical pillars are used.

As a proof of concept for potential applications, encapsulation of fullerene molecules has been achieved by trapping them during the reversible 2D to 3D transition, while the structure is being formed. The observed process constitutes a new way to encapsulate large molecules that cannot easily diffuse into the porous material.

SCIENTIFIC HIGHLIGHTS

Battery materials research: from commercial chemistries to new concepts

Materials research is crucial in all battery technologies ranging from commercial chemistries to pre-competitive alternatives and also emerging concepts



Electrochemical profile corresponding to a Ca//TiS$_2$ cell at 100 ºC and synchrotron X-ray diffraction patterns XRD collected at different stages of TiS$_2$ reduction and after full reoxidation, with peaks corresponding to new phases formed labelled as 1, 2 and 3. Bottom: Three dimensional Ca distribution representation obtained by differential absorption tomography at the Ca L2 edge. Three Ca regions were identified: "high absorption external Ca" (red) with Δµ=3.2±0.9 µm^{-1}, "low absorption external Ca" (orange) with Δµ=1.0±0.3 µm-1 and "intercalated Ca" (pink) inside the TiS2 particle with Δµ=0.4±0.1 µm^{-1}.

Our current research interests are fully focused in rechargeable battery materials covering a wide spectrum from commercial traditional systems, such as Ni based, to promising alternatives such as Na-ion to fully new concepts as Ca metal. Specific emphasis is set in tailoring structure and microstructure of electrode materials to maximise electrochemical performance and in the development of new materials.

Some of the recent achievements involve elucidating the crystal structure of the nickel battery positive electrode material in the fully charged state, which consists of metastable β-NiOOH. This has been possible through a joint approach involving NMR and FTIR spectroscopies, powder neutron diffraction and DFT calculations. The results confirm that structural changes occur during the β-Ni(OH)2/β-NiOOH transformation in each electrochemical cycle. [1]

In the field of Na-ion batteries, hard carbons were prepared from different precursors (phenolic resin and commercially available cellulose and lignin) under different pyrolysis and processing conditions using industrially adapted syntheses protocols. The study of their microstructural features enabled to assess that the nature of the precursor and the temperature of pyrolysis are the major factors determining the carbon yield and the surface area, the latter one having a major effect on the useful electrochemical capacity. [2]

Last but not least, a comparative study of the electrochemical intercalation of Ca^{2}+ and Mg^{2}+ in layered TiS$_2$ using alkylcarbonate based electrolytes was carried out. Reversible electrochemical Ca^{2}+ insertion was assessed both using X-ray diffraction and differential absorption X-ray tomography at the Ca L2 edge. Different new phases are formed upon M^{2+} insertion, their amount and composition being dependent on M^{2+} and the experimental conditions. [3]

Overall, crystal chemistry is a very useful tool in battery research, enabling tailoring structure and microstructure of electrode materials to maximise electrochemical performance for traditional technologies and development of new materials for emerging technologies.

[1] Montse Casas-Cabanas,[1] Maxwell D. Radin,[2] Jongsik Kim,[3 †] Clare P. Grey,[3,4] Anton Van der Ven,[2] M.Rosa Palacín[5]

[1] CIC energiGUNE, Spain
[2] Materials Department, University of California, Santa Barbara, USA
[3] Chemistry Department, Stony Brook University, USA (present address: Department of Chemistry, Dong-A University, Busan, Korea)
[4] Chemistry Department, Cambridge University, UK
[5] Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Spain

[2] Enrigue Irisarri,[1] Negar Amini,[2] Steve Tennison,[2] Camelia Matei Ghimbeu,[3,4] Joana Gorka,[3] Cathie Vix-Guterl,[3,4] Alexandre Ponrouch,[1,5] M. Rosa Palacin[1,5]

[1] Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Spain
[2] CarbonTex Ltd, England
[3] Université de Strasbourg, Université de Haute-Alsace, Institut de Science des Matériaux de Mulhouse, CNRS, France
[4] Réseau sur le Stockage Electrochimique de l'énergie (RS2E), CNRS, France
[5] ALISTORE ERI, European Research Institute

[3] Deyana Tchitchekova,[1] Alexandre Ponrouch,[1] Roberta Verrelli,[1] Thibault Broux,[1] Carlos Frontera,[1] Andrea Sorrentino,[2] Fanny Barde,[3] Neven Biskup,[4] M.Elena Arroyo-de Dompablo[5] and M.Rosa Palacín[1]

[1] Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Spain
[2] MISTRAL Beamline – Experiments Division, ALBA Synchrotron Light Source, Spain
[3] Toyota Motor Europe, Research & Development 3, Advanced Technology 1, Belgium
[4] Instituto Pluridisciplinar, Universidad Complutense de Madrid, Spain
[5] Departamento de Química Inorgánica, Universidad Complutense de Madrid, Spain

[1] The nickel battery positive electrode revisited: stability and structure of the beta-NiOOH phase
Journal of Materials Chemistry A 6, 19256-19265 (2018)
[2] Optimization of Large Scale Produced Hard Carbon Performance in Na-Ion Batteries: Effect of Precursor, Temperature and Processing Conditions
Journal of the Electrochemical Society 165 (16), A4058-A4066 (2018)
[3] Electrochemical Intercalation of Calcium and Magnesium in TiS2: Fundamental Studies Related to Multivalent Battery Applications
Chemistry of Materials 30 (3), 847-856 (2018)

SCIENTIFIC HIGHLIGHTS

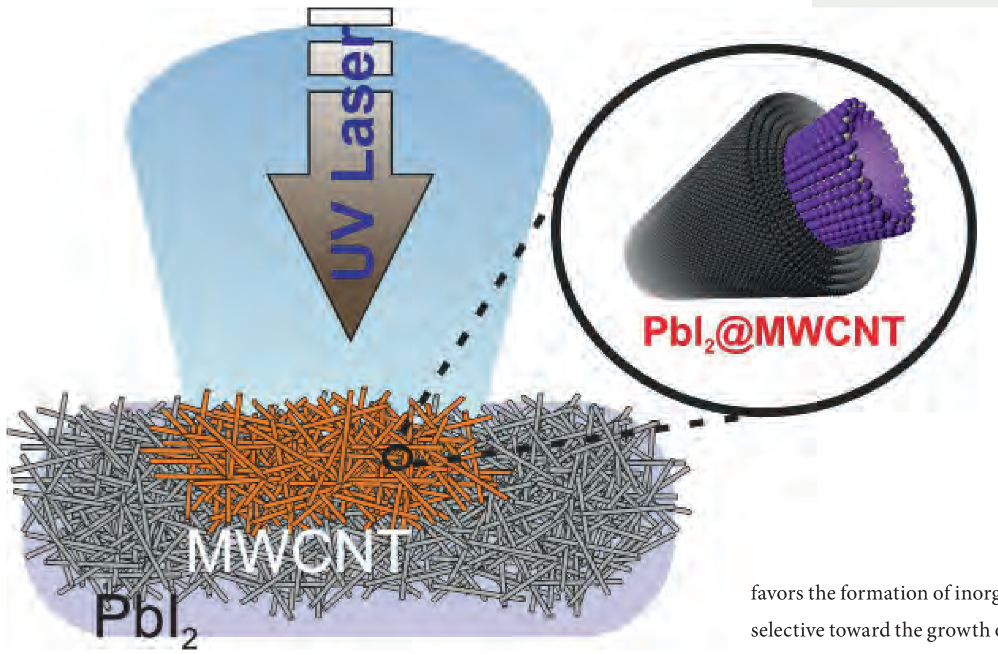
Ultrafast laser filling of PbI_2 into carbon nanotubes: tubular van der Waals heterostructures exhibiting photogeneration of carriers

Stefania Sandoval,[1] Dejan Kepić,[1,2] Ángel Pérez del Pino,[1] Enikö György,[1] Andrés Gómez,[1] Martin Pfannmoeller,[3] Gustaaf Van Tendeloo,[3] Belén Ballesteros,[4] and Gerard Tobias[1]

[1] Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Spain
[2] Vinča Institute of Nuclear Sciences, Serbia
[3] Electron Microscopy for Materials Research (EMAT), University of Antwerp, Belgium
[4] Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC and BIST, Spain

Selective Laser-Assisted Synthesis of Tubular van der Waals Heterostructures of Single-Layered PbI_2 within Carbon Nanotubes Exhibiting Carrier Photogeneration
ACS Nano 12, 6648-6656 (2018)

Cylindrical van der Waals heterostructures of a conductive (CNT) and a light sensitive material (PbI_2) have been prepared which conductivity can be tuned upon illumination



Schematic representation of the laser-assisted filling of carbon nanotubes.

The electronic and optical properties of two-dimensional layered materials allow the miniaturization of nanoelectronic and optoelectronic devices in a competitive manner. Even larger opportunities arise when two or more layers of different materials are combined. We have reported on an ultrafast energy efficient strategy, using laser irradiation, which allows bulk synthesis of crystalline single-layered lead iodide in the cavities of carbon nanotubes by forming cylindrical van der Waals heterostructures . In contrast to the filling of van der Waals solids into carbon nanotubes by conventional thermal annealing, which favors the formation of inorganic nanowires, the present strategy is highly selective toward the growth of monolayers forming lead iodide nanotubes. The irradiated bulk material bearing the nanotubes reveals a decrease of the resistivity as well as a significant increase in the current flow upon illumination. Both effects are attributed to the presence of single-walled lead iodide nanotubes in the cavities of carbon nanotubes, which dominate the properties of the whole matrix. The present study brings in a simple, ultrafast and energy efficient strategy for the tailored synthesis of rolled-up single-layers of lead iodide (i.e., single-walled PbI_2 nanotubes), which we believe could be expanded to other two-dimensional (2D) van der Waals solids. In fact, initial tests with ZnI_2 already reveal the formation of single-walled ZnI_2 nanotubes, thus proving the versatility of the approach.

SCIENTIFIC HIGHLIGHTS

Visualizing degradation and defects in hybrid perovskite solar cells

Zhuoneng Bi,[1,2] Xabier Rodríguez-Martínez,[2] Clara Aranda,[3] Enrique Pascual-San-José,[3] Alejandro R. Goñi,[3,4] Xueqing Xu,[2] Antonio Guerrero,[1] Andrés Gómez,[3] Sandy Sánchez,[5] Antonio Abate,[5,6] and Mariano Campoy-Quiles[3]

[1] Institute of Advanced Materials (INAM), Spain
[2] Guangzhou Institute of Energy Conversion, China
[3] Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Spain
[4] ICREA, Spain
[5] Adolphe Merkle Institute, Switzerland
[6] Helmholtz-Zentrum Berlin für Materialien und Energie, Germany

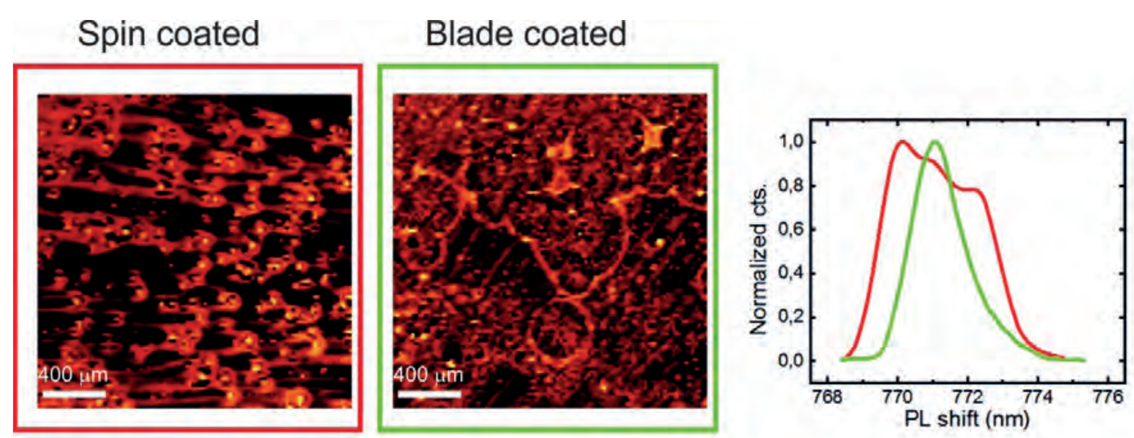
[1] *Defect tolerant perovskite solar cells from blade coated non-toxic solvents*
Journal of Material Chemistry A, 6, 19085-19093 (2018)
[2] *Topological distribution of reversible and non-reversible degradation in perovskite solar cells.*
Nano Energy, 45, 94-100 (2018)

While hybrid perovskites are tolerant to structural defects during fabrication, they present strong reversible and non-reversible degradation paths upon light exposure

Metal halide perovskites are emerging as a solution processed, high efficient photovoltaic technology. Hybrid perovskites offer very outstanding properties including high absorption coefficient, micron diffusion length and tunable bandgap. However, the stability of this class of material is still a key challenge for industrialization. With the aid of advanced imaging techniques, it is shown that perovskites are tolerant to structural defects [1] and they also present reversible and non-reversible degradation paths [2].

Efficient perovskite solar cells have been manufactured fulfilling industry requirements including large scale coating technique (doctor blading) and development of inks from non-toxic solvents [1]. The morphology-performance dependence in perovskite films processed by spin and blade coating is investigated by co-local photoluminescence (PL) and photocurrent maps (see image). The blade coated perovskite from non-toxic solvents leads to spherulitic growth which is shown to be beneficial for the device performance. The chemical defects are located at the grain boundaries of the spherullites and do not have detrimental impact on the photogenerated charges. [1]

Moreover, the degradation of the perovskite solar cells at the nanoscale level is addressed by comparing the photoconductive atomic force microscopy and photoluminescence maps. Two different degradation mechanisms are clearly identified: fully reversible behavior within the bulk of the perovskite crystal grains and a non-reversible degradation confined at the perovskite grains boundaries. Additionally, the movement of a degradation front is detected, from the boundaries towards the bulk of the grains. The study suggests that, in order to improve the perovskite stability, grain boundaries need to be minimized or passivated. [2]



Comparison between photoluminescence shift map for spin coated and bade coated perovskite solar cells. Statistical distribution of the data for the same spin coated (red line) and blade coated (green line) devices presented in the images

Antonio Sánchez-Díaz, Xabier Rodríguez-Martínez, Laura Córcoles-Guija, Germán Mora-Martín and Mariano Campoy-Quiles

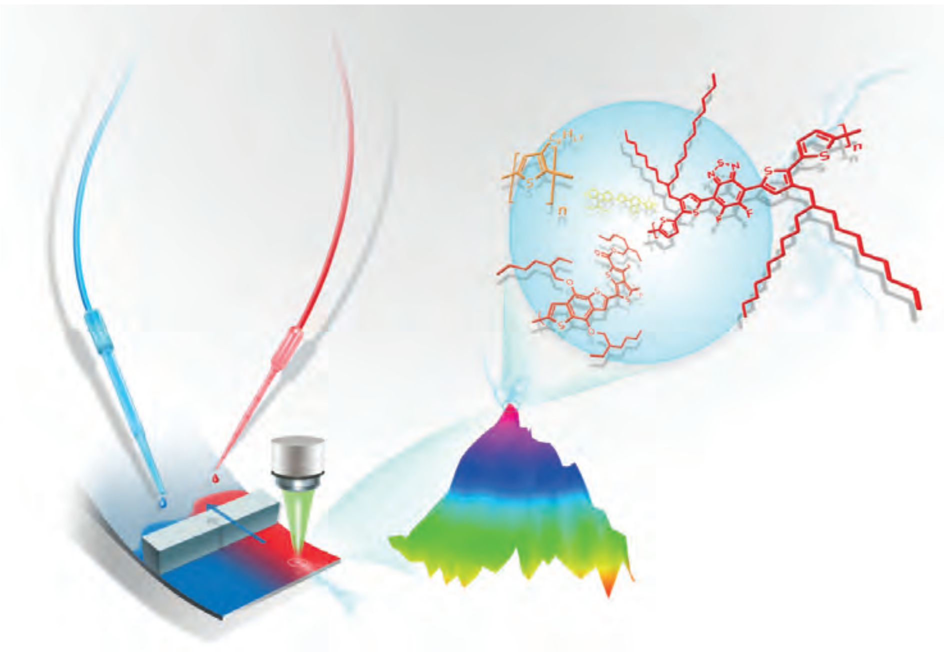
Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Spain

High-Throughput Multiparametric Screening of Solution Processed Bulk Heterojunction Solar Cells. Advanced Electronic Materials, 4, 1700477 (2018)

RL1 SCIENTIFIC HIGHLIGHTS

The evaluation of organic photovoltaic material goes "Fast and Flurrious"

Accelerating more than 50 times the process of optimization of novel photovoltaic materials, at a fraction of the material cost



Artist's rendering of the high-throughput combinatorial methodology. From doctor-bladed devices with composition gradients to non-invasive Raman and photocurrent imaging to identify the values of thickness and composition that result in maximum performance. Artist: Gustavo Regalado

Organic photovoltaic have experienced unprecedented improvement due to the synthesis of novel high-performing materials. Over the last years, thousands of novel organic semiconductors have been screened to evaluate their potential in photovoltaics. One of the major bottlenecks in the material evaluation is, however, the large amount of resources, time and material required for the device optimization. The authors circumvent this bottleneck by shifting from fabrication-intense to measurement-intensive assessment methods, enabling rapid multi-parametric optimization of novel organic photovoltaic systems.

The developed platform combines the fabrication of samples with gradients in the parameters of interest and advanced electrical and optical co-local evaluation images. The gradient sample is manufactured by doctor blading varying the blade speed profile (thickness gradients) with multichannel dispenser (composition gradients) and position-temperature dependent hot plate (annealing gradients). Then photocurrent and Raman maps enable the correlation of device performance and the thickness, composition and annealing temperature. The main advantage of this high-throughput methodology is that it allows a reduction in the evaluation times up to two orders of magnitude, and, at the same time, it saves around 90% of material. To show the generality of this high-throughput approach, three different photovoltaic system were optimized, namely PCDTBT:PC70BM, PTB7-Th:PC70BM and PffBT4T-2OD:PC70BM, employing less than 10 mg of each material in the entire process, yielding efficiencies of 5 %, 8 %, and 9.5 %, respectively.

Claudia Fasolato[1], Marta De Luca[1], Doriane Djomani[2], Laetitia Vincent[2], Charles Renard[2], Giulia Di Iorio[1], Vincent Paillard[3], Michele Amato[4], Riccardo Rurali[5], and Ilaria Zardo[1]

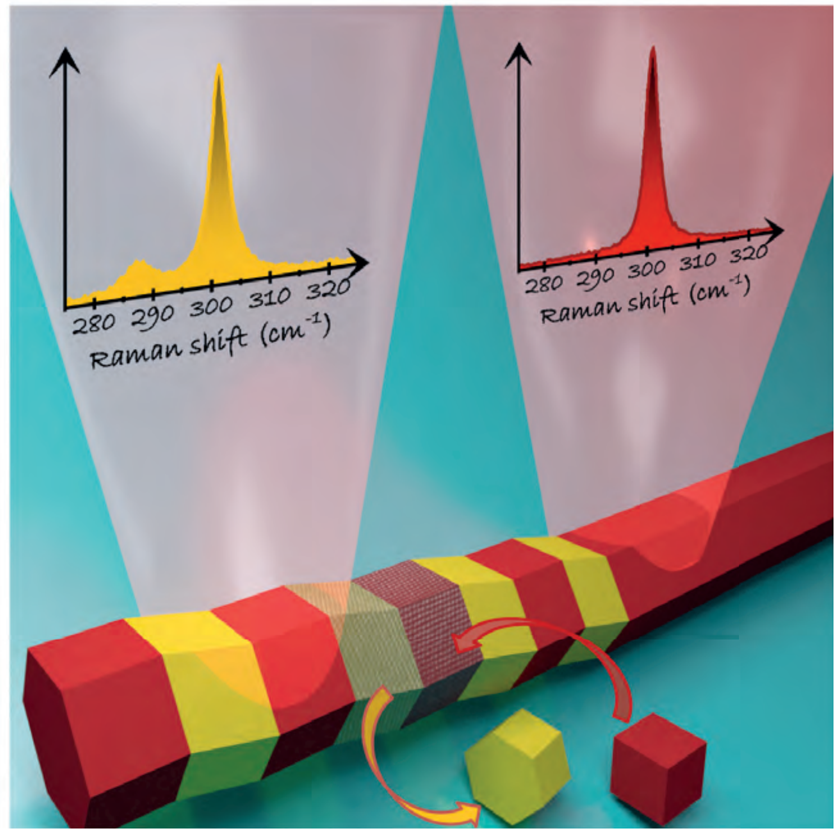
[1] Departement Physik, Universität Basel, Switzerland
[2] Centre de Nanosciences et Nanotechnologies (C2N), CNRS, Univ. Paris-Sud, UniversitéParis-Saclay, France
[3] CEMES, University of Toulouse, CNRS, France
[4] Laboratoire de Physique des Solides (LPS), CNRS, Univ. Paris-Sud, Université Paris-Saclay, France
[5] Institut de Ciència de Materials de Barcelona (ICMAB–CSIC), Spain

Crystalline, Phononic, and Electronic Properties of Heterostructured Polytypic Ge Nanowires by Raman Spectroscopy Nano Letters, 18, 11, 7075-7084 (2018)

RL1 SCIENTIFIC HIGHLIGHTS

In-depth analysis of novel semiconductor polymorphs

A combination of Raman spectroscopy and theoretical calculations provides unprecedented insight into crystal phase engineering in semiconducting nanostructures



Artist view of a heterostructured Ge nanowire where cubic (in red) and hexagonal (in dark yellow) domains are alternated. Sketches of the Raman spectra acquired are also shown. Two segments of the nanowire are textured with the corresponding TEM image.

Recent advances in the synthetic growth of nanowires --rod shaped semiconductors of nanometric size-- have given access to crystal phases that in bulk are only observed under extreme pressure conditions. The advent of these novel polymorphs, such as hexagonal Ge, promises to overcome some of the limitations that have prevented them to find application in photonics and optoelectronics thus far. The bandgap of hexagonal Ge is predicted to be direct, a fact that could have important implications with respect to the long-standing goal of designing a Ge-based light-emitting materials. Experimental data on these novel materials are scarce and are sometimes limited by the quality of the sample.

In this work, we used Raman spectroscopy, a common technique to probe the vibrational properties of materials and demonstrate its versatility when it comes to the determination of the main crystalline, phononic, and electronic properties of one of the most challenging type of nanostructure: a nanoscale sample with constant material composition, but different crystal phases. Theoretical calculations played a crucial role in understanding and interpreting the experimental results, especially because, due to its novelty, there are no reference data on hexagonal Ge.

The general procedure that we establish can be applied to several types of nanostructures.

RL1 SCIENTIFIC HIGHLIGHTS

Symmetric supercapacitors made of flexible electrodes grown by laser-based technique

An environmentally friendly laser technique was developed for the growth of nitrogen doped reduced graphene oxide and transition metal oxide coatings for energy storage applications

Ángel Perez del Pino,[1] Andreu Martınez Villarroya,[1] Alex Chuquitarqui,[1] Constantin Logofatu,[2] Dino Tonti,[1] Eniko György[1]

[1] Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Spain

[2] National Institute for Materials Physics, Romania

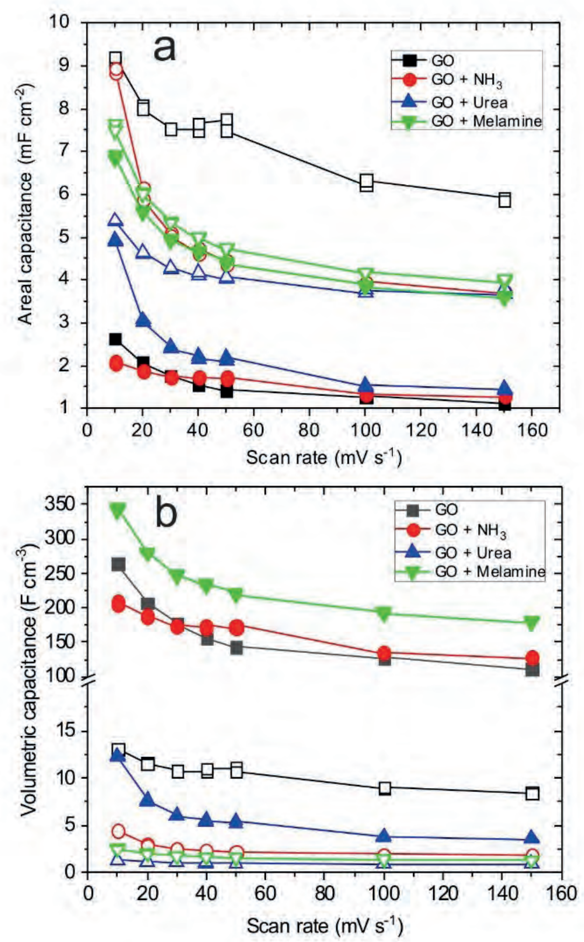
Reactive laser synthesis of nitrogen-doped hybrid graphene-based electrodes for energy storage

Journal of Materials Chemistry A, 6, 16074–16086 (2018)

Graphene-based electrodes were deposited onto metallic or gold-coated polymer substrates. The technique that we developed allows for the chemical transformation and simultaneous deposition of graphene oxide (GO) and GO-NiO nanoparticles. Nitrogen inclusion into the structure of GO was achieved through the addition to the irradiated aqueous target dispersions containing the nanoentities, GO platelets and NiO nanoparticles, nitrogen containing organic compounds (ammonia, urea, or melamine). The obtained flexible electrodes reveal high electrochemical charge storage performance (Figure) as well as outstanding long-term charge–discharge stability.

Addition of melamine to the graphene oxide-NiO dispersions leads to the synthesis of the electrodes with the highest energy storage performance. Melamine, as nitrogen containing precursor, leads to the formation of pyrrolic / amine, graphitic quaternary, and pyridinic nitrogen functional groups. Amine groups and graphitic nitrogen doping of GO are known to reduce the intrinsic resistance of graphene platelets and thus, ensure better electron transfer through the active material, improving the electrodes' capacitive performance. Moreover, graphitic and pyridinic nitrogen exhibit large dipole moments that greatly enhance the wettability of graphene materials in aqueous electrolyte solutions, leading to capacitance enhancement. Besides, pyridinic and pyrrolic nitrogen groups are electrochemically active, participating in redox reactions.

The developed fabrication method is cost-effective, fast, and environmentally friendly, characterized by an enormous versatility for the growth of functional nanocomposite coatings. Moreover, the work opens up new possibilities for the synthesis and deposition of new compounds, through the light induced chemical reactions taking place during the irradiation of organic materials.



(a) Areal and (b) volumetric capacitance of the deposited nitrogen doped reduced graphene oxide (GO) and transition metal oxide electrodes

RL2 SCIENTIFIC HIGHLIGHTS

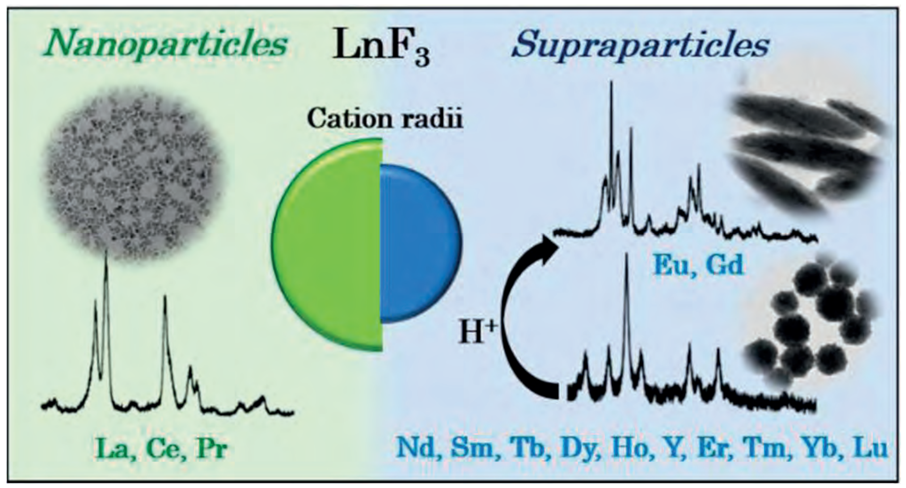
Unraveling the surface of nanoparticles: From aggregates to patchy Rare Earth Fluoride (ReF_3) Nanoparticles

Jordi Martínez-Esaín,[1,2] Teresa Puig,[2] Xavier Obradors,[2] Josep Ros,[1] Ramón Yáñez,[1] Jordi Faraudo[2],*and Susagna Ricart[2],*

[1] Departament de Química, Universitat Autònoma de Barcelona, Spain.

[2] Institut de Ciència de Materials de Barcelona, ICMAB-CSIC, Spain.

LnF_3 nanocrystals are synthesized and their different behavior is studied by a combination of experimental and all-atomic molecular dynamics simulations. We show here that the deep knowledge of the surface is a powerful tool to control the final size, shape and behavior of the nanoparticles



The study not only reveals the dependence of the crystalline structure with used metal and pH, but also the achievement of assembled particles depending on the final shape of nanocrystals.

Surface chemistry serves a fundamental role as the bridge between nanocrystal design and their final applications. In the study LnF_3 nanocrystals are synthesized using co-precipitation method with citrate stabilization, as commonly is used to allow the fast, easy and reproducible synthesis of several nanoscaled structures in water. General trends related to the behavior of LnF_3 nanocrystals are highlighted due to their broad range of application in several fields (e.g. medical applications). The same demeanor for all lanthanide (III) cations is expected due to the internal role of their f-orbitals. However we found that the use of different lanthanide elements is crucial in the final size, shape, assembly and crystalline structure. Fifteen Rare Earth elements (plus Y) were studied and the mechanism for the formation of the aggregates or patches and the properties of the obtained nanocrystals are characterized by a combination of experimental techniques and all-atomic molecular dynamics simulations. The crystallographic phase is tuned by changing the pH of the reaction. General trends are unraveled for each lanthanide, giving a classification where the metal-cation size is the pivotal key. Therefore, a different crystal structure and surface chemistry distributions are obtained, depending on the used lanthanide, pH and its final NCs shape. Nowadays, the accurate control of the interface between NC surface and stabilizers become in a hard and tedious work to enhance the intricate bridge, arriving to a future deep range of applications. Further studies towards an accurate and selective control over surface serves a fundamental role as the bridge between nanocrystal design and their final applications.

Tunable Self-Assembly of YF_3 Nanoparticles by Citrate-Mediated Ionic Bridges
Journal of the American Chemical Society, 140, 6, 2127-2134 (2018)

Faceted-Charge Patchy LnF(3) Nanocrystals with a Selective Solvent Interaction
Angewandte Chemie-International Edition, 130, 14963-14967 (2018)

Tailoring the Synthesis of LnF(3) (Ln = La-Lu and Y) Nanocrystals via Mechanistic Study of the Coprecipitation Method
Langmuir, 34, 22, 6443-6453 (2018)

RL2 SCIENTIFIC HIGHLIGHTS

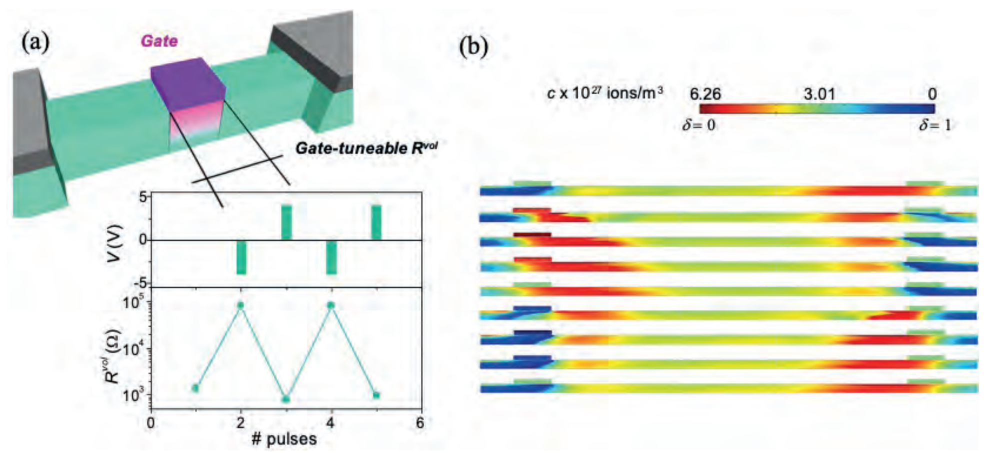
Non-volatile Metal-Insulator Transition in high temperature superconducting through field-induced oxygen diffusion

Alejandro Fernandez-Rodriguez,[1] Juan Carlos Gonzalez-Rosillo,[1] Xavier Granados,[1] Mariona Coll,[1] Bernat Bozzo,[1] Rafael Ortega-Hernandez,[1,2] Jordi Suñé,[2] Xavier Obradors,[1] Teresa Puig,[1] Narcís Mestres,[1] Anna Palau[1]

[1] Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Spain

[2] Dept. d'Enginyeria Electrònica, Universitat Autònoma de Barcelona, Spain

This work shows the potential of reversible, non-volatile electrochemical oxygen doping for a systematic tuning of the carrier density in $YBa_2Cu_3O_{7-\delta}$ films



(a) Schematic illustration of a transistor-like device (top). Voltage pulses and volume bridge resistance evolution obtained for a 50 nm thick YBa2Cu3O7-δ device
(b) Simulation of oxygen diffusion at different stages of the switching process, after the application of a sinusoidal voltage pulse. Colors show the oxygen concentration.

Modulation of carrier concentration in strongly correlated oxides offers the unique opportunity to induce Metal–insulator transitions (MITs) between different electronic phases which dramatically change their physical properties [1]. Particularly interesting are strongly correlated high-temperature superconducting cuprates, in which a reversible modulation of their critical temperature transition can be produced by means of an electric field as the external control parameter. Great progress has been made by inducing electrostatic doping through a ferroelectric polarization or by using a dielectric or electrolyte gating [2]. However, ultrathin superconducting layers and large electric fields must be used to observe significant carrier modulation.

We propose an original approach based on the reversible modulation of non-volatile superconducting–insulator phase transition in YBa2Cu3O7-δ films, through oxygen diffusion, that offers several technological and scientific breakthroughs as compared with modulations based on pure electrostatic doping. The key advantage the possibility to induce a volume phase transition (not just confined at the vicinity of the interface between the film and the gate electrode but spanning hundreds of nm away from the gate contact). We analyse different device configurations in which the lateral conduction of a bridge is controlled by gate-tuneable vertical and lateral oxygen motion, providing the basis for the design of robust, homogeneous and flexible transistor-like devices (Figure a), which may operate both at room temperature or exploit their superconducting nature. We analyse the experimental results in light of a theoretical mode, which incorporates thermally activated and electrically driven volume oxygen diffusion (Figure b)

Electrochemical Tuning of Metal Insulator Transition and Nonvolatile Resistive Switching in Superconducting Films
ACS Applied Materials & Interfaces, 10, 36, 30522-30531 (2018)

[1] Morosan et al. Advanced Materials, 24, 4896 (2012)
[2] Ahn, et al. Science 1999, 284, 1152; Crassous et al. Phys. Rev. Lett. 2011, 107, 247002; Leng, et al. Phys. Rev. Lett., 107, 027001 (2011) Nano Energy, 45, 94-100 (2018)

Ziliang Li,[1] Natalia Chamorro,[2] Ferran Valles,[1] Cornelia Pop,[1] Bernat Mundet,[1] Victor Rouco,[1] Mariona Coll,[1] Jaume Gazquez,[1] Roger Guzman,[1] Joffre Gutierrez,[1] Bohores Villarejo,[1] Flavio Pino,[1] Josep Ros,[2] Susagna Ricart,[1] Anna Palau,[1] Xavier Obradors,[1] Teresa Puig[1]

[1] Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Spain

[2] Departament de Química, Facultat de Ciències, Universitat Autònoma de Barcelona, Spain

[1] Epitaxial $YBa_2Cu_3O_{7-x}$ nanocomposite films and coated conductors from $BaMO_3$ (M = Zr, Hf) colloidal solutions.
Supercond. Sci. Technol. 31, 044001 (2018)

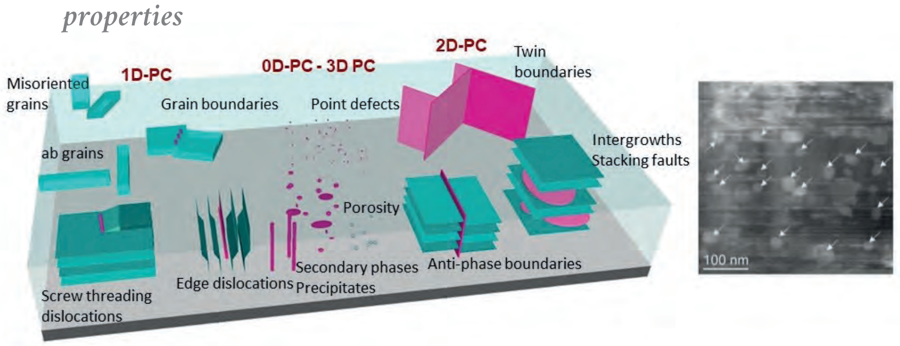
[2] Disentangling vortex pinning landscape in chemical solution deposited superconducting $YBa_2Cu_3O_{7-x}$ films and nanocomposites.
Supercond. Sci. Technol. 31, 034004 (2018)

[3] Angular flux creep contributions in $YBa_2Cu_3O_{7-delta}$ nanocomposites from electrical transport measurements.
Scientific Reports 8, 5924 (2018)

RL2 SCIENTIFIC HIGHLIGHTS

High temperature superconducting nanocomposites: A plethora for vortex pinning centers

The potentiality of preformed nanoparticles to control vortex pinning and dynamics of chemical solution nanocomposites is disentangled by correlating preparation, microstructure and properties



Schematic representation of the different defects that may contribute to pin vortices in HTS nanocomposites (a), scanning transmission electron microscopy image of a YBCO nanocomposite with the addition of 20 %mol of preformed $BaZrO_3$ nanoparticles, where the interaction with stacking faults is observed (b)

High temperature superconducting nanocomposites are a new class of materials that arose in the last decade based on the potentiality of introducing artificial pinning centers of nanometric size in $REBa_2Cu_3O_{7-x}$ (REBCO, RE=rare earth). The capability of introducing non-superconducting nanometric secondary phases was realized by different growth techniques (pulsed laser deposition, metalorganic chemical vapor deposition, chemical solution deposition). Initially, all were based on the spontaneous segregation of secondary phases during the epitaxial growth of REBCO. Recently, we pioneered the fabrication of solution-derived nanocomposites using preformed nanoparticles prepared by solvothermal methods through their stabilization in REBCO precursor solutions.

Here we demonstrate [1], for the first time, that non-reactive $BaZrO_3$ and $BaHfO_3$ perovskite preformed nanoparticles are suitable for growing high quality epitaxial films, and coated conductors with a homogeneous distribution and controlled particle size. This study could be extended to thick nanocomposite films, up to 0.8 µm, with a single deposition using ink jet printing. Nanocomposites up to 20 %–25 % mol without any degradation of the superconducting properties are achieved. However, the vortex pinning effects induced by these nanoparticles requires of an extensive study of the electrical transport properties as function of temperature, magnetic field and orientation of the magnetic field.

We need to distinguish between the different defects and contributions that interfere in the results correlating with corresponding microstructure. A quantitative analysis of vortex pinning strength and energies [2], associated with different kinds of natural and artificial pinning defects, enables us to unravel the different pining regions of the H–T phase diagram, which provides a unique tool to design the best vortex pinning landscape under different operating conditions.

This study is then extended to the vortex dynamics regime, studying the angular dependence of the flux creep properties of nanocomposites, for the first time, from electrical transport measurements [3].

Amparo Fuertes

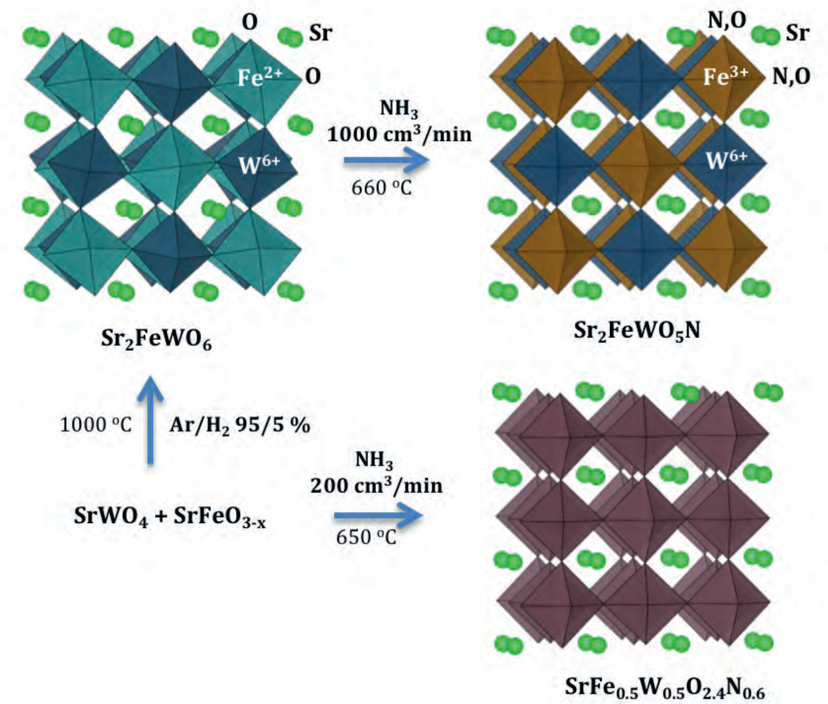
Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Spain

Synthetic approaches in oxynitride chemistry
Progress in Solid State Chemistry 51, 63-70 (2018)

RL3 SCIENTIFIC HIGHLIGHTS

Accessing new functional oxynitride materials

The major challenge in the chemistry of oxynitride materials is the control and reproducibility of the synthesis and the development of new preparative methods



Synthesis of cation ordered Sr_2FeWO_5N and disordered $SrFe_{0.5}W_{0.5}O_{2.4}N_{0.6}$. The cation disordered perovskite was obtained by ammonolysis of a 1:1 mixture of SrWO4 and $SrFeO_3$-x prepared by a citrate route. This mixture was used to prepare the oxidic Sr_2FeWO_6 at 1000 oC under Ar/H_2 (5 %) that was further topochemically ammonolysed at 660 oC to obtain the cation ordered double perovskite oxynitride.

Mixed anion oxides are emerging materials showing a variety of physical and chemical properties. Among them oxynitrides are widely investigated because of important photocatalytic, dielectric, luminescent and electronic properties. Nitrides show more positive free energies of formation than oxides because of the higher stability of N_2 molecule with respect to O_2 and the unfavourable electron affinity of nitrogen compared to oxygen. However the stability of oxynitrides is higher than for nitrides, and they easily form from oxides in presence of reactive gases as NH3.

The notable development of new oxynitride materials in the last years is a consequence of the improving of synthetic methodologies. Research in the field is increasingly showing that despite the lower thermodynamic stability of nitrides the N^{3-} anion can be easily stabilized in any structural type shown by oxides. Nitriding in ammonolysis reactions is governed by kinetic factors and for more reducible cations the oxynitrides are isolated as metastable compounds that with prolonged time decompose into complex oxides and binary metal nitrides. Recent examples of solution methods in supercritical ammonia show the obtention of highly crystalline powders and small single crystals. The development of crystal growth methods is challenging but necessary to provide large single crystals for measuring physical properties. Within the group of transition metals the majority of oxynitrides have been reported for the groups 4, 5 and 6. Among them the tantalum compounds are the most investigated because of their photocatalytic and dielectric properties. The stabilization of more reducible later transition metals is difficult under the conventional ammonolysis conditions used for Ti, Zr or Ta oxynitrides. However new oxynitrides of more electronegative Cr, Fe, Mn or Zn have been recently prepared at lower temperatures from adequate precursors in the ammonolysis reaction (Figure) or under high pressure. These show interesting electronic properties such as antiferromagnetism (for $LnCrO_{3-x}N_x$ and Sr_2FeWO_5N), ferromagnetism (for Sr_2FeMoO_5N) and helicoidal spin order (for $MnTaO_2N$).

[1] Ceravola R, Oró-Solé J, Black AP, Ritter C, Puente Onrech I, Mata I, Molins E, Frontera C, Fuertes A. Topochemical synthesis of cation ordered double perovskite oxynitrides. Dalton Trans., 46, 5128-5132 (2017

RL3 SCIENTIFIC HIGHLIGHTS

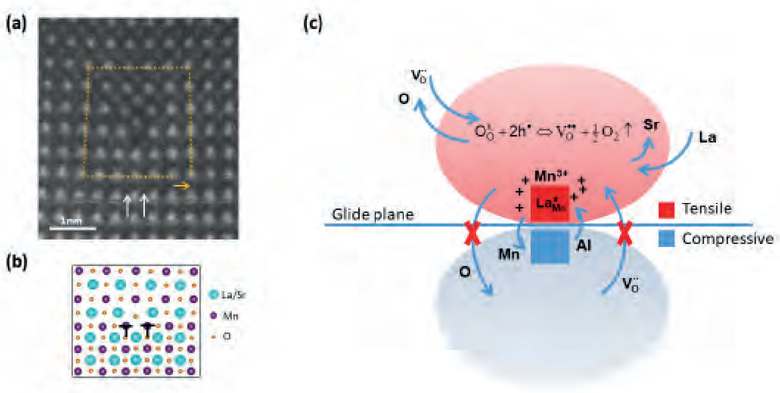
Cross talks between strain and chemistry at dislocations

New insight into the nanochemistry and electronic structure of an oxide dislocation core: oxygen vacancies singled out and quantified

Núria Bagués,[1,2] José Santiso,[2] Bryan D. Esser,[3] Robert E. A. Williams,[3] Dave W. McComb,[3] Zorica Konstantinovic,[4] Lluís Balcells,[1] and Felip Sandiumenge[1*]

[1] Institut de Ciència de Materials de Barcelona, ICMAB-CSIC, Spain.
[2] Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC and BIST, Spain.
[3] Center for Electron Microscopy and Analysis. The Ohio State University, USA.
[4] Center for Solid State Physics and New Materials, Institute of Physics Belgrade, University of Belgrade, Serbia.

The Misfit Dislocation Core Phase in Complex Oxide Heteroepitaxy
Adv. Funct. Mater. 28, 170443 (2018)



(a) Atomic resolution high angle annular dark field image of misfit dislocation. The two arrows indicate the position of the two extra half planes of the dissociated core. Dotted lines draw a Burgers circuit. (b) Atomic model of the dislocation core. (c) Schematic illustration of the basic mechanisms operating in the MD core. The redox reaction indicated in the tensile region is displaced to the right, favoring the formation of electron donor oxygen vacancies. The imbalance between the rate of Sr diffusion out of the core region and the concentration of vacancies results in a positive charge in the tensile region

Dislocations are topological defects ubiquitous in crystals, which despite having been conceptually conceived more than eight decades ago, have largely remained in the drawers of oddities in materials science labs owing to the obstinate inaccessibility of their ~ 1nm cores. This is particularly true for dislocations in oxides, where electrostatic interactions arising from their ionic character can define the core structure and the defect chemistry in the associated strain field.

The strong sensitivity of the defect chemistry, particularly oxygen vacancy formation energies, to dislocation strains, otherwise provide a rich scenario for the development of new confined states. In this sense, dislocations are emerging as the one-dimensional analogue of ferroelastic or ferroelectric domain walls, where strain and symmetry breaking promote the development of localized states exhibiting different properties from those of the host crystal.

The transformation of such defects from passive into potentially active functional elements, however, necessitates a deep understanding of their chemical and electronic structure. In [1], we combine different atomic resolution imaging and spectroscopic techniques in the transmission electron microscope to determine the complex structure of misfit dislocations in the perovskite type $La_{0.67}Sr_{0.33}MnO_3/LaAlO_3$ heteroepitaxial system. While the position of the film–substrate interface is blurred by cation intermixing, oxygen vacancies selectively accumulate at the tensile region of the dislocation strain field. Such accumulation of vacancies is accompanied by the reduction of manganese cations in the same area, with associated chemical expansion effects contributing to accommodate the dislocation strain. The formation of oxygen vacancies is only partially electrically compensated and results in a positive net charge $q \approx +0.3 \pm 0.1$ localized in the tensile region of the dislocation, while the compressive region remains neutral. These results highlight a prototypical core model for perovskite-based heteroepitaxial systems and offer insights for a predictive manipulation of misfit dislocation properties.

RL3 SCIENTIFIC HIGHLIGHTS

A new Iron (III) oxide phase from ε-Fe_2O_3 under high pressures

Synchrotron-based diffraction and spectroscopy experiments combined with ab-initio calculations unveiled the fate of ε-Fe_2O_3 under isostatic compression: transforming to a new polymorph through a spin crossover transition

Juan Ángel Sans,[1] Virginia Monteseguro,[2,3] Gaston Garbarino,[2] Martí Gich,[4] Valerio Cerantola,[2] Vera Cuartero,[2,5] Manuel Monte,[2] Tetsuo Irifune,[6,7] Alfonso Muñoz,[8] and Catalin Popescu[9]

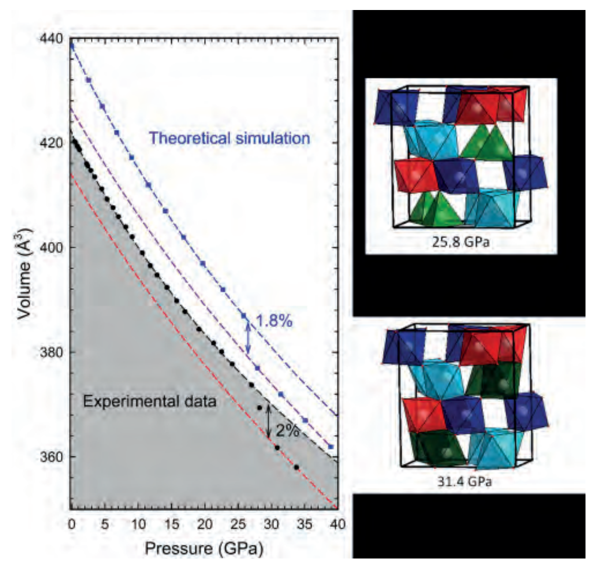
[1] Instituto de Diseño para la Fabricación y Producción Automatizada, MALTA Consolider Team, Universitat Politècnica de València, Spain.
[2] European Radiation Synchrotron Facility 38043, France. [3] ICMUV. MALTA Consolider Team, Universitat de València, Spain. [4] Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Spain
5 Centro Universitario de la Defensa de Zaragoza, Spain. [6] Ehime University, Japan. [7] Earth-Life Science Institute, Tokyo Institute of Technology, Japan. [8] Departamento de Física, Instituto de Materiales y Nanotecnología, MALTA Consolider Team, Universidad de La Laguna, Spain. [9] ALBA Synchrotron, Spain

Stability and nature of the volume collapse of ε-Fe_2O_3 under extreme conditions
Nature Communications, 9, 4554 (2018)

Mirric oxide (Fe_2O_3) has been widely studied in many fields from geophysics and biomedicine to technological applications. At ambient conditions it is found in form of five polymorphs with quite different properties. Among them, ε-Fe_2O_3 presents giant coercivity and has been lately found as a nanomineral in basaltic rocks [1], opening the possibility of its relevant presence in the Earth's interior. However, an important prerequisite is the stability of ε-Fe_2O_3 at extreme conditions, which has motivated the high pressure study of this oxide.

ε-Fe_2O_3 presents an orthorhombic structure with four polyhedral units: a regular octahedron, two distorted octahedra and a regular tetrahedron (Figure). By X-ray absorption fine structure (EXAFS) the deformation of polyhedral units were monitored under increasing pressures and revealed a remarkable stability, altered by a sudden change in the average interatomic distances at 27 GPa, the limiting pressure to access the upper Earth's mantle. This structural anomaly is also reflected by a collapse of the unit cell volume revealed by pressure dependent X-ray diffraction. The analysis of the diffraction patterns at different pressures allowed obtaining the pressure-volume equation of state which was reproduced, including the volume collapse, by ab-initio theoretical simulations. These calculations also indicated the phase stability up to 1800 K and provided its structural characteristics above the volume collapse, which were found to be compatible with the experimental diffraction data.

In particular, in the new high pressure ε'-phase, one of the irregular octahedrons and the regular tetrahedron become very distorted octahedral units, closer to a 5+1 coordination. Synchrotron-based Mössbauer spectroscopy measurements indicated that the ε to ε' transformation is a spin crossover transition.



Evolution of the unit cell volume of ε-Fe_2O_3 under compression. Experimental data (black circles), theoretically simulated data (blue squares) and the fits to 3rd order Birch-Murnaghan equation of state (dashed lines). The structure of ε-Fe_2O_3 just below the volume collapse and above it (ε'–phase) as obtained by ab-initio calculations are presented on the right side.

[1] Xu, H., Lee, S., and Xu, H. Luogufengite: A new nano-mineral of Fe2O3 polymorph with giant coercive field. Am. Mineral. 102, 711–719 (2017).

Blai Casals,[1] Andrea Schiaffino,[1] Arianna Casiraghi,[2] Sampo J. Hämäläinen,[2] Diego López González,[2] Sebastiaan van Dijken,[2] Massimiliano Stengel,[1,3] and Gervasi Herranz[1]

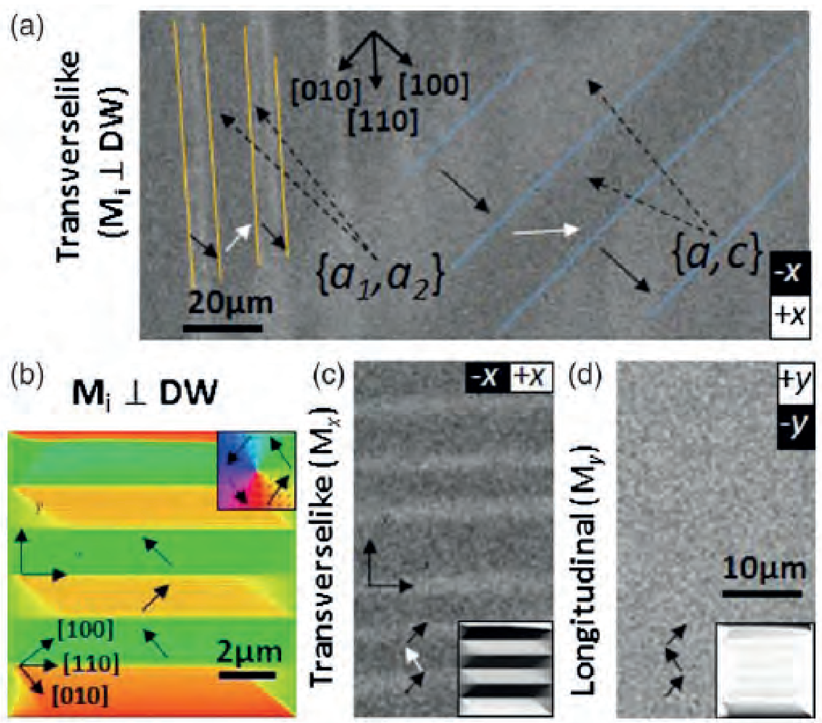
[1] Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Spain
[2] NanoSpin, Department of Applied Physics, Aalto University School of Science, Finland
[3] ICREA–Institució Catalana de Recerca i Estudis Avançats, Spain

Low-Temperature Dielectric Anisotropy Driven by an Antiferroelectric Mode in SrTiO3
Physical Review Letters 120, 217601 (2018)

RL3 SCIENTIFIC HIGHLIGHTS

Ferroelastic domains in motion under electric fields

Optical imaging and first-principles modeling unveil the physics of domain motion driven by electric fields in ferroelastic $SrTiO_3$ crystals



(a) Map of ferroelastic domains obtained by magneto-optical imaging. The images show the presence of {a1, a2} and {a,c} ferroelastic twins, revealed by imprinting of ferroelastic domains into a magnetostrictive film on top of $SrTiO_3$. Micromagnetic simulations of the magnetic state shown in (b) are in agreement with the spatial distribution of magnetic domains imprinted on the magnetostrictive film (shown in (c) and (d) by the underlying ferroelastic twins in $SrTiO_3$.

By altering the chemical composition of $SrTiO_3$ or by straining the crystals, a remarkable wide scope of physical phenomena emerge, including superconductivity, ferroelectricity, 2D-transport or magnetism. This notable versatility makes of $SrTiO_3$ a paradigmatic material of oxide electronics. Another fundamental feature of $SrTiO_3$ is the transition from a cubic to a tetragonal low-temperature phase, whereby ferroelastic domains form in the crystals. There is also evidence that electric polarity emerges at domain walls, which is, a priori, an unexpected outcome, as the material itself is not polar.

Given these considerations, a natural question arises about how electric fields interact with ferroelastic domains and, in particular, whether the polar character of domain walls drives the motion of ferroelastic domains or if, on the contrary, the dielectric properties of $SrTiO_3$ prevail on the dynamics of domains. To answer this question, we imaged the evolution of ferroelastic domains in situ (Figure), carefully controlling the orientation of the applied fields with respect to the orientation axis of the domains. By combining in-situ imaging with numerical modeling based on first-principles density-functional theory, we conclude that it is the dielectric anisotropy of tetragonal $SrTiO_3$, rather than the intrinsic domain wall polarity, what drives the motion of the ferroelastic twins. The underlying mechanism relies on the excitation of a particular IR-active lattice mode below the tetragonal transition, which we predict to be a general characteristic of perovskites.

Ignasi Fina,[1] Jike Lyu,[1] Fanmao Liu,[1] Raúl Solanas,[1] Guillaume Sauthier,[2] Andrew M. Rappe,[3] Josep Fontcuberta,[1] and Florencio Sánchez[1]

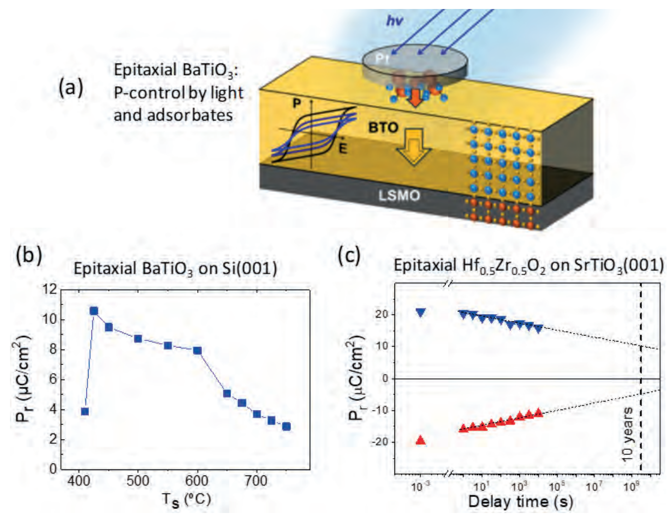
[1] Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Spain
[2] Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC and BIST, Spain
[3] Department of Chemistry, University of Pennsylvania, Philadelphia, USA

[1] Tailoring Lattice Strain and Ferroelectric Polarization of Epitaxial BaTiO3 Thin Films on Si(001), Scientific Reports 8, 495 (2018)
[2] Control of the polarization of ferroelectric capacitors by the concurrent action of light and adsorbates, ACS Applied Materials & Interfaces 10, 23968-23975 (2018).
[3] Robust ferroelectricity in epitaxial Hf1/2Zr1/2O2 thin films, Applied Physics Letters 113, 082902 (2018)

RL3 SCIENTIFIC HIGHLIGHTS

Ferroelectric $BaTiO_3$ and doped-HfO_2: epitaxy and control of polarization

The ferroelectric polarization of epitaxial oxide films is controlled by growth kinetics and by concurrent action of light and adsorbates



(a) Sketch of a Pt/$BaTiO_3$/$La_{2/3}Sr_{1/3}MnO_3$ capacitor under illumination, with adsorbates in the Pt/ $BaTiO_3$ interface.
(b) Dependence on deposition temperature of the remnant polarization of epitaxial $BaTiO_3$ films integrated epitaxially with Si(001).
(c) Epitaxial $Hf_{0.5}Zr_{0.5}O_2$ films with retention time longer than 10 years.

The classical methods to tune polarization of ferroelectric films require chemical substitutions or selection of a particular substrate. We have developed two alternative methods that are more flexible, permitting tailoring polarization without requiring changes in film composition or substrate. One strategy, illustrated with the paradigmatic ferroelectric $BaTiO_3$, is based on imposing kinetic limitations during epitaxial growth. The balance between kinetics and thermodynamics fixes the amount of point defects in the deposited films. The defects produce lattice expansion of $BaTiO_3$, determining the unit cell tetragonality and ultimately the ferroelectric polarization. This method, that allows obtaining a particular polarization without changing composition or substrate, is demonstrated with $BaTiO_3$ films integrated epitaxially on Si(001) wafers [1].

The second strategy permits dynamic control of the polarization by using light radiation. Under illumination, photoinduced carriers in semiconductors and photodissociated adsorbates modify the electrostatic screening at the surface of ferroelectric films and modify the switchable polarization. We have shown that water-related adsorbates at the surface of $BaTiO_3$ enable a substantial modulation (up to 75 %) of the switchable remanent polarization by light. As ferroelectric perovskites hold promises of enhanced photovoltaic efficiency in solar cells and photocatalytic activity, these findings may get a far reaching relevance for novel applications of [2].

The recent discovery of ferroelectricity in doped HfO_2 represents a breakthrough towards commercial permanent memories based in ferroelectrics. The metastable ferroelectric phase of HfO_2 is obtained in polycrystalline films, and epitaxial ferroelectric HfO_2 films have been rarely achieved. However, epitaxial films are needed for better understanding of the properties and prototyping devices of nanometric dimensions. We have stabilized the ferroelectric phase of $Hf_{0.5}Zr_{0.5}O_2$ films in epitaxial films, which present high polarization that depends strongly on the thickness and demonstrating by the first time for epitaxial films absence of wake up effect, long retention and high endurance against fatigue. [3]

Laura López-Mir,[1] Carlos Frontera,[1] Hugo Aramberri,[1] Karim Bouzehouane,[2] Jose Cisneros-Fernández,[1] Bernat Bozzo,[1] Lluís Balcells,[1] Benjamin Martínez[1]

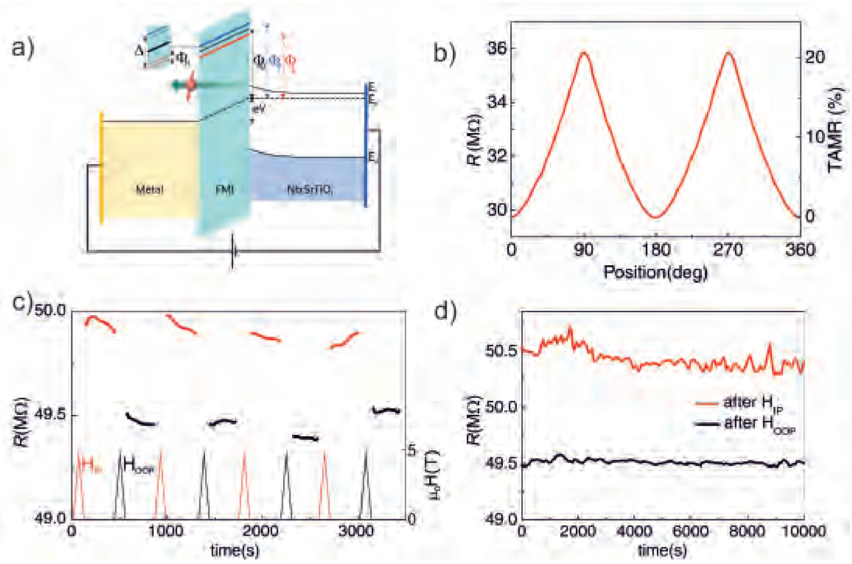
[1]Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Spain
[2]Unité Mixte de Physique, CNRS-Thales, France

Anisotropic sensor and memory device with a ferromagnetic tunnel barrier as the only magnetic element
Scientific Reports, 8, 861 (2018)

RL3 SCIENTIFIC HIGHLIGHTS

Storing information in a ferromagnetic insulating barrier

Magnetic anisotropy converts a tunnel junction device, in which the only magnetic material is the barrier, into a memory devicesize, shape and behavior of the nanoparticles



a) Schematics of the band diagram of our device with forward applied bias V. F0 is the tunneling barrier that splits into F and F⁻ for spin up and spin down electrons due to i) the exchange splitting D and the effect of the magnetic field (FH).

b) Resistance and TAMR of the sample with respect to the orientation of the applied field (9T): perpendicular plane (OOP) at q=0°, 180° and in plane (IP) for q=90°, 270°.

c) Resistance measured during 300s after applying/releasing a field of 5T OOP (black) and IP (red). Schematic of magnetic field pulses is depicted at the bottom.

d) Long time measurement (105 s) of the two resistance states after a 9T pulse IP (red) and OOP (black).

Multiple spin functionalities are tested on Pt/$La_2Co_{0.8}Mn_{1.2}O_6$/Nb:$SrTiO_3$, a device composed by a ferromagnetic insulating (FMI) barrier sandwiched between nonmagnetic electrodes. FMIs are scarce in nature, as ferromagnetic interactions are typically of exchange-type mediated by charge carriers, and they can play an important role in spintronics as an efficient way to obtain polarized currents when used as spin filters. In our device, the only magnetic element is $La_2Co_{0.8}Mn_{1.2}O_6$ barrier. Moreover, $La_2Co_{0.8}Mn_{1.2}O_6$ thin films present strong perpendicular magnetic anisotropy whose origin lies in the large spin-orbit interaction of Co_2+which is additionally tuned by the strain of the crystal lattice.[1] This anisotropy is largely reflected in the transport properties of the junction presenting tunneling anisotropic magnetoresistance (TAMR) values up to 30% at low temperatures, in addition to an estimated spin filtering efficiency of 99.7%.[2] These results are corroborated by DFT-based calculations. We demonstrate that the DOS of La_2CoMnO_6 has a fully polarized spin-down character above the Fermi level. On the other hand, our calculations estimate a difference in the tunnel barrier height of 8 meV when magnetization changes from OOP to IP, and an exchange splitting of 0.2 eV, in good agreement with values fitted experimentally. Furthermore, we found that the junction can operate as an electrically readable magnetic memory device. Our results probe the existence of a non-volatile bistable resistive state that can be switched by applying magnetic field pulses in perpendicular or parallel directions. Thus, the findings of this work demonstrate that a single ferromagnetic insulating barrier with strong magnetocrystalline anisotropy is sufficient for realizing sensor and memory functionalities in a tunneling device based on TAMR.

[1] L. López-Mir, R. Galceran, J. Herrero-Martín, B. Bozzo, J. Cisneros-Fernández, E. V. Pannunzio Miner, A. Pomar, L. Balcells, B. Martínez, C. Frontera, Phys. Rev. B 2017, 95, 224434.
[2] L. López-Mir, C. Frontera, H. Aramberri, K. Bouzehouane, J. Cisneros-Fernández, B. Bozzo, L. Balcells, B. Martínez, Sci. Rep. 2018, 8, DOI 10.1038/s41598-017-19129-5.

RL3 SCIENTIFIC HIGHLIGHTS

Influence of the magnetic field direction on the magnetoelectric properties of an incommensurate conical improper multiferroic

The complete magnetic and ferroelectric H-T phase diagrams for magnetic fields along the special magnetic directions were determined in a Dzyaloshinskii–Moriya multiferroic crystal with conical antiferromagnetic structure

Irene Urcelay-Olabarria,[1] Eric Ressouche,[2] Vsevolod Yu Ivanov,[3] Vassil Skumryev,[4] Zhaosheng Wang,[5] Yurii Skourski,[5] Anatoly M. Balbashov,[6] Yu. F. Popov,[7] Gennadii P. Vorob'ev,[7] Navid Qureshi,[8] José Luís García-Muñoz,[9] and Alexander A. Mukhin[3]

[1] Zientzia eta Teknologia Fakultatea, Universidad del País Vasco, UPV/EHU, Spain, [2]Université Grenoble Alpes, CEA, INAC, MEM, France, [3] Prokhorov General Physics Institute, RAS, Russia, [4] Institució Catalana de Recerca i Estudis Avancats (ICREA) and Universitat Autònoma de Barcelona, Spain, [5] Hochfeld-Magnetlabor Dresden (HLD-EMFL) Helmholtz-Zentrum Dresden-Rossendorf, Germany, [6] Moscow Power Engineering Institute, Russia, [7] Faculty of Physics, M.V. Lomonosov Moscow State University, Russia

[8] Institut Laue Langevin, France, [9]Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Spain

Influence of the magnetic field on the stability of the multiferroic conical spin arrangement of $Mn_{0.80}Co_{0.20}WO_4$

Physical Review B 98(13) 134430 [10pp] (2018)

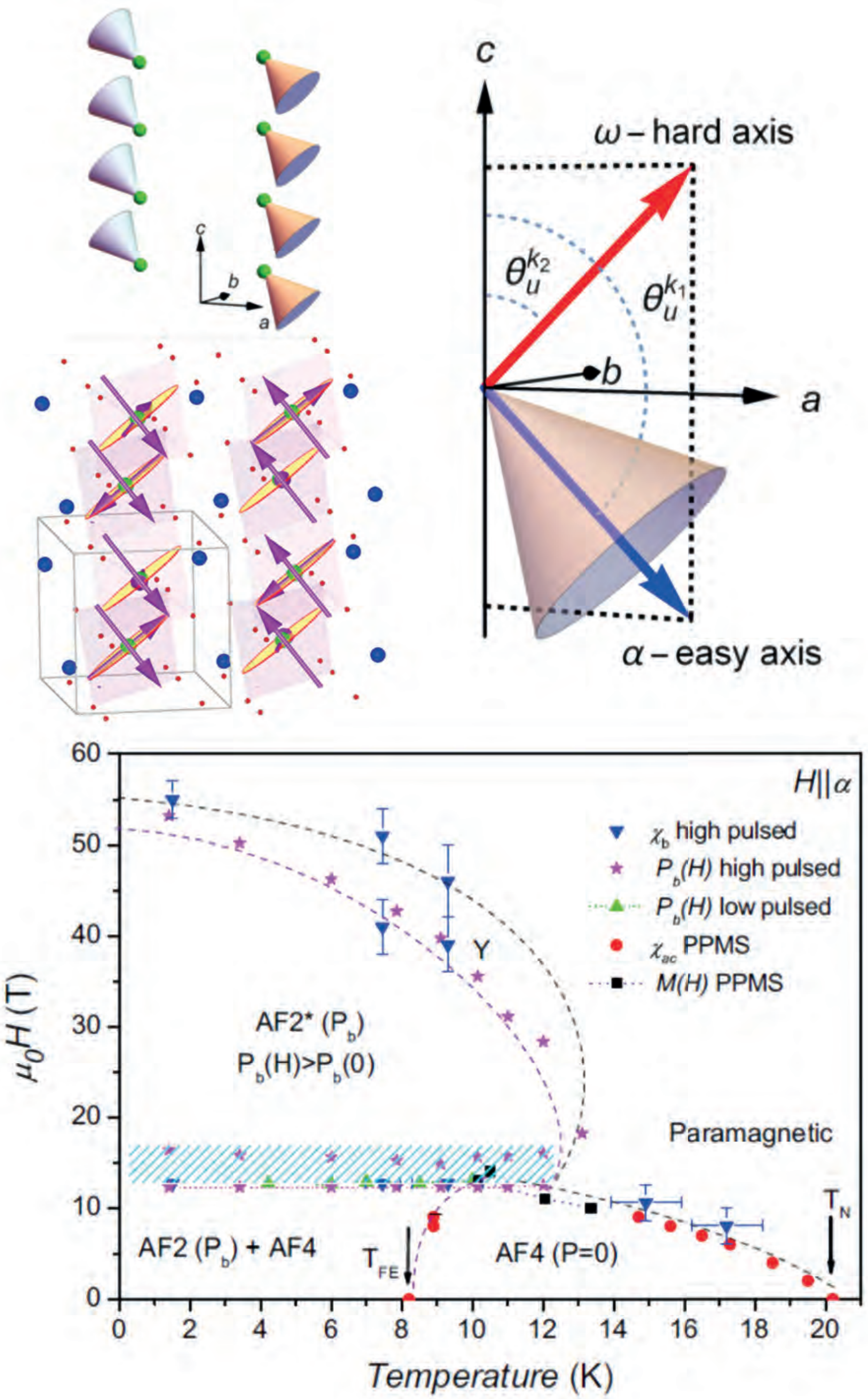
Understanding the interplay between magnetism and ferroelectricity in improper multiferroics is of interest in fundamental and applied research. In previous studies we showed the appearance of ferroelectricity in Dzyaloshinskii-Moriya Mn1-xCoxWO4 crystals (x≥0.15) due to the stabilization of a rare double-k spin configuration: a transverse conical AFM order, composed of AFM collinear (AF4) and incommensurate (ICOM) cycloidal orders. The objective of the present study was the construction of the complete magnetoelectric phase diagrams for the principal magnetic directions.

The magnetic and pyroelectric responses to magnetic fields were characterized along the main axes of the conical spin arrangement in quality crystals of $Mn_{0.80}Co_{0.20}WO$ grown by floating zone: the easy α and hard ω axes, and the b axis. The rotation plane (ωb) of the cycloidal spins is perpendicular to the easy magnetic axis of AF4 (α). ω is the magnetically hard direction within the ac plane (α ⊥ ω). The magnetic order evolution was studied by single-crystal neutron diffraction (D23, ILL) up to 12 T, and by magnetometry (ac, dc) up to 60 T (at ICMAB and the EMFL Lab. at Dresden). The dielectric polarization was measured up to 20/60 T in static/pulsed fields. Several magnetoelectric transitions were thoroughly investigated:

A: Suppression of the conical antiferromagnetic structure under field H//α. The complete magnetoelectric phase diagrams were determined for H//ω and H//b, with the field applied along the two elliptical axes of the cycloid in the conical structure. These components can be separately suppressed under field producing a fan-like magnetic configuration. In this phase transition (AF2+AF4 →AF3+AF4) the ferroelectric Pb state transforms to a paraelectric phase. At higher fields the paraelectric AF3 (COM) and AF4 (ICOM) components are successively suppressed.

B: Conical to cycloidal structure transformation and polarization in H//α axis. Marked differences were found in the H//α topology respect to the magnetoelectric transitions in the previous configurations (H//ω and H//b). An increase of the electric polarization accompanies the first metamagnetic transition (Pb(H)> Pb(0)) with H//α. The COM AF4 spin ordering is transferred to the AF2* magnetic cycloid, which exhibits enhanced elliptical amplitudes (AF2+AF4 →AF2*). Increasing further the field, and before the forced FM (paramagnetic) state, another intermediate magnetic phase (Y phase, with no polarization) was detected.

For all the phases the symmetry dictated relationships between magnetic order and the polarization tensor have been analyzed. The obtained results might be common for other magnetic materials possessing conical antiferromagnetic structures.



Conical antiferromagnetic structure in the ground state of ferroelectric $Mn_{0.80}Co_{0.20}WO_4$. H-T magnetoelectric phase diagram of a $Mn_{0.80}Co_{0.20}WO_4$ crystal for magnetic field along the α easy axis. Sketch of the magnetic and crystallographic axes drawn together with the conical surface that envelopes the spins

Massimiliano Stengel[1,2] and David Vanderbilt[3]

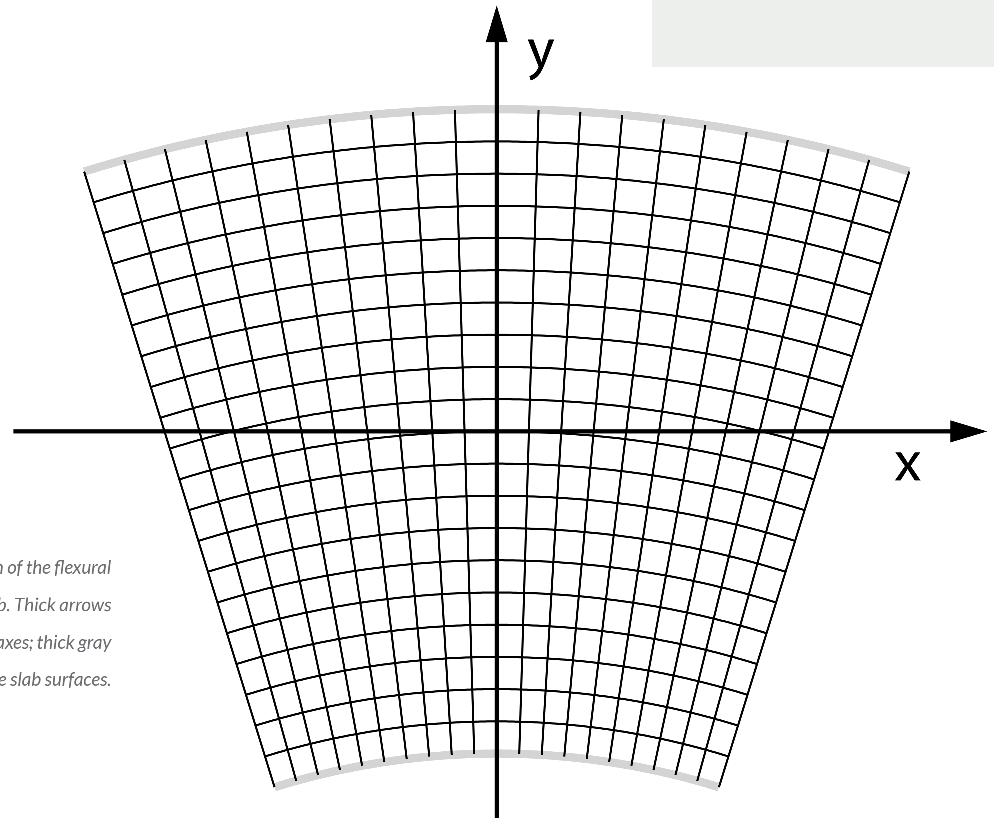
[1] Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Spain
[2] ICREA–Institució Catalana de Recerca i Estudis Avançats, Spain
[3] Department of Physics and Astronomy, Rutgers University, USA

Quantum theory of mechanical deformations
Physical Review B 98, 125133 (2018)

RL3 SCIENTIFIC HIGHLIGHTS

Bending electrons

A curvilinear-frame representation of the time-dependent Schrödinger equation sheds light onto the intricacies of complex electromechanical couplings such as flexoelectricity



Schematic illustration of the flexural deformation of a slab. Thick arrows indicate the Cartesian axes; thick gray curves indicate the slab surfaces.

Mechanical stress is arguably the simplest type of external field that can be applied to a crystalline solid. What happens to the electronic wavefunctions in the course of a deformation, however, is nowhere simple; on the contrary, interesting functionalities can emerge that are nowadays under the spotlight of researchers and engineers alike. An example of such functionalities is flexoelectricity, which describes the electrical polarization response to the gradient of a strain. (Figure)

During the last five years or so, we have made tremendous advances towards the development of a "modern" theory of flexoelectricity, and only very recently we have reached the stage where first-principles calculations for realistic materials can be performed with relative ease. Achieving this goal forced us to rethink the methodological bases of density-functional theory from their very root: strain gradients break translational symmetry and this is a major obstacle for the established approaches. Here, we address this issue by representing the Schrödinger equation in the curvilinear "co-moving" frame of the deformed crystal; the main advantage is that the perturbation no longer changes the boundary conditions of the Hamiltonian, and can be more easily dealt with.

Apart from the methodological advances, which have already been used in public code implementations, our work also unveils some peculiar and unsuspected aspects of flexoelectricity, e.g. its relationship to the theory of orbital magnetism. These results are an important milestone towards a fundamental understanding of phenomena where an electrical polarization results from a spatially inhomogeneous configuration of the crystal.

Sergi Riera-Galindo, Adrián Tamayo, Marta Mas-Torrent

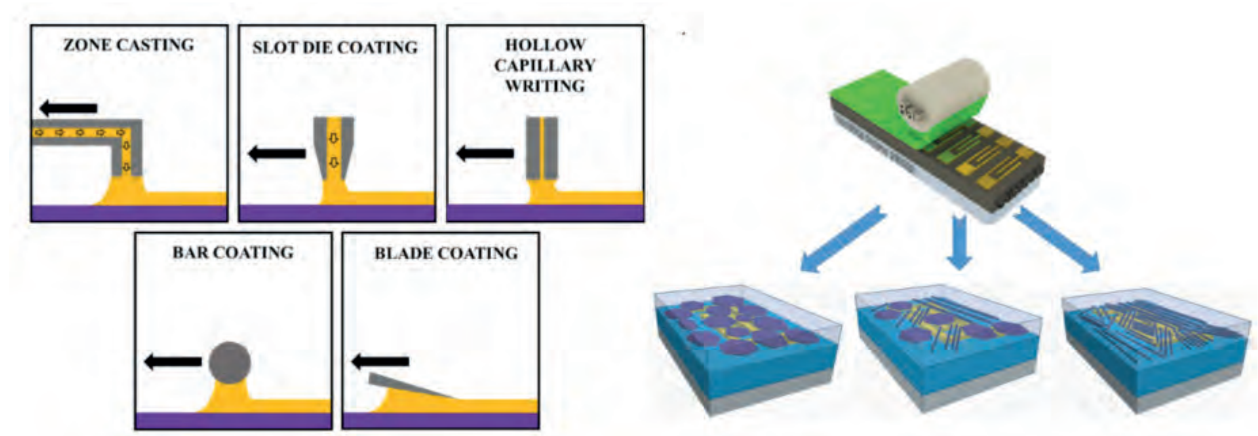
Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Spain

Role of Polymorphism and Thin-Film Morphology in Organic Semiconductors Processed by Solution Shearing
ACS Omega, 3, 2, 2329 (2018)

RL4 SCIENTIFIC HIGHLIGHTS

The role of polymorphism and thin film morphology in organic semiconductors processed by solution shearing

The control of polymorphism and thin film morphology in small molecule organic semiconductor thin films deposited by solution-shearing techniques is reviewed. To gain insights into the thin film crystallization is crucial to achieve high performing devices with high reproducibility



Left. Schematic illustration of some of the most common solution shearing deposition techniques.

Right. 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

Organic semiconductors (OSCs) have emerged as promising materials for cost-effective production of new flexible electronic devices since they can be processed from solution and at temperatures compatible with polymeric substrates. In particular, small molecule OSCs have been applied as active materials in organic field-effect transistors (OFETs) exhibiting impressive field-effect mobility values. To raise industrial interest though, it is crucial that such deposition techniques are simple, cheap and compatible with up-scaling and high throughput processes such as roll-to-roll. In this direction, solution shearing techniques are highly appealing (Figure, left). However, small molecule OSCs are prone to structural modifications due to the presence of weak van der Waals intermolecular interactions. Therefore, the control of the crystallization in these materials is pivotal to achieve a high device-to-device reproducibility.

In this review article we report on the influence of polymorphism and morphology on the electrical characteristics of OFETs fabricated by solution-shearing techniques. We show that by modifying the coating parameters such as the coating speed or the temperature, among others, a control of the thin film morphology and structure can be achieved leading to optimized device performances (Figure, right). Further, the main characterization techniques for thin film structure are reviewed, highlighting the in situ characterization tools which can provide crucial insights into the crystallization mechanisms.

RL4 SCIENTIFIC HIGHLIGHTS

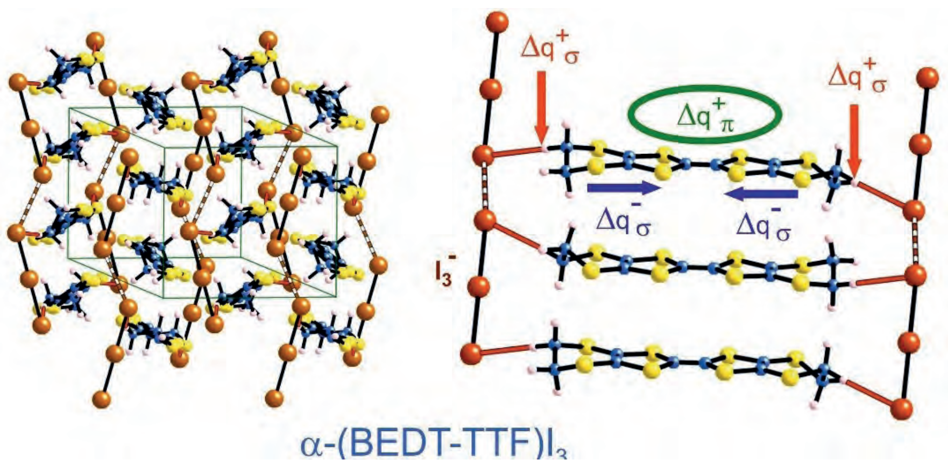
Anions are not naïve players in molecular conductors

Anions are usually considered to act simply as electron donors or acceptors in molecular conductors but they play an essential role in directing their structural and electronic properties.

Jean-Paul Pouget,[1] Pere Alemany[2] and Enric Canadell[3]

[1]Laboratoire de Physique des Solides, CNRS UMR 8502, Université Paris-Sud, Université Paris Saclay, France
[2]Departament de Ciència de Materials i Química Física and Institut de Química Teòrica i Computacional (IQTCUB), Universitat de Barcelona, Spain
[3]Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Spain

Donor–anion interactions in quarter-filled low-dimensional organic conductors
Materials Horizons, 5, 590-640 (2018).



Crystal structure of α–(BEDT-TTF)$_2$I$_3$ and diagram showing how the development of a positive s charge in the H atom making a hydrogen bond with the anion and a positive π charge in the central core of BEDT-TTF are correlated through a negative σ charge shift

Anions have often been considered to act essentially as a source or a sink of electrons in molecular conductors. However there is now growing evidence that they play an essential role in directing the structural and hence electronic properties of many of these systems. In this review the basic interactions and different ground states occurring in molecular conductors are considered. How anions influence the structure of donor stacks and often guide them toward different types of transitions (charge and anion ordering transitions, charge and/or spin density waves, etc.) is discussed in detail.

The well-known Bechgaard and Fabre salts are used to illustrate how anions play a crucial role in directing these prototype one-dimensional conductors through complex phase diagrams resulting from the competition between different conducting and localized states. For instance, the anion ordering transitions exert a strong control of the low-temperature transport properties (metallic, spin density wave, superconductivity, etc) of the Bechgaard (TMTSF)$_2$X (X: PF$_6$, ClO$_4$, NO$_3$, etc.) salts. The anions also have a crucial role in imposing the nature of the charge localized and charge ordered phases of the Fabre salts, (TMTSF)$_2$X (X: PF$_6$, ClO$_4$, ReO$_4$, etc.).

Two-dimensional molecular conductors are also subject to the control of anions. The important role played by hydrogen bonding and the conformational flexibility of donors related to BEDT-TTF is illustrated by several examples as for instance: (i) the concerted action of anion shifts and hydrogen bonding modulation in δ-(EDT-TTF-CONMe$_2$)$_2$Br, (ii) the structural and charge ordering instability of α-(BEDT-TTF)$_2$I$_3$, (iii) the puzzling one-dimensional instability of α-(BEDT-TTF)$_2$KHg(SCN)$_4$, and (iv) the role of the anions in the order-disorder and metal to insulator transitions of θ-(BEDT-TTF)$_2$RbM´ (SCN)$_4$ (M´ = Co, Zn) salts.

RL4 SCIENTIFIC HIGHLIGHTS

Electron accumulative molecules: possible candidates for molecular electronics

Metallacarboranylviologen compounds are able to accept up to five electrons and to donate one in single electron steps at accessible potentials and in a reversible way

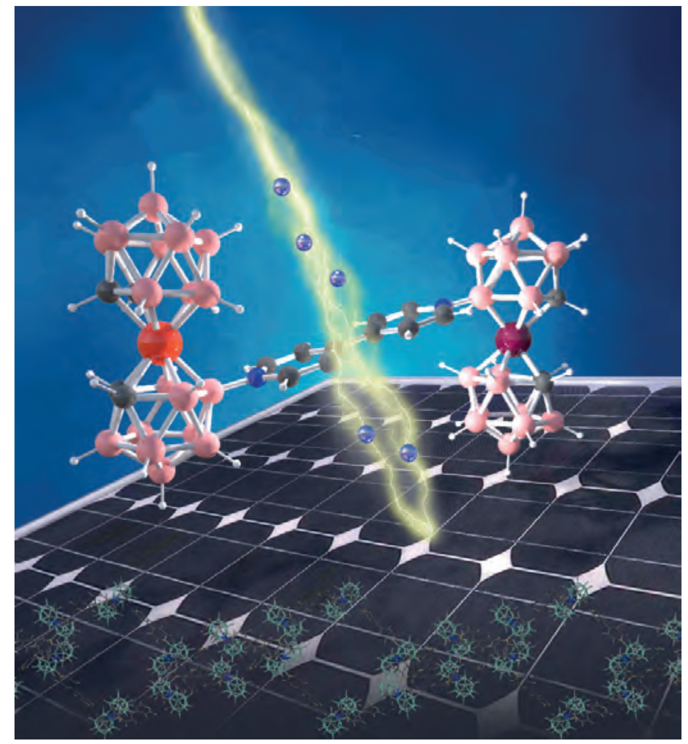
Ana B. Buades,[1] Víctor Sanchez Arderiu,[1] David Olid-Britos,[1] Clara Viñas,[1] Reijo Sillanpää,[2] Matti Haukka,[2] Xavier Fontrodona,[3] Markos Paradinas,[1] Carmen Ocal,[1] and Francesc Teixidor[1]

[1] Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Spain
[2] Dept. of Chemistry, University of Jyväskylä, Finland
[3] Dept. de Química and Serveis Tècnics de Recerca, Universitat de Girona, Spain

Electron Accumulative Molecules.
Journal of the American Chemical Society 140, 2957−2970 (2018).

A procedure leading to the formation of a B-N(aromatic) bond in an anionic sandwich metallabisdicarbollide cluster, [3,3'-M(1,2-C$_2$B$_9$H$_{11}$)2]- (M=Co,Fe,[2]-), was developed. It consists of a parallel decomposition reaction to generate a reactive electrophile and a synthesis reaction to generate the B-N bond. This has paved the way to produce the metallacarboranylviologen [M(C$_2$B$_9$H$_{11}$)(C$_2$B$_9$H$_{10}$)-NC$_5$H$_4$-C$_5$H$_4$N-M'(C$_2$B$_9$H$_{11}$)(C$_2$B$_9$H$_{10}$)] (M=M'=Co, Fe and M= Co and M'=Fe) and semi(metallacarboranyl) viologen [3,3'–M(8-(NC$_5$H$_4$-C$_5$H$_4$N–1,2-C$_2$B$_9$H$_{10}$)(1',2'-C$_2$B$_9$H$_{11}$)] (M=M'=Co, Fe) electron cumulative molecules with Fe, Co or a mix of both.

These molecules are able to accept up to five electrons and to donate one in single electron steps at accessible potentials and in a reversible way. By targeted synthesis and corresponding electrochemical tests, each Electron Transfer (ET) step has been assigned to specific fragments of the molecules. The molecules were carefully characterized and the electronic communication between both metal centers (when this situation applies) has been definitely observed through the co-planarity of both pyridine fragments. The structural characteristics of these molecules imply a low reorganization energy that is a requirement for low energy ET processes. This makes them electronically comparable to fullerenes, but on their side these metallacarboranylviologen compounds are much more soluble than C60 and its derivatives in the same or much related solvents, but most importantly that they offer a wider range of solvents of different nature.



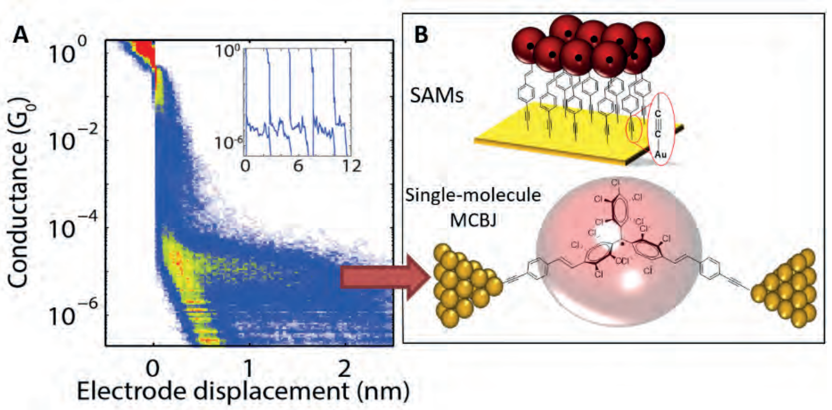
Metallacarboranylviologen compounds, which are much more soluble than C60 and its derivatives, are able to accept up to five electrons and to donate one in single electron steps at accessible potentials and in a reversible way.

The fact that these new compounds are very soluble in common organic solvents makes them possible candidates for molecular electronics and molecular materials in general. The electronic transfer from one molecule to another has been clearly demonstrated as well as their self-organizing capacity. We consider that these molecules thanks to their easy synthesis, ET, self-organizing capacity, wide range of solubility and easy processability can find important application in any area where ET is paramount.

RL4 SCIENTIFIC HIGHLIGHTS

Improving the stability of the electrode-molecule interface

In this work, we show that Au-C bond can provide a robust and well-defined anchoring geometry for single molecule junctions



A 2D conductance vs electrode displacement histogram of the radical molecule constructed from 2500 consecutive traces at RT and 0.2 V bias voltage. The inset shows some selected individual traces. B Scheme of the SAM (top) and MCBJ (bottom) based on the novel organic radical.

Francesc Bejarano,[1] Ignacio Jose Olavarria-Contreras,[2] Andrea Droghetti,[3] Ivan Rungger,[4] Alexander Rudnev,[5,6] Diego Gutierrez,[1] Marta Mas-Torrent,[1] Jaume Veciana,[1] Herre S. J. van der Zant,[2] Concepció Rovira,[1] Enrique Burzurí,[2,7] and Núria Crivillers[1]

[1]Department of Molecular Nanoscience and Organic Materials, Institut de Ciència de Materials de Barcelona (ICMAB- CSIC) and CIBER-BBN, Spain
[2]Kavli Institute of Nanoscience, Delft University of Technology, The Netherlands
[3]Nano-Bio Spectroscopy Group and European Theoretical Spectroscopy Facility (ETSF), Universidad del País Vasco (UPV/EHU), Spain
4 National Physical Laboratory, United Kingdom
[5]Department of Chemistry and Biochemistry, University of Bern, Switzerland
[6]Russian Academy of Sciences A. N. Frumkin Institute of Physical Chemistry and Electrochemistry RAS, Russia
[7]IMDEA Nanoscience, Spain

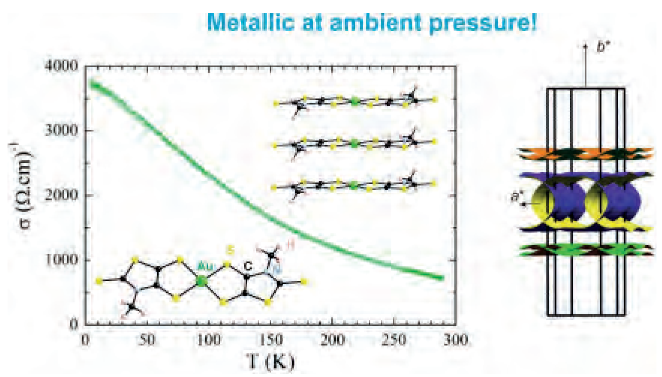
Robust Organic Radical Molecular Junctions Using Acetylene Terminated Groups for C-Au Bond Formation
Am. Chem. Soc. 140, 5, 1691-1696 (2018)

The molecule/electrode contact plays a fundamental role in the performance of molecular electronic devices since it directly affects the charge transport across the interface. The search for a more stable molecule–electrode bond, a well-defined interface geometry, and more conductive interfaces is the driving force to pursue robust and efficient molecule based devices. Interestingly, some recent works have shown that the formation of covalent highly directional σ-bonded C–Au junctions provides high conductance at the single-molecule level. In this field, we are very much interested in exploring organic paramagnetic and electroactive molecules which are attracting interest as core components of molecular electronic and spintronic devices. In this work, we reported the synthesis of a persistent organic radical bearing one and two terminal alkyne groups to spontaneously form Au–C σ bonds. On the one hand, the formation and stability of self-assembled monolayers was achieved and, the electron transport through the SAMs and single-molecule junctions at room temperature was studied. We first demonstrated that the magnetic character is preserved after covalent bonding. Strikingly, it was shown that the investigated system allows for drastic improvements in the reproducibility of single molecule conductance measurements and bond strength when compared to other commonly used contacts such as S-Au. Through a detailed comparison with a similar thiophene functionalized derivative, we proved that the Au–C bond provides a more robust and better-defined anchoring geometry as supported by DFT calculations. Our findings open the door to more reproducible spintronics devices based on multifunctional molecules.

RL4 SCIENTIFIC HIGHLIGHTS

New facets of molecular conductors

Molecular conductors still have many uncovered facets like silver-based single molecule metals and anilate-based small polaron hopping conductors



Temperature dependence of the conductivity (left) and Fermi surface (right) of the single component ambient pressure stable metal, [Au(Me-thiazdt)2].

Yann Le Gal,[1] Thierry Roisnel,[1] Pascale Auban-Senzier,[2] Nathalie Bellec,[1] Jorge Íñiguez,[3] Enric Canadell,[4] Dominique Lorcy,[1] Suchithra Ashoka Sahadevan,[5,6] Alexandre Abhervé,[5] Noemi Monni,[6] Cristina Sáenz de Pipaón,[7] José R. Galán-Mascarós,[7,8] Joao C. Waerenborgh,[9] Bruno J. C. Vieira,[9] Sébastien Pillet,[10] El-Eulmi. Bendeif,[10] Pere Alemany,[11] Maria L. Mercuri,[6] Narcis Avarvari[5]

[1]Université de Rennes, CNRS, ISCR (Institut des Sciences Chimiques de Rennes) - UMR 6226, France
[2]Laboratoire de Physique des Solides UMR 8502, CNRS-Université de Paris-Sud, France
[3]Materials Research and Technology Department, Luxembourg Institute of Science and Technology (LIST), Luxembourg
[4]Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Spain
[5]Laboratoire MOLTECH-Anjou UMR 6200, UFR Sciences, CNRS, Université d'Angers, France
[6]Dipartimento di Scienze Chimiche e Geologiche, Universitá degli Studi di Cagliari, Italy
[7]Institute of Chemical Research of Catalonia, BIST, Spain
[8]ICREA, Spain
[9]Centro de Ciéncias e Tecnologias Nucleares, Instituto Superior Técnico, Universidade de Lisboa, Portugal
[10]Université de Lorraine, CNRS, France
[11]Departament de Ciència de Materials i Química Física and Institut de Química Teórica i Computacional (IQTCUB), Universitat de Barcelona, Spain

[1] Stable metallic state of a neutral radical single-component conductor at ambient pressure.
J. Am. Chem. Soc. 140, 6998-7004 (2018).
[2] Conducting Anilate-Based Mixed-Valence Fe(II)Fe(III) Coordination Polymer: Small-Polaron Hopping Model for Oxalate-Type Fe(II)Fe(III) 2D Networks
J. Am. Chem. Soc. 140, 12611-12621 (2018).

The field of molecular conductors continuously offers new surprises and accomplishments because of the broad tunability range offered by their molecular components. Two of these still uncovered features are the recent preparation of silver-based ambient pressure single molecule metals and anilate-based new two-dimensional semiconductors.

Based on the properties of the two-band conductors it was predicted that stable metals without any doping could exist. This prediction was first confirmed by the preparation of Ni[tmdt]2, a 3D molecular metal. The more challenging preparation of a stable 1D or pseudo-1D metal has been more involved. As a result of a long term experimental-theoretical collaboration between the groups of D. Lorcy (Rennes) and E. Canadell (ICMAB) in order to design the necessary structural and electronic requirements it has been finally possible to prepare and characterize, the first single component ambient pressure stable metal built from chains of neutral radicals, [Au(Me-thiazdt)2]. This system is immune to the ubiquitous Mott and Peierls type instabilities and keeps the room temperature metallic conductivity down to very low temperatures.

The coexistence of electrical conductivity and magnetic ordering in mixed valence FeII/FeIII two-dimensional oxalate-based coordination polymers has recently stimulated a large interest. Up to now the oxalate-based materials were found to be poor conductors. However the related anilate-based systems are very good semiconductors, opening the way towards the preparation of multifunctional conducting materials based on these extended coordination materials.

RL4 SCIENTIFIC HIGHLIGHTS

Halogen interactions and rotor dynamics at the nanoscale

Variable temperature proton spin-lattice relaxation experiments and crystallography as well as DFT calculations decode the complex dynamics of crystalline molecular rotors at the nanoscale

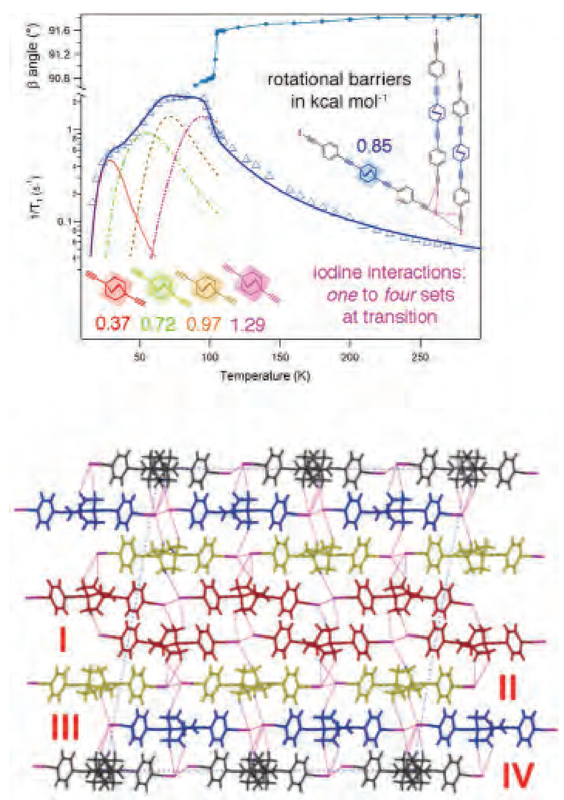
Crystalline arrays of molecular rotors with complex dynamics such as correlated motions and multiple rotational potentials, thermal dynamics coupled to lattice elasticity with a change in the crystal birefringence response or coupled to the electronic response of the system as in switchable dielectrics, and the emerging phenomenon of quantum dissipation addressing the difference of dynamics of the rotors in solids with different electrical properties are of intense current interest. The control of complex dynamic molecular systems at the nanoscale is an essential issue for the development of molecular machines capable of performing useful work. Materials design that includes deliberate use of halogen- and hydrogen-bonding interactions, as well as variable-temperature X-ray and 1H spin-lattice relaxation experiments, and calculations of rotational barriers, provide an in-depth understanding of the switching mechanism of the rotational barriers and of the frequency of associated rotational motion.

We have observed that the monoclinic unit cell of a single crystal of the rod-like molecular rotor shown in the figure, abruptly changes below 105 K, experiencing an expansion by seven times its volume to encompass three and a half independent rotators at 90 K. As a result, after the transition there is a static modulation wave of arrays of halogen interactions. The remarkable finding is that the total 1H spin-lattice relaxation rate of unprecedented complexity to date in molecular rotors, can be decoded, on the basis of DFT calculations which provide understanding on how the H…H and H…I interactions influence the rotational motion, as the weighted sum of the relaxation rates of the four contributing rotors relaxation rates, each with distinguishable exchange frequencies reflecting Arrhenius parameters with different activation barriers and attempt frequencies. This allowed understanding how the dynamics of molecular rotors are able to decode structural information from their surroundings with remarkable nanoscale precision.

Sergey Simonov,[1,2] Leokadiya Zorina,[1,2] Pawel Wzietek,[3] Antonio Rodríguez-Fortea,[4] Enric Canadell,[5] Cécile Mézière,[1] Guillaume Bastien,[1] Cyprien Lemouchi,[1] Miguel A. Garcia-Garibay,[6] and Patrick Batail[1]

[1] Laboratoire MOLTECH-Anjou, CNRS UMR 6200, Université d'Angers, France
[2] Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka, Russia
[3] Laboratoire de Physique des Solides, CNRS UMR 6502, Université de Paris-Sud, France
[4] Departament de Química Física i Inorgànica, Universitat Rovira i Virgili, Spain
[5] Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Spain
[6] Department of Chemistry and Biochemistry, University of California, Los Angeles, USA

Static Modulation Wave of Arrays of Halogen Interactions Transduced to a Hierarchy of Nanoscale Change Stimuli of Crystalline Rotors Dynamics
Nano Letters 18, 3780-3784 (2018)



(top) Variable-temperature ^{1}H spin–lattice relaxation time $T1^{-1}$ at 57 MHz for 1,4-bis((4´-(iodoethynyl)phenyl)ethynyl) bicyclo[2.2.2]octane rotor and curves for each of the four components of the total relaxation (T < Tc).
(bottom) The four different arrays of molecular rotators at 90 K, below the phase transition, because of the static modulation wave of halogen interactions.

RL4 SCIENTIFIC HIGHLIGHTS

Organic electroactive molecules on surfaces for the development of electronic devices

Electroactive molecules assembled on substrates have been employed for the development of: 1) a water actuator that operates at low voltage and 2) a reliable n-type organic field-effect transistor

The self-assembly of organic electroactive molecules on surfaces can lead to the development of advanced electronic devices with additional advantages compared to their inorganic counterparts such as low-cost, compatibility with flexible substrates or low-voltage operation. In this direction, we highlight here two recent works.

In the first work [1], a single self-assembled monolayer of an anthraquinone derivative is covalently anchored on a conducting indium-tin oxide (ITO) substrate. By the application of a voltage, the redox state of the molecule can be switched which, in turn, modifies significantly the wetting properties of the substrate. This effect has been exploited for droplets actuation at low voltage. The device was further integrated in a microfluidic system to perform mixing and dispensing on sub-nanoliter scale. Further, vehiculation of cells across microfluidic compartments was made possible by taking full advantage of surface electrowetting in culture medium.

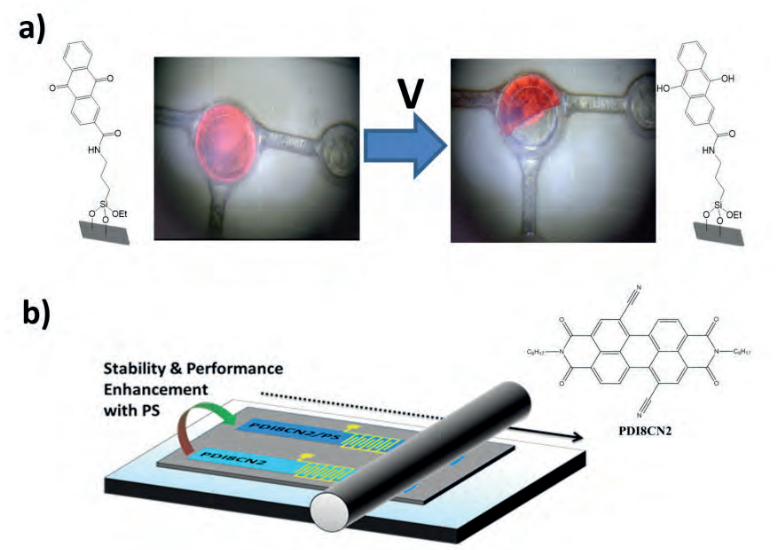
In the second work [2], crystalline thin films of organic electroactive molecules can be applied as active semiconducting materials in field-effect transistors (OFETs). In particular, solution-processed n-type OFETs are essential elements for developing large-area, low-cost, and all organic logic/complementary circuits. Nonetheless, the development of air-stable n-type organic semiconductors (OSCs) lags behind their p-type counterparts. The trapping of electrons at the semiconductor–dielectric interface leads to a lower performance and operational stability. In this second work, we report printed small-molecule n-type OFETs based on a blend of an electron acceptor molecule with a binder insulating polymer. The latter enhances the device stability due to the improvement of the semiconductor–dielectric interface quality and a self-encapsulation of the OSC. Both combined effects prevent the fast deterioration of the device.

Maria Serena Maglione,[1] Antonio Campos,[1] Sergi Galindo-Riera,[1] Joaquim Puigdollers,[2] Stefano Casalini,[1] Stamatis Georgakopoulos,[1] Marianna Barbalinardo,[3] Vitaliy Parkula,[3] Núria Crivillers,[1] Concepció Rovira,[1] Pierpaolo Greco,[3] Marta Mas-Torrent[1]

[1]Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Spain
[2]Department Enginyeria Electrònica, Universitat Politècnica de Catalunya, Spain
[3]Scriba Nanotecnologie, Italy

[1] Fluid Mixing for Low-Power 'Digital Microfluidics' Using Electroactive Molecular Monolayers, Small, 1703344 (2018).

[2] Reduction of Charge Traps and Stability Enhancement in Solution-Processed Organic Field-Effect Transistors Based on a Blended n-Type Semiconductor, ACS Appl. Mater. Interfaces, 10, 18, 15952 (2018).



A) Microfluidic system embedded on an ITO surface functionalized with a self-assembled monolayer of an anthraquinone derivative. Upon de application of a voltage the molecules are reduced and the water actuation is controlled.
B) Deposition of the organic semiconductor PDI8CN2 by bar-assisted meniscus shearing. The blending of the material with polystyrene (PS) enhances the device response

RL4 SCIENTIFIC HIGHLIGHTS

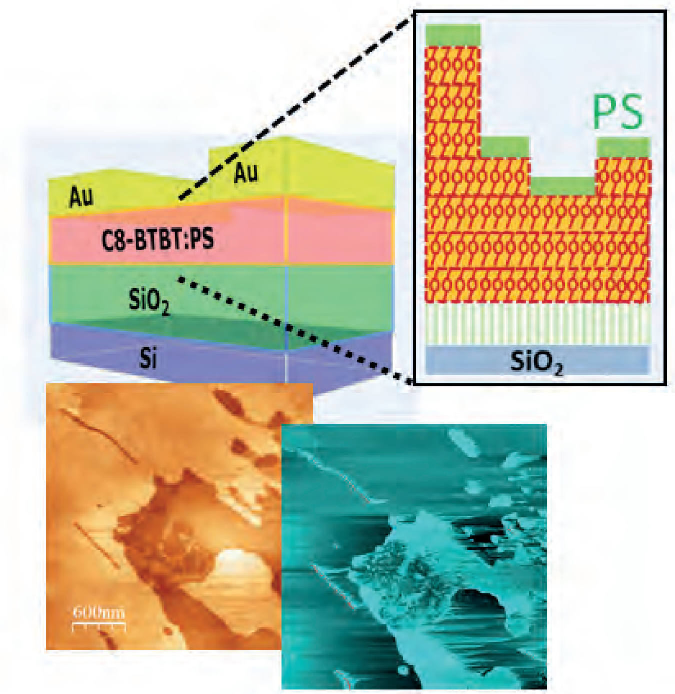
Nanoscale phase separation of organic blends as key for high-performance OFETs

Ana Pérez-Rodríguez,[1] Inés Temiño,[1] Carmen Ocal,[1] Marta Mas-Torrent,[1,2] Esther Barrena[1]

[1]Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Spain
[2]CIBER-BBN, Spain

Decoding the Vertical Phase Separation and Its Impact on C8-BTBT/PS Transistor Properties
ACS Applied Materials & Interfaces, 10, 8, 7296-7303 (2018)

The nanoscale investigation of OFETs by means of a combination of FFM and KPFM allows unveiling the nanoscale phase separation in organic blend that play a major role in the high-performance of solution-processed OFETs and identifying optimization routes



Schematic view of the three-layer stratification in the blend. Topography lateral force image by FFM (blue image) showing the frictional contrast caused by the two materials in the blend

As core component of integrated circuits, the realization of high-performance organic field effect transistors (OFETs) from solution processing requires uniform and crystalline films with optimal electronic properties. One of the advances in the solution manufacturing process is raised from the idea of blending small conjugated semiconductor molecules with an amorphous insulating polymer to combine the advantageous properties of the individual components. This strategy has led to an overall rise in the charge carrier mobility and an improvement of device processability, reproducibility, and stability [1]. The key of superior performance of OFETs fabricated with blended films seems to be the spontaneous vertical phase separation of the two material components. In this article we elucidate the structural details at nanoscale level of blends based on a relevant OSC, 2,7-dioctyl[1]-benzothieno[3,2-b][1]benzothiophene (C8-BTBT) and polystyrene (PS) by employing friction force microscopy (FFM) to identify the two different blend constituents [2]. The results reveal a three-layer stratification: a C8-BTBT crystalline layer (for efficient carrier transport) sandwiched between two PS layers, one at the bottom acting as a passivating dielectric layer and a PS-rich skin layer on the top (⊠1 nm) conferring stability to the devices. The investigation of the electronic properties at the nanoscale by Kelvin Probe Force Microscopy (KPFM) demonstrates that contact resistance is the critical factor limiting the device performance, which is significantly improved by doping the contacts with a molecular dopant. Our findings, obtained via a combination of FFM and KPFM, allows identifying optimization routes for high-throughput solution-processed OFETs.

[1] Temiño, I.; Del Pozo, F. G.; Ajayakumar, M. R.; Galindo, S.; Puigdollers, J.; Mas-Torrent, M. A. Adv. Mater. Technol. 2016, 1, 1600090
[2] Yuan, Y.; Giri, G.; Ayzner, A. L.; Zoombelt, A. P.; Mannsfeld, S. C. B.; Chen, J.; Nordlund, D.; Toney, M. F.; Huang, J.; Bao, Z. Nat. Commun. 2014, 5, 3005

RL4 SCIENTIFIC HIGHLIGHTS

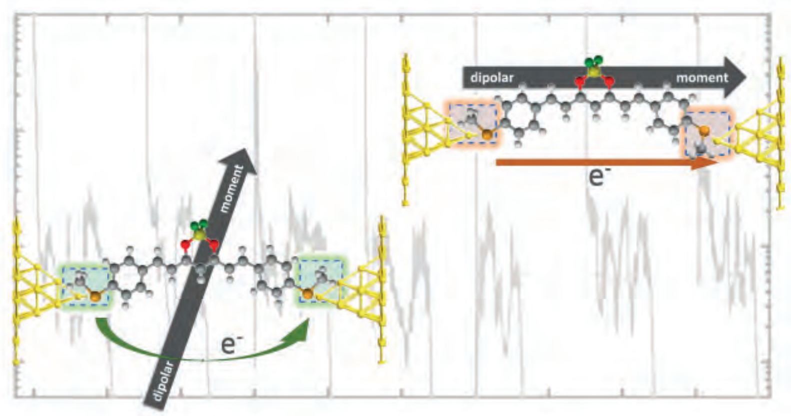
Boron-(β-diketone) compounds foster interplay between applied bias voltage and molecular dipole toward the achievement of bistability conductance measurements

Ignacio José Olavarría-Contreras,[1] Alvaro Etcheverry-Berríos,[2] Wenjie Qian,[3] Cristian Gutiérrez-Cerón,4 Aldo Campos-Olguín,[2] E. Carolina Sañudo,[5,6] Diana Dulić,[4] Eliseo Ruiz,[5,7] Núria Aliaga-Alcalde,[3,8] Monica Soler[2] and Herre S. J. van der Zant[1]

[1]Kavli Institute of Nanoscience, Delft University of Technology, The Netherlands.
[2]Departamento de Ingeniería Química, Biotecnología y Materiales, Facultad de Ciencias Físicas y Matemáticas, Universidad de Chile, Chile
[3]Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Spain
4Departamento de Física, Facultad de Ciencias Físicas y Matemáticas, Universidad de Chile, Chile
[5]Departament de Química Inorgànica i Orgànica, Universitat de Barcelona, Spain
[6]Institut de Nanociència i Nanotecnologia, Universitat de Barcelona, Spain
[7]Institut de Química Teòrica i Computacional, Universitat de Barcelona, Spain
[8]ICREA (Institució Catalana de Recerca i Estudis Avançats), Spain

Electric-field induced bistability in single-molecule conductance measurements for boron coordinated curcuminoid compounds
Chem. Sci., 9, 6988-6996 (2018)

MCBJ measurements show the possibility of having two conductance states in the same trace experiment by studying a boron-curcuminoid compound which different conformations rise to changes in the molecular dipole moment meanwhile measuring providing the observed bistability



Left. Schematic illustration of some of the most common solution shearing deposition techniques. Right. 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

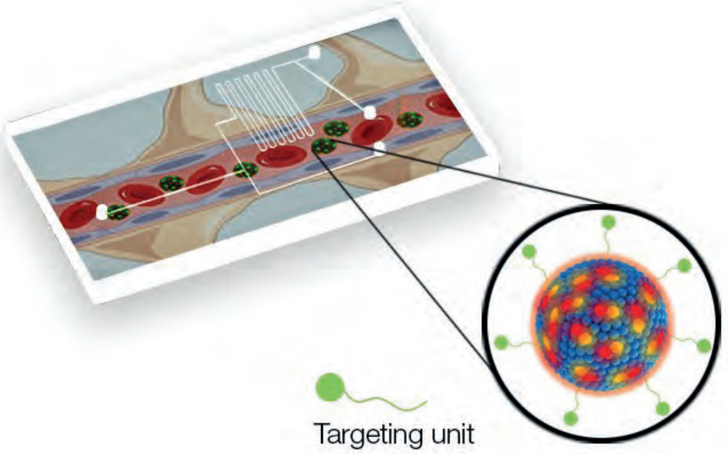
Mechanically-controlled break junction (MCBJ) experiments in a family of curcuminoid molecules (CCMoids) was explored. Single electron transport information was gathered using them as nanowires sandwiched between Au electrodes. The molecular set was formed by CCMoids with different S-based ending groups (MeS-, RS- (R = S-thiocarbamate) and 3-Thiophene-) akin to the electrodes and the coordination compounds achieved by the binding of CuII and BF2 moieties to such organic molecules. The nature of the side groups provided a gradient of conductance values where RS- sites gave conductance values one order of magnitude higher than the MeS- analogs. The coordination to CuII with respect to the free ligand did not provided drastic changes in the electronic transport; however, in the case of the MeS-CCM-BF2 system, the switching between two conductance values in individual traces was observed. The sum of additional MCBJ experiments in an extended family of molecules and the use of theoretical calculations, (providing models of the systems attached to the electrodes) revealed the relationship between the orientation of the dipole moment of the molecules within the junction and the bistability measurements

RL5 SCIENTIFIC HIGHLIGHTS

Stable fluorescent nanovesicles as new probes for bioimaging

New fluorescent nanovesicles have been developed, using compressed $C0_2$ technology developed in-house, to produce efficient probes for bioimaging applications

In the frame of a Marie-Curie Initial Training Network (ITN), Nano-2-fun, new fluorescent nanoparticles with superior stability and remarkable optical properties, bearing fluorescent organic dyes, have been developed. These fluorescent nanovesicles have already proved to be efficient probes for in vivo and in vitro imaging and have potential applications as biomarkers in bio-imaging, diagnostic, biomedical applications and theranostics [1](combined therapeutic and diagnostic functionalities). The preparation of the fluorescent nanovesicles offers a great potential for the development of multifunctional nanovesicles integrating for example drugs (such as proteins, small molecules or even genetic material), targeting peptides, and fluorescent imaging agents. Moreover, the fluorescent nanovesicles can incorporate simultaneously several dyes, obtaining probes for more complex applications, such as multicolour imaging. This platform is especially effective for the conveyance of non-water-soluble dyes whose optical properties are usually not stable in physiological media, but remain efficient after incorporation in nanovesicles [2].

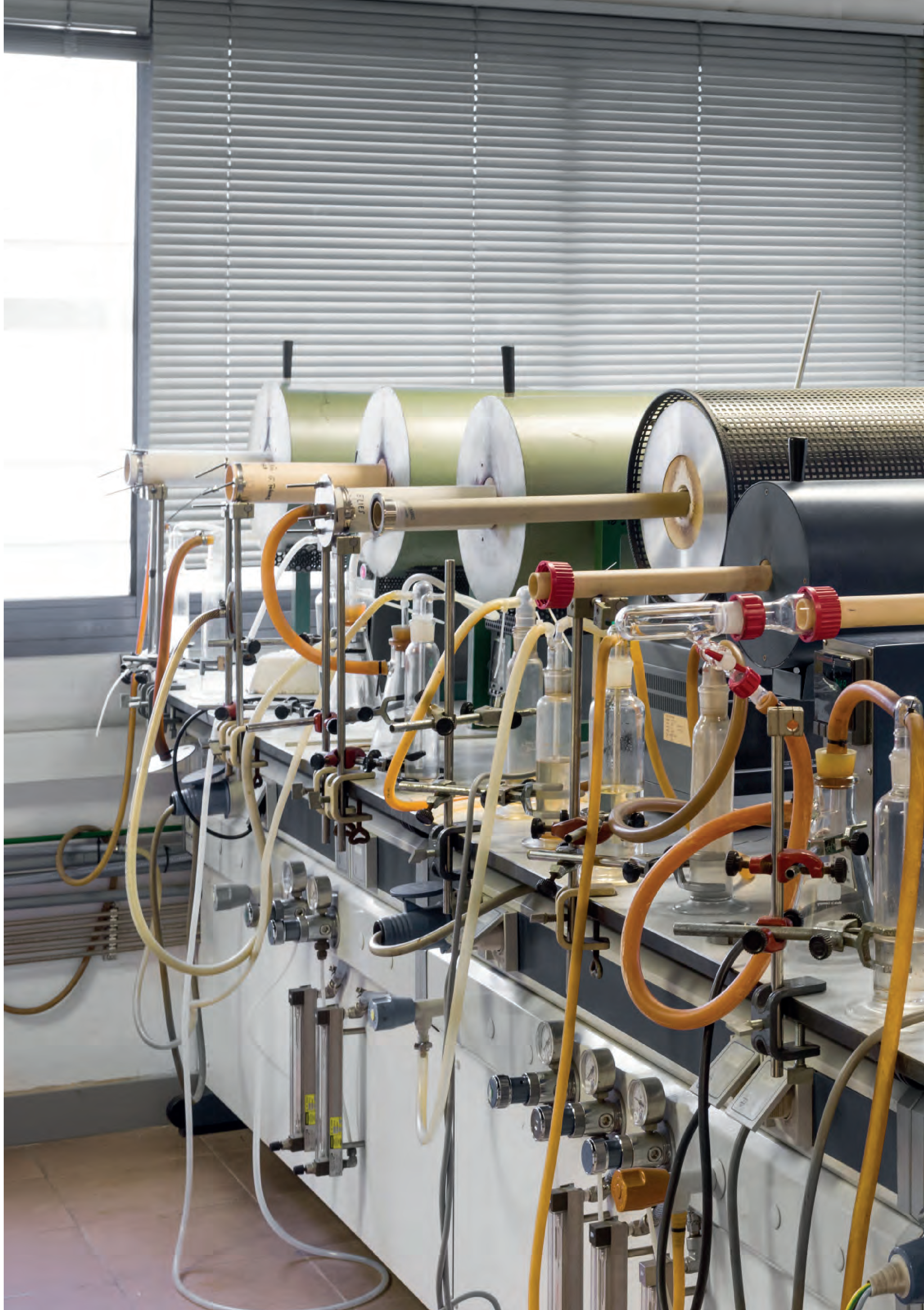


Example of the use of the new developed fluorescent nanovesicles, embed in an in vitro diagnostic assay, specifically an organ-on-chip simulating endothelial cells environment

Antonio Ardizzone,[1] Davide Blasi,[1] Siarhei Kurhuzenkau,[2] Danilo Vona,[3] Sílvia Illa-Tuset[1,4] Arnulf Rosspeintner,[5] Jordi Faraudo,[1] Angela Punzi,[3] Mykhailo Bondar,[6] Emiliano Altamura,[3] David Hagan,[7] Natascia Grimaldi,[1] Eric W. Van Stryland,[7] Anna Painelli,[2] Cristina Sissa,[2] Santi Sala,[1] Natalia Feiner,[8] Eric Vauthey,[5] Lorenzo Albertazzi,[8] Gianluca M. Farinola,[3] Imma Ratera,[1] Jaume Veciana,[1] and Nora Ventosa,[1].

[1] Institut de Ciències de Materials de Barcelona (ICMAB-CSIC), Spain.
[2] Dipartimento di Scienze Chimiche, della Vita e della Sostenibilità Ambientale Università di Parma, Italy.
[3] Dipartimento di Chimica Università degli Studi di Bari Aldo Moro, Italy.
[4] Theoretical Sciences Unit, JNCASR, India.
[5] Department of Physical Chemistry, University of Geneva, Switzerland.
[6] Institute of Physics, National Academy of Sciences of Ukraine, Ukraine.
[7] The College of Optics and Photonics (CREOL), University of Central Florida, USA
[8] Institute of Bioengineering of Catalonia (IBEC), Spain

[1] Highly Stable and Red-Emitting NanovesiclesIncorporatingLipophilic Diketopyrrolopyrroles for Cell Imaging, Chemistry a European Journal 24, 11386 - 11392 (2018)
[2] Nanostructuring Lipophilic Dyes in Water Using Stable Vesicles, Quatsomes, as Scaffolds and Their Use as Probes for Bioimaging Small 14 1703851 (2018)



RL5 SCIENTIFIC HIGHLIGHTS

Quatsomes as a topical delivery platform

We report the study of a topical drug delivery platform and how it can tune its mechanical properties, depending on the micro-surrounding and constituting molecules.

Visual representation of a future product based on Quatsomes for the topical delivery of pharmaceutical or cosmetic ingredients

Berta Gumí-Audenis,[1, 2 3] Sílvia Illa-Tuset[4], Luca Costa,[5] Natascia Grimaldi,[4, 6] Laia Pasquina-Lemonch,[1, 4] Lidia Ferrer-Tasies6, Fausto Sanz,[1,2,3] Jaume Veciana,[3, 4] Imma Ratera,[3, 4] Jordi Faraudo,[4] Nora Ventosa,[3, 4] and Marina I. Giannotti,[1, 2, 3]

[1]Institute for Bioengineering of Catalonia (IBEC), The Barcelona Institute of Science and Technology (BIST), Spain.
[2]Departament de Ciència dels Materials i Química Física, Universitat de Barcelona, Spain.
[3]Centro de Investigación Biomédica en Red (CIBER), Spain.
[4]Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Spain.
[5]Centre de Biochimie Structurale (CBS), CNRS UMR 5048–UM–INSERM U 1054, France.
6Nanomol Technologies SL, Mòdul de Recerca B, Campus Universitari de Bellaterra, Spain.

[1] Insights into the structure and nanomechanics of aquatsome membrane by force spectroscopymeasurements and molecular simulations, Nanoscale , 10, 23001 - 23011, 2018.
[2] Pulling lipid tubes from supported bilayers unveilsthe underlying substrate contribution to themembrane mechanics, Nanoscale, 10, 14763 - 14770, 2018.

The response of cells to the exposure of nanomaterials is crucial for determining their safety in their multiple uses; however, the majority of the in vitro experiments use monolayered cell cultures, 2D cell cultures. Multiple studies highlight the different toxicological response, phenotype, metabolism and composition of cells grown on 2D systems (petri dishes, plastic flat surfaces) compared to their growth in 3D systems, a more realistic environment.

3D in vitro cell culture approaches emerged to obtain in vitro cell culture systems that recapitulate realistically and physiologically the environment of cells and to increase the applicability of NPs and drugs. These 3D in vitro approaches also aim at reducing and optimizing the translation of new drugs to the market following the three R notion (Replace, Reduce and Refine).

Here, we have analyzed how the exposed surface of the cells, as well as the environment where cells grow, can influence the interaction and uptake of superparamagnetic iron oxide nanoparticles (SPIONs). We exposed three different cell lines (MDAMB-231, HL60 and bEnd3) grown at different environments with increasing concentrations of SPIONs. We evaluated parameters analyzing the morphological changes of the cell, iron uptake and cell viability. Results showed that upon exposure to SPIONs, cell viability and morphology are more affected when cells are growing in 3D systems, indicating that the increase of exposed surface area of the cells is a strong parameter to take in account when evaluating SPIONs or other materials or drugs. Our results clearly reinforce the use of more realistic environments, such as 3D, for the design of new drug delivery systems.

RL5 SCIENTIFIC HIGHLIGHTS

Spherical and hollow bacterial cellulose structures; a novel material to promote long-term stemness of mouse embryonic stem cells (mESC)

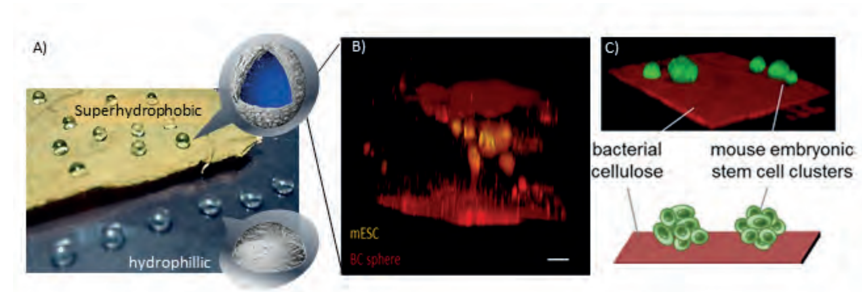
Taking advantage of hydrophobic surfaces and in a single step, we produced 3D hollow cellulose structures. We also showed that bacterial cellulose promotes the long-term maintenance of stemness in mouse embryonic stem cell

Anna Laromaine,[1] Tina Tronser,[2] Ivana Pini,[2] Sebastià Parets,[1] Pavel A. Levkin[2,3] and Anna Roig[1]

[1]Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Spain
[2]Institute of Toxicology and Genetics, Karlsruhe Institute of Technology (KIT), Germany
[3]Institute of Organic Chemistry, Karlsruhe Institute of Technology (KIT), Germany

Bacterial Cellulose Promotes Long-Term Stemness of mESC
ACS Applied Materials & Interfaces10, 19, 16260-16269 (2018)

Free-standing three-dimensional hollow bacterial cellulose structures with controlled geometry via patterned superhydrophobic-hydrophilic surfaces
Soft Matter, 14, 3955-3962 (2018)



A) Image indicating the hydrophobic-hydrophilic surfaces to grow of bacterial cellulose.3D structures. B) 3D reconstruction of confocal images (overlay) showing mESC growing within the structure after two days of culture. Scale bar 100 µm. Red color: Safranin O, BC sphere; yellow color: GFP, mESC Oct4-eGFP. C) Three-dimensional reconstruction of confocal images of mESC Oct4-eGFP (green) cultured on BC (red) indicating the no-differentiation of the stem cells and maintenance of the stemness

Cellulose, one of the most abundant biopolymer on earth, emerges as a green, sustainable and natural material for many industrial applications. Especially interesting is the biosynthesized cellulose produced by organisms which represent a suitable alternative to manufacture biodegradable and renewable materials with low energy consumption.

Production of 3D freestanding structures with control in shape and made of biocompatible polymers entails high complexity; however these structures show great potential in tissue engineering, as soft 3D cell scaffolds or as drug delivery systems. The *Soft Matter* publication presents an in situ single-step process to produce self-standing 3D-BC structures with controllable wall thickness, size and geometry made of bacterial cellulose (BC). Hollow spheres and convex domes could be easily obtained by tuning the hydrophobicity of the surfaces and interestingly, mouse embryonic stem cells (mESC) could be cultivated inside. Moreover, volume of the inoculum and time of culture further define the resulting 3D-BC structures.

The ACS Appl. Mater. Interfaces manuscript reports for the first time on the use of bacterial cellulose films to inhibit the differentiation of mESC for many days improving the cultivation of mouse embryonic fibroblast (MEF)-free in comparison to the MEF-supported conventional culture. Stem cells possess unique properties, such as the ability to self-renew and the potential to differentiate into a various cell types. These make them highly valuable in regenerative medicine and tissue engineering. In this work, also showed that the culture of mESCs on these flexible, free-standing BC membranes enable the quick and facile manipulation and transfer of stem cells between culture dishes, both of which significantly facilitate the use of stem cells in routine culture and various applications.

Witold I. Tatkiewicz,[1,2] Joaquin Seras-Franzoso,[2,3] Elena Garcia-Fruitós,[2,3] Esther Vazquez,[2,3] Adriana R. Kyvik,[1,2] Judith Guasch,[1,2,4] Antonio Villaverde,[2,3] Jaume Veciana,[1,2] Imma Ratera[1,2,4]

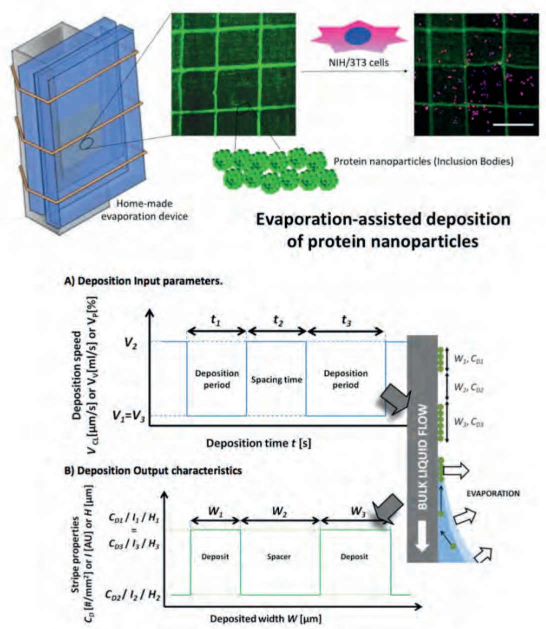
[1]Institut de Ciència de Materials de Barcelona (CSIC), Spain
[2]Centro de Investigación Biomédica en Red de Bioingeniería, Biomateriales y Nanomedicina (CIBER-BBN), Spain
[3]Institut de Biotecnologia i de Biomedicina (IBB) and Departament de Genètica i de Microbiologia, UAB, Spain
[4]Dynamic Biomaterials for Cancer Immunotherapy, Max Planck Partner Group, ICMAB-CSIC, Spain

Surface-Bound Gradient Deposition of Protein Nanoparticles for Cell Motility Studies, ACS Applied Materials & Interfaces, 10, 25779–25786 (2018)

RL5 SCIENTIFIC HIGHLIGHTS

Decoration of surfaces *à la carte* with gradients of protein nanoparticles for high-throughput studies on cell motility

A versatile evaporation-assisted methodology based on the coffee-drop effect is described to deposit nanoparticles on surfaces, obtaining for the first time patterned gradients of protein nanoparticles (pNPs) by using a simple custom-made device



Top. Left: Schematic view of the custom-made device designed for evaporation-assisted pattern deposition of pNPs. Right: Substrate functionalized with pNP of the Green Fluorescent Protein (GFP) at different concentrations and gradients used for high-throughput cell motility studies. Bottom. Scheme of an operational protocol consisting of three consecutive steps (i = 1, 2, 3) with deposition input parameters (Vi) and output characteristics (CDi, Ii, or Hi), presented on separate plots, resulting in the deposition of three stripes.

Cells accommodate to their external environment and therefore to various stimuli such as ramps of soluble biomolecules and gradients of topography or stiffness by moving to their preferred conditions. Reproducing these gradients in vitro is one of the most popular and effective approaches to study cell motility. There is no straightforward technique that allows obtaining surface-bound protein particle gradients from their colloidal suspensions. One way to tackle this shortcoming is the emerging field of evaporation-assisted deposition methods, based on the widely known "coffee-drop effect".

Protein Nanoparticles (pNPs) are nontoxic and mechanically stable particles with sizes ranging from ca. 50 to 500–600 nm. They have functional amyloid structure and are under exploration as drug delivery systems and as biochemical and topographical modifiers of surfaces at nanoscales and microscales for cell-guiding studies. We have previously used these materials for surface decoration with geometrical patterns at constant pNP concentrations for cell guidance. Nevertheless, to the best of our knowledge, they have not been used to produce surface-bound gradients of pNPs.

In this work, a versatile evaporation-assisted methodology based on the coffee-drop effect is described to deposit nanoparticles on surfaces, obtaining for the first time patterned gradients of protein nanoparticles (pNPs) by using a simple custom-made device. In this way, fully controllable patterns with specific periodicities consisting of stripes with different widths and distinct nanoparticle concentration as well as gradients can be produced over large areas (~10 cm2) in a fast (up to 10 mm2 /min), reproducible, and cost-effective manner using an operational protocol optimized by an evolutionary algorithm. This method can be readily applied to a flat surface, that is, it does not require masks, stamps, replicas, surface functionalizations, or any other type of labelling. The developed method opens the possibility to decorate surfaces "a-la-carte" with pNPs enabling different categories of high-throughput studies on cell motility.

Maria Milla, Si-Ming Yu, Anna Laromaine

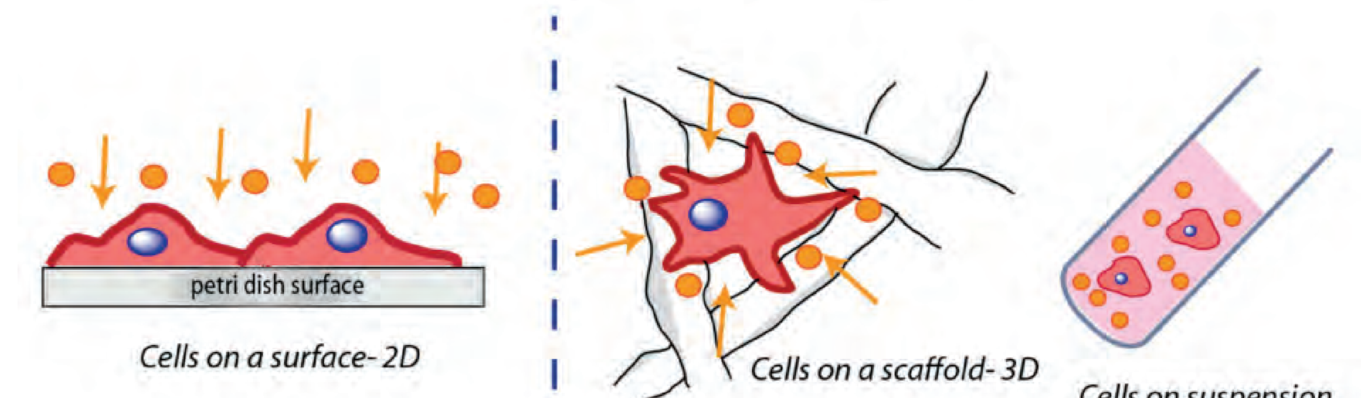
Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Spain

Parametrizing the exposure of superparamagnetic iron oxide nanoparticles in cell cultures at different in vitro environments
Chemical Engineering Journal 340, 173-180, (2018)

RL5 SCIENTIFIC HIGHLIGHTS

Iron oxide nanoparticles evaluated in vitro at different 2D and 3D cell culture environments

Exposed surface area of cells is an essential parameter to take in account in the evaluation of toxicity of nanomaterials



A 2D conductance vs electrode displacement histogram of the radical molecule constructed from 2500 consecutive traces at RT and 0.2 V bias voltage. The inset shows some selected individual traces. B Scheme of the SAM (top) and MCBJ (bottom) based on the novel organic radical.

The response of cells to the exposure of nanomaterials is crucial for determining their safety in their multiple uses; however, the majority of the in vitro experiments use monolayered cell cultures, 2D cell cultures. Multiple studies highlight the different toxicological response, phenotype, metabolism and composition of cells grown on 2D systems (petri dishes, plastic flat surfaces) compared to their growth in 3D systems, a more realistic environment.

3D in vitro cell culture approaches emerged to obtain in vitro cell culture systems that recapitulate realistically and physiologically the environment of cells and to increase the applicability of NPs and drugs. These 3D in vitro approaches also aim at reducing and optimizing the translation of new drugs to the market following the three R notion (Replace, Reduce and Refine).

Here, we have analyzed how the exposed surface of the cells, as well as the environment where cells grow, can influence the interaction and uptake of superparamagnetic iron oxide nanoparticles (SPIONs). We exposed three different cell lines (MDAMB-231, HL60 and bEnd3) grown at different environments with increasing concentrations of SPIONs. We evaluated parameters analyzing the morphological changes of the cell, iron uptake and cell viability. Results showed that upon exposure to SPIONs, cell viability and morphology are more affected when cells are growing in 3D systems, indicating that the increase of exposed surface area of the cells is a strong parameter to take in account when evaluating SPIONs or other materials or drugs. Our results clearly reinforce the use of more realistic environments, such as 3D, for the design of new drug delivery systems.

Nuria Portolés-Gil,[1] Arianna Lanza,[2] Núria Aliaga-Alcalde,[1,3] José A. Ayllón,[4] Mauro Gemmi,[2] Enrico Mugnaioli,[2] Ana M. López-Periago[1] and Concepción Domingo[1]

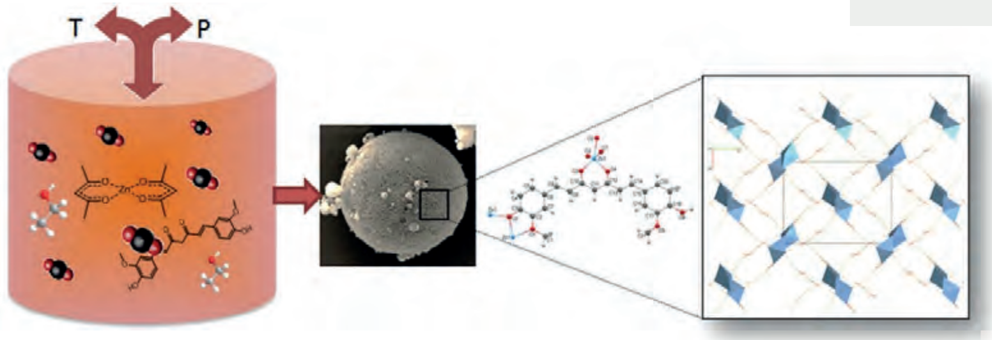
[1]Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Spain
[2]Center for Nanotechnology Innovation@ NEST, Istituto Italiano di Tecnologia, Italy
[3]ICREA, Institució Catalana de Recerca i Estudis Avançats, Spain
[4]Departamento de Química Analítica, Universidad de Barcelona, Spain

Crystalline Curcumin bioMOF Obtained by Precipitation in Supercritical CO_2 and Structural Determination by Electron Diffraction Tomography
ACS Sustainable Chemistry & Engineering, 6, 12309-12319 (2018)

RL5 SCIENTIFIC HIGHLIGHTS

Preparation of curcumine bio-metal-organic-frameworks (bio-MOFs)

This article analyses the use of supercritical CO_2 green technology in the reactive crystallization processes of a bio-MOF composed by curcumin and Zn (II) metal centres



Scheme of the formation of curcumin–based bio-MOF and its crystal structure

The attained success in controlling the structure, functionality and porosity of MOFs materials has led to the development of numerous applications, most notably in gas adsorption, energy conversion and storage, and medicine. Medical applications would require constructions made of biocompatible building blocks, which drive on the development of the topic of metal–biomolecule frame-works or bioMOFs. In this article, a new phase with a [Zn(curcumin)]n composition, termed sc-CCMOF-1, is presented. In previous research we have demonstrated that 1D to 3D coordination polymers can be prepared in scCO2 through reactive crystallization by the right choice of building blocks with suitable solubility in this fluid.

In this case, the developed $scCO_2$ methodology allowed the precipitation in high yields of the small-sized crystalline material, which was characterized by the use of the recently developed electron diffraction tomography method applied to the resolution of sub-micrometric crystals. A remarkable 3D macrostructure with a complex morphology was obtained.

To analyse the crystallization mechanism, multiple identical runs were performed under similar experimental conditions to study in each time period the crystal growth progress ex-situ by X-ray diffraction and scanning electron microscopy. These experiments indicated that the process to achieve the sc-CCMOF-1 in a crystalline form involves the formation of amorphous or semi-crystalline metastable phases that derived into hierarchical stable and crystalline nano-flower aggregates. In addition, a potential therapeutic application of the bio-MOF was tested by studying the released of the curcumin molecule at neutral pH. The obtained results indicate that the curcumin dissolution process was faster from the synthesized MOF than from the pristine curcumin. The dynamic micro-porosity of the bio-MOF appears to provide the advantage of speeding dissolution by facilitating water diffusion to the interior of the bioMOF, thus increasing the bioavailability.

Isabel Fuentes,[1] Tania García-Mendiola,[2] Shinichi Sato,[3] Marcos Pita,[2] Hiroyuki Nakamura,[3] Encarnación Lorenzo,[2] Francesc Teixidor,[1] Fernanda Marques,[4] and Clara Viñas[1]

[1] Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Spain.
[2] Departamento Química Analítica y Análisis Instrumental, Universidad Autónoma de Madrid, Spain
[3] Laboratory for Chemistry and Life Science, Institute of Innovative Research, Tokyo Institute of Technology, Japan.
[4] Centro de Ciências e Tecnologias Nucleares (C2TN), Instituto Superior Técnico, Universidade de Lisboa, Portugal.

Metallacarboranes on the road to anticancer therapies: cellular uptake, DNA interaction and biological evaluation of cobaltabisdicarbollide ([COSAN]-).
Chemistry-A European Journal 2018, 24, 17239 – 17254

Free-standing three-dimensional hollow bacterial cellulose structures with controlled geometry via patterned superhydrophobic-hydrophilic surfaces
Soft Matter, 14, 3955-3962 (2018)

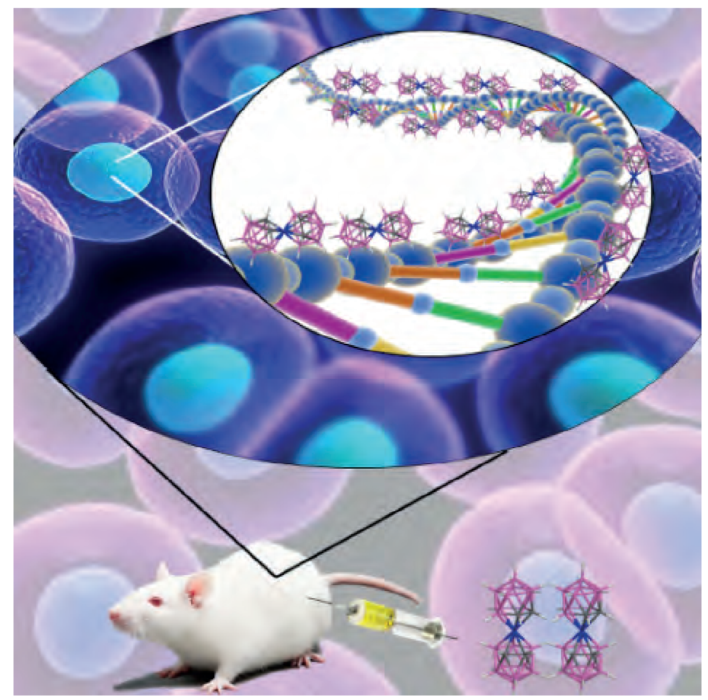
RL5 SCIENTIFIC HIGHLIGHTS

Metallacarboranes on the road to anticancer therapies

This work demonstrates that the pristine Na[3,3'-M(1,2-closo-$C_2B_9H_{11})_2$], [COSAN]-, molecules enter into the cells cytoplasm reaching the nucleus The strong interaction between Na[COSAN] and CT-dsDNA has been demonstrated and the formed nanohybrid biomaterial fully characterized. The non-cytotoxic profile of [COSAN]- has been demonstrated on V79 fibroblast cells.

The most studied metallacarborane is cobaltabisdicarbollide [3,3'-M(1,2-closo-C_2B_9H11)2]- (M= Co, Fe) that are metal sandwich complexes similar to ferrocene and as this one, have a nice reversible electroactive couple, M^{3+}/ M^{2+}, but unlike ferrocene they are water-soluble. Metallacarboranes are becoming a subject of growing interest to the broad chemical community owing to their unique combination of features and properties, including the rigidity of the cages and their relative rotary motion, hydrophobicity, as well as chemical and thermal stability due to delocalized charge.

Herein we focus on the studies of relevant tumor cell uptake and intracellular [COSAN]- distribution by cells, its accumulation in the cell nucleus, which is a particularly desirable target, because the nucleus is the cells' control center in which DNA and transcription machinery reside. The interaction of [COSAN]- with DNA is detailed studied. The interaction of [Na·2.5H_2O][COSAN] with double stranded calf thymus DNA in aqueous solutions and physiological media by spectroscopic measurements (IR and RAMAN) is studied in detail. Once proved the interaction, melting temperature, ultraviolet-visible spectrophotometry, cyclic voltammetry, circular dicroism, dynamic light scattering and 11B{1H} NMR techniques have been used to discern on the nature of such interaction, which is intercalative or electrostatic depending on the ionic strength of the solution. Optical and electronic microscopies (TEM and CryoTEM) displayed better understanding of this interaction with regard to its potential applications. Finally, biodistribution studies of the Na[COSAN] in normal mice were run. After administration, Na[COSAN] was distributed into many organs but mainly accumulates in the RES, including liver and spleen. At 1h the formation of aggregates by plasma protein interaction play a role in the biodistribution profile accumulating mostly in the lungs. Na[COSAN], which display low toxicity and high uptake by relevant cancer cells accumulating boron within the nucleus, could act as a suitable compound for further developments as BNCT agents.

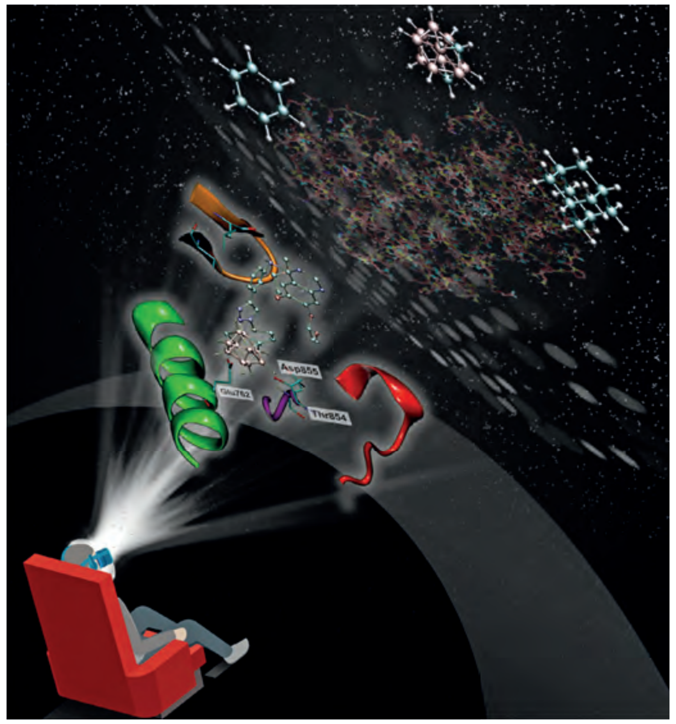


[3,3'-Co(1,2-closo-$C_2B_9H_{11})_2$]-, which can self-assembly and present no relevant cytotoxicity, interacts with ds-DNA

RL5 SCIENTIFIC HIGHLIGHTS

Potential boron-based drugs for glioma treatment

This work demonstrates that Erlotinib-decorated with 3D-boron-rich-cluster resulted in an anti-EGFR lead molecule with IC50 value of 2.3 nM, 10-fold higher than the parent Erlotinib.



The comparative docking analysis of EGFR inhibitor incorporating closo-carborane with compounds bearing bioisoster-substructures, demonstrated the relevance of the 3D aromatic-boron-rich moiety for interacting into the EGFR ATP binding region.

Marcos Couto,[1,2,3] María Fernanda García,[3] Catalina Alamón,[1] Mauricio Cabrera,[4] Pablo Cabral,[3] Alicia Merlino,[5] Francesc Teixidor,[2] Hugo Cerecetto[1,3] and Clara Viñas[2]

[1] Grupo de Química Medicinal, Lab. Química Orgánica, Fac. de Ciencias, Univ. de la República Iguá. Uruguay.
2 Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Spain.
[3] Área de Radiofarmacia, Centro de Investigaciones Nucleares, Fac. Ciencias, Univ. de la República, Uruguay.
[4] Lab. I + D Moléculas Bioactivas, Centro Universitario Paysandú, CenUR Litoral Norte, Univ. de la República, Uruguay.
[5] Lab. Química Teórica y Computacional, Instituto de Química Biológica, Fac. Ciencias, Univ. de la República, Uruguay.

[1] Discovery of Potent EGFR Inhibitors through the Incorporation of a 3D-Aromatic-Boron-Rich-Cluster into the 4-Anilinoquinazoline Scaffold: Potential Drugs for Glioma Treatment.
Chemistry-A European Journal 24, 3122 – 3126 (2018)

The epidermal growth factor receptor (EGFR, ErbB1), is a transmembrane glycoprotein that consists of an extracellular binding domain, a single hydrophobic transmembrane segment, and an intracellular protein tyrosine kinase domain. Icosahedral carboranes have roughly the same molecular volume as adamantane (148 Å^3 vs 136 Å^3) but is more hydrophobic. As a consequence of their electronic structure, carboranes are aromatic and are therefore used as bioisosteres for phenyl groups. Icosahedral boron clusters have emerged as interesting alternatives and promising scaffolds to be used in pharmaceutical drug design. However, these clusters have been an underexplored moiety in the development of EGFR kinase inhibitors.

In our previous studies we reported new anilinoquinazoline-icosahedral borane hybrids as glioma targeting for potential use in cancer therapy. The anti-glioma activity of the most powerful compound against glioma cells, a 1,7-closo-derivative, displayed at least 3.3 times higher activity than the parent drug erlotinib. According to the cytotoxic effects on normal glia cells, the hybrids were selective for epidermal growth factor receptor (EGFR)-overexpressed tumor cells. These boron carriers could be used to enrich glioma cancer cells with boron for cancer therapy.

In this article [1] we report that EGFR inhibitor incorporating closo-carborane has been shown to have higher affinity than Erlotinib. The comparative docking analysis with compounds bearing bioisoster-substructures, demonstrated the relevance of the 3D aromatic-boron-rich moiety for interacting into the EGFR ATP binding region. The capability to accumulate in glioma cells, the ability to cross the blood-brain barrier and the stability on simulated biological conditions render these molecules as lead compounds for further structural modifications to obtain dual action drugs to treat glioblastoma.

RL5 SCIENTIFIC HIGHLIGHTS

Remote control of neural cell behavior using induced dipoles in electroactive conducting implanted materials

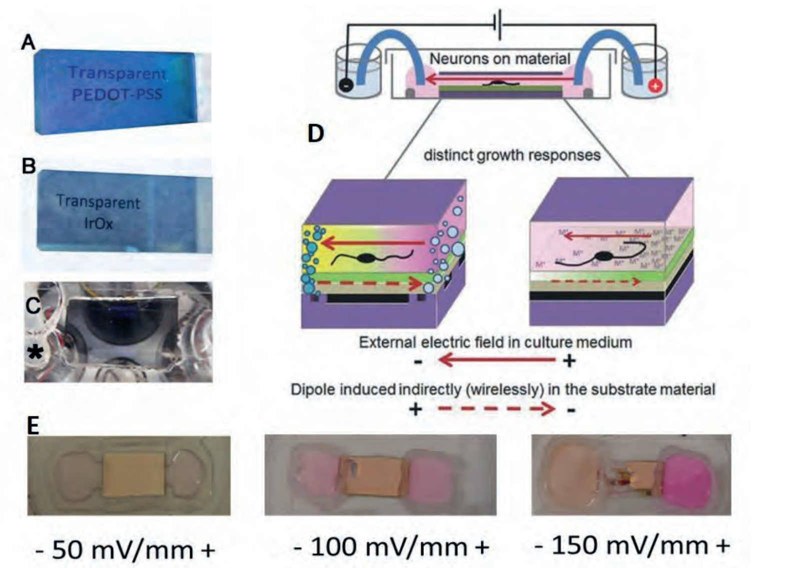
Electrostimulation of neurons is possible through the induced dipoles on implanted transparent conductive materials, with distinct effects depending on the material and its intercalation properties

Ann M. Rajnicek,[2] Zhiqiang Zhao[2], Javier Moral-Vico[1], Ana M. Cruz[2], Colin D. McCaig[2], and Nieves Casañ-Pastor[1]

[1]Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Spain
[2]School of Medical Sciences-University of Aberdeen, UK

Controlling Nerve Growth with an Electric Field Induced Indirectly in Transparent Conductive Substrate Material
Advanced Healthcare Materials 7, 1800473 (2018)

Electrostimulation of the Central nervous system to alleviate neurological symptoms or trying to repair damaged tissue is possible through implanted electrodes in direct electrical contact to a power source. When using intercalation materials like Iridium Oxide and its hybrids with nanocarbons as electrodes, the charge capacity of the final electrode is enlarged several orders of magnitude, with a simultaneous decrease of impedance. In those cases DC fields render neural repair in short periods of time. Nano-structuring induced by the coupling of iridium oxide around carbon nanotubes or graphene yields stable coatings with large cyclability not present for graphite combinations or even for IrOx alone. This work shows a significant discovery that opens a new possibility: response of neural cells is also possible using electrodes without direct contact to the power source. Immersed conducting materials in the biological media, with an external field applied by remote external electrodes, render a local dipole between the borders of the material that, in turn, may induce chemical reactions for certain potentials.



Remote electrostimulation of neural cells through induced dipoles on A-C) metals and transparent nanostructured conducting materials. D) Cell geometry for remote control and E) pH changes observed at the poles of gold/titanium coatings for small and large voltages.

This effect is known as bipolar electrochemistry, and the final induced dipole potential depends on the applied external field, the material and the geometry of the electrochemical cell. Within the electrochemical safe window of water, intercalation of ions and ionic gradients along the material occur, yielding gradients that modulate the cell growth. The observed neural effects are quite distinct depending on the material. Thus, Iridium oxide materials favor speed of dendrite growth, while PEDOT conducting polymers favor growth turning towards a specific direction. In contrast noble metals show smaller or no effects. Electroactive materials are believed to act differently thanks to the ionic gradients created within the material depending on the specific intercalation properties. Thus, iridium oxide is truly a hydrated oxohydroxide that allows H+, Na+, K+ and OH- intercalation/deintercalation processes at negative and positive poles. PEDOT-PSS on the other hand, has a large PSS anion that cannot move out of the structure and that results in cation intercalation only. Diffusion of ions is also different for both types of materials, and result in a different impedance behavior. The significance of the observation is related to the design of new implants in biological systems, when electrostimulation is planned, and allow to explore a new remote control procedure, even in cases where electrodes need to be transparent (retina).

Justo Cabrera-González,[1] Blanca M. Muñoz-Flores,[2] Clara Viñas,[1] Arturo Chávez-Reyes,[3] H. V. Rasika Dias,[5] Víctor M. Jiménez-Pérez [2] and Rosario Núñez[1]

[1]Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Spain
[2]Universidad Autónoma de Nuevo León, Facultad de Ciencias Químicas, Ciudad Universitaria, México.
[3]Centro de Investigación y de Estudios Avanzados del IPN, Unidad Monterrey, México.
[4]Department of Chemistry and Biochemistry, The University of Texas at Arlington, USA

Organotin dyes bearing anionic boron clusters as cell-staining fluorescent probes
Chemistry A-European Journal 24, 5601–5612 (2018)

RL5 SCIENTIFIC HIGHLIGHTS

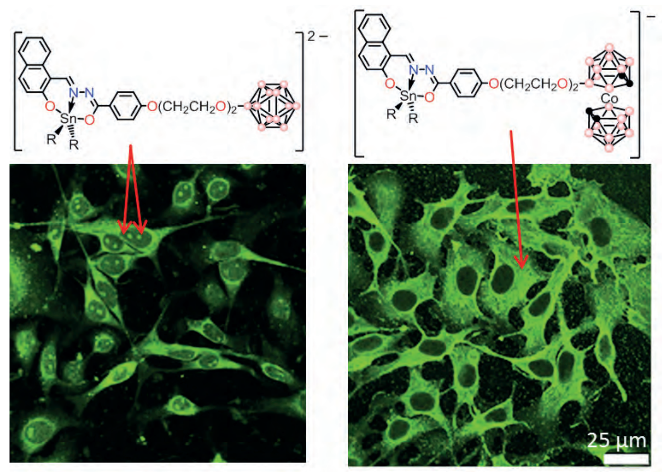
Boron clusters bearing Tin complexes: efficient and specific cell-staining conjugates

The results presented herein demonstrate the key role played by the boron clusters, closo-dodecaborate and cobaltabisdicarbollide, in the cell staining properties of organotin dyes. Whilst those bearing the closo-dodecaborate produce nucleoli and cytoplasmic staining, cobaltabisdicarbollide-containing dyes only produce cytoplasm staining. The remarkable fluorescence staining properties showed by these compounds make them excellent candidates as cell-staining fluorescent probes

Boron clusters are three-dimensional rigid compounds with high thermal and chemical stability. Due to their intriguing electronic properties and their biological compatibility, our group and others have been interested in the development of carborane-containing dyes with potential applications in biomedicine and material sciences. Amongst the wide variety of biomedical techniques, Fluorescence Bioimaging has emerged as an important tool for cell and tissue visualisation, with organotin Schiff-base compounds proving to act as cytoplasm markers in vitro.

Therefore, incorporation of boron clusters in the structure of organotin complexes is an attractive chemical strategy, not only to modulate their photophysical properties, but also to change their cellular internalization behavior. Herein the design of novel fluorescent organotin compounds bearing closo-dodecaborate ([B12H12]2-) and cobaltabisdicarbollide (COSAN) is described, and their cytoplasm and nucleoli staining in vitro (B16F10 cells) is studied.

Organotin compounds bearing an aliphatic chain displayed fluorescent quantum yields (FF) around 24-34 %. Solution-state photophysical studies showed a considerably increase in the FF up to 49 % when the aliphatic chain is replaced by the [B12H12]2- moiety, whereas those bearing COSAN moieties showed lower quantum yield values (3-7 %). Despite this, the fluorescence intensity still allows the analysis of all the compounds by confocal microscopy (see Figure). Two noteworthy conclusions arise



Celullar localization by confocal microscopy of organotin complexes bearing closo-dodecaborate (left) and cobaltabisdicarbollide (right)

from the study of these confocal images. Firstly, there is a striking improvement in solubility for those boron cluster-containing complexes, and no aggregation is observed, neither in the cell media nor on the cell membrane. Secondly, the presence of each boron cluster in the structure produces a different staining effect; those bearing [B12H12]2- produce nucleoli and cytoplasmic staining, while the COSAN-containing dyes are only detected in the cytoplasm.

The striking results obtained for the in vitro studies, highlight the suitability of these boron cluster-containing organotin complexes as potential candidates for cell labelling agents towards medical diagnosis in clinical biopsies.

PROJECTS, PUBLICATIONS AND AWARDS

Research Projects

By the end of 2018, nine researchers of the ICMAB had been granted with ten projects of the European Research Council (ERC). The ERC operates according to a "curiosity-driven", or "bottom-up", approach, allowing researchers to identify new opportunities in any field of research. Accordingly, the portfolio ERC funded projects spans a wide range of topics and research questions. At the ICMAB we have projects on superconducting tapes, organic energy materials, cancer therapy and diagnosis, graphene-based devices, flexoelectricity, photonic and optoelectronic devices, molecular electronic devices, calcium and magnesium-based batteries and materials for the future 5G technology.

Our researchers have also been awarded with many other European and National projects (MSCA, INFRAEDI, COST ACTIONS, I+D RETOS...). Check them out in our Annual Report 2018 website!!

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)Tallahassee (USA)

Núria ALIAGA-ALCALDE (2017)
Efficient electronic transport at room temperature by T-shaped molecules in graphene based chemically modified three-terminal nanodevices (Tmol4TRANS)

Gerard TOBIAS (2017)
Nanoengineering of Radioactive Seeds for Cancer Therapy and Diagnosis (NEST)

Martí GICH (2019)
Ferrites-by-design for Millimeter-wave and Terahertz Technologies (FeMiT)

Starting Grants

Agustín MIHI (2015)
Photonic electrodes for enhanced light management in Optoelectronic devices (ENLIGHTMENT)

Marta MAS-TORRENT (2012)
Surface self-assembled molecular electronic devices: logic gates, memories and sensors (e-GAMES)

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 (LAB-TECH)

Publications

Scientific Outputs

ICMAB confirmed its leadership in excellence in science in the Nature Index 2019, which was based on published research articles from 1 January 2018 to 31 December 2018. The Institute was the first in the ranking among the CSIC centers, in terms of research outputs. CSIC was the first research institute in Spain, was ranked 54th in the world ranking, and the 4th of the government institutions. The Nature Index database is an indicator to value the impact of the research outputs, and compare it to other research institutes of the world and within the CSIC. The Nature Index tracks the author affiliations collected from high quality scientific articles published in 82 high-quality science journals independently selected by a panel of active scientists.

Our Institute is characterized by its high quality research outcomes and by its highly talented people. At the end of 2018, we counted with 5,223 publications, and more than 144,000 citations, with an average ratio of more than 26 citations per paper and a total h index of 137.

During 2018, ICMAB researchers have written 226 articles in international peer-review science journals of various disciplines: chemistry, physics, materials, nanotechnology, photonics, energy, superconductivity, biochemistry, etc., with an average impact factor of 6.30. The Lead index (articles with corresponding author from the ICMAB) is 57 %.

According to the Scimago Journal Ranking (SJR), 88 % of the papers were in first quartile (Q1) journals, 72 % in first decile (D1) journals, and 16 % were published in journals with impact factor above 10 (data from Journal Citation Reports 2018).

70 publications from 2018 are currently Open Access (31 %), either through the gold route (in Open Access journals) or the green route, in Digital CSIC, the institutional repository of the Spanish National Research Council, which organizes, preserves and provides open access to CSIC research outputs. Moreover, 1 publication of 2018 is considered "highly cited paper" by the Web of Science, i.e. it is in the top 1 % mostly cited in its category and year worldwide.

Scientific Collaborations

The internationality and interdisciplinary of our researchers is also confirmed by the high number of collaborations with other countries' institutions. In 2018, the International Collaboration (IC), i.e., articles with co-authors from other countries, were 71%: the ICMAB had 273 collaborations with researchers from 44 countries, being the top 10 countries: Italy, France, USA, Germany, England, Switzerland, Belgium, Luxembourg, Japan and China.

The ICMAB researchers collaborates mainly with universities (549 collaborations), research institutes, hospitals, synchrotrons and other large facilities or state agencies (348 collaborations), and in a minor way with other CSIC centers (33 collaborations), private companies (18 collaborations) and other consortiums and institutions (6 collaborations).

Regarding the collaborations with large facilities, 51 articles in 2018 are co-authored by researchers from these installations, such as ALBA Synchrotron (24), EMAT-Electron Microscoy for Materials Sci-Univ-Antwerp (3), Diamond-Diamond Light Source, Elettra-Elettra Sincrotrone Trieste, ILL-Institut Laue Langevin, LMA at INA-Lab. de Microscopías Avanzadas at INA, Oak Ridge NL MatSci Div, (2 collaborations), and ISIS-ISIS Neutron and Muon Source, ALS-Advanced Light Source and Soleil Synchrotron (1 collaboration).

The CSIC centers with which we most collaborated in 2018 are the ICN2 (23) and the IMB-CNM (6) (located at the UAB Campus), and the ICMA (Zaragoza), CFM (San Sebastián), IIBB (Barcelona) and INCAR (Oviedo) (1 collaboration each).

SCIENTIFIC HIGHLIGHTS

Publications

TOP JOURNALS WITH IF>10

The journals with Impact Factor (IF) higher than 10 in which the researchers have published an article are the following (data from Journal Citation Reports 2018) :

1.- Chemical Society Reviews (40.443)

Understanding ageing in Li-ion batteries: a chemical issue

Palacin, MR. DOI: 10.1039/c7cs00889a

2.- Nature Photonics (31.583)

Hydroxypropyl cellulose photonic architectures by soft nanoimprinting lithography

Espinha, A; Dore, C; Matricardi, C; Alonso, MI; Goni, AR; Mihi, A.
DOI: 10.1038/s41566-018-0152-1

3.- Advanced Materials (25.809)

Ultrathin Semiconductor Superabsorbers from the Visible to the Near-Infrared

Molet, P; Garcia-Pomar, JL; Matricardi, C; Garriga, M; Alonso, MI; Mihi, A.
DOI: 10.1002/adma.201705876

An Unprecedented Stimuli-Controlled Single-Crystal Reversible Phase Transition of a Metal-Organic Framework and Its Application to a Novel Method of Guest Encapsulation

Tan, FC; Lopez-Periago, A; Light, ME; Cirera, J; Ruiz, E; Borras, A; Teixidor, F; Vinas, C; Domingo, C; Planas, JG.
DOI: 10.1002/adma.201800726

4.- Advanced Energy Materials (24.884)

Optical Analysis of Oxygen Self-Diffusion in Ultrathin CeO_2 Layers at Low Temperatures

Neuderth, P; Hille, P; Marti-Sanchez, S; de la Mata, M; Coll, M; Arbiol, J; Eickhoff, M.
DOI: 10.1002/aenm.201802120

5.- Nature Chemistry (23.139)

Self-assembly of polyhedral metal-organic framework particles into three-dimensional ordered superstructures

Avci, C; Imaz, I; Carne-Sanchez, A; Pariente, JA; Tasios, N; Perez-Carvajal, J; Alonso, MI; Blanco, A; Dijkstra, M; Lopez, C; Maspoch, D. DOI: 10.1038/NCHEM.2875.

6.- Advanced Science (15.804)

Coercivity Modulation in FeCu Pseudo-Ordered Porous Thin Films Controlled by an Applied Voltage: A Sustainable, Energy-Efficient Approach to Magnetoelectrically Driven Materials

Evangelia Dislaki, Shauna Robbennolt, Mariano Campoy‐Quiles, Josep Nogués, Eva Pellicer, Jordi Sort. DOI: 10.1002/advs.201800499

7.- Advanced Functional Materials (15.621)

Ultrathin Semiconductor The Misfit Dislocation Core Phase in Complex Oxide Heteroepitaxy

Bagues, N; Santiso, J; Esser, BD; Williams, REA; McComb, DW; Konstantinovic, Z; Balcells, L; Sandiumenge, F. DOI: 10.1002/adfm.201704437

8.- Nano Energy (15.548)

Topological distribution of reversible and non-reversible degradation in perovskite solar cells

Gomez, A; Sanchez, S; Campoy-Quiles, M; Abate, A. DOI: 10.1016/j.nanoen.2017.12.040

9.- Journal of The American Chemical Society (14.6957)

Robust Organic Radical Molecular Junctions Using Acetylene Terminated Groups for C-Au Bond Formation

Bejarano, F; Olavarria-Contreras, IJ; Droghetti, A; Rungger, I; Rudnev, A; Gutierrez, D; Mas-Torrent, M; Veciana, J; van der Zant, HSJ; Rovira, C; Burzuri, E; Crivillers, N.
DOI: 10.1021/jacs.7b10019

Electron Accumulative Molecules

Buades, AB; Arderiu, VS; Olid-Britos, D; Vinas, C; Sillanpaa, R; Haukka, M; Fontrodona, X; Paradinas, M; Ocal, C; Teixidor, F. DOI: 10.1021/jacs.7b12815

Tunable Self-Assembly of YF_3 Nanoparticles by Citrate -Mediated Ionic Bridge

Martinez-Esain, J; Faraudo, J; Puig, T; Obradors, X; Ros, J; Ricart, S; Yanez, R.
DOI: 10.1021/jacs.7b09821

Stable Metallic State of a Neutral-Radical Single-Component Conductor at Ambient Pressure

Le Gal, Y; Roisnel, T; Auban-Senzier, P; Bellec, N; Iniguez, J; Canadell, E; Lorcy, D.
DOI: 10.1021/jacs.8b03714

Conducting Anilate-Based Mixed-Valence Fe(II)Fe(III) Coordination Polymer: Small-Polaron Hopping Model for Oxalate-Type Fe(II)Fe(III) 2D Networks

Sahadevan, SA; Abherve, A; Monni, N; de Pipaon, CS; Galan-Mascaros, JR; Waerenborgh, JC; Vieira, BJC; Auban-Senzier, P; Pillet, S; Bendeif, EE; Alemany, P; Canadell, E; Mercuri, ML; Avarvari, N. DOI: 10.1021/jacs.8b08032

10.- Materials Horizons (14.356)

Donor-anion interactions in quarter-filled low-dimensional organic conductors

Pouget, JP; Alemany, P; Canadell, E.
DOI: 10.1039/c8mh00423d

11.- ACS Nano (13.903)

Minimalist Prion-Inspired Polar Self-Assembling Peptides

Diaz-Caballero, M; Navarro, S; Fuentes, I; Teixidor, F; Ventura, S.
DOI: 10.1021/acsnano.8b00417

Selective Laser-Assisted Synthesis of Tubular van der Waals Heterostructures of Single-Layered PbI_2 within Carbon Nanotubes Exhibiting Carrier Photogeneration

Sandoval, S; Kepic, D; del Pino, AP; Gyorgy, E; Gomez, A; Pfannmoeller, M; Van Tendeloo, G; Ballesteros, B; Tobias, G.
DOI: 10.1021/acsnano.8b01638

Gold Nanoparticle Plasmonic Superlattices as Surface-Enhanced Raman Spectroscopy Substrates

Matricardi, C; Hanske, C; Garcia-Pomar, JL; Langer, J; Mihi, A; Liz-Marzan, LM.
DOI: 10.1021/acsnano.8b04073

12.- Nano Letters (12.279)

Combining Adhesive Nanostructured Surfaces and Costimulatory Signals to Increase T Cell Activation

Judith Guasch, Marco Hoffmann, Jennifer Diemer, Hossein Riahinezhad, Stefanie Neubauer, Horst Kessler, Joachim P. Spatz. DOI: 10.1021/acs.nanolett.8b02588

Crystalline, Phononic, and Electronic Properties of Heterostructured Polytypic Ge Nanowires by Raman Spectroscopy

Claudia Fasolato, Marta De Luca, Doriane Djomani, Laetitia Vincent, Charles Renard, Giulia Di Iorio, Vincent Paillard, Michele Amato, Riccardo Rurali, Ilaria Zardo.
DOI: 10.1021/acs.nanolett.8b03073

Direct Mapping of Phase Separation across the Metal-Insulator Transition of $NdNiO_3$

Daniele Preziosi, Laura Lopez-Mir, Xiaoyan Li, Tom Cornelissen, Jin Hong Lee, Felix Trier, Karim Bouzehouane, Sergio Valencia, Alexandre Gloter, Agnès Barthélémy, Manuel Bibes.
DOI: 10.1021/acs.nanolett.7b04728

Static Modulation Wave of Arrays of Halogen Interactions Transduced to a Hierarchy of Nanoscale Change Stimuli of Crystalline Rotors Dynamics

Sergey Simonov, Leokadiya Zorina, Pawel Wzietek, Antonio Rodríguez-Fortea, Enric Canadell, Cécile Mézière, Guillaume Bastien, Cyprien Lemouchi, Miguel A. Garcia-Garibay, Patrick Batail. DOI: 10.1021/acs.nanolett.8b00956

13.- Angewandte Chemie-international Edition (12.257)

Faceted-Charge Patchy LnF_3 Nanocrystals with a Selective Solvent Interaction

Jordi Martínez-Esaín, Prof. Teresa Puig, Prof. Xavier Obradors, Prof. Josep Ros, Dr. Ramón Yáñez, Dr. Jordi Faraudo, Dr. Susagna Ricart
DOI: 10.1002/anie.201806273

14.- Nature Communications (11.878)

Stability and nature of the volume collapse of ε–$Fe2O_3$ under extreme conditions

J. A. Sans, V. Monteseguro, G. Garbarino, M. Gich, V. Cerantola, V. Cuartero, M. Monte, T.Irifune, A. Muñoz, C. Popescu
DOI: 10.1038/s41467-018-06966-9

15.- Small (10.856)

Combining X-Ray Whole Powder Pattern Modeling, Rietveld and Pair Distribution Function Analyses as a Novel Bulk Approach to Study Interfaces in Heteronanostructures: Oxidation Front in FeO/$Fe3O_4$ Core/Shell Nanoparticles as a Case Study

Rodrigo U. Ichikawa, Alejandro G. Roca, Alberto López‐Ortega, Marta Estrader, Inma Peral, Xabier Turrillas, Josep Nogués
DOI: 10.1002/smll.201800804

Fluid Mixing for Low-Power 'Digital Microfluidics' Using Electroactive Molecular Monolayers

Maria Serena Maglione, Stefano Casalini, Stamatis Georgakopoulos, Marianna Barbalinardo, Vitaliy Parkula, Núria Crivillers, Concepció Rovira, Pierpaolo Greco, Marta Mas-Torrent. DOI: 10.1002/smll.201703344

Nanostructuring Lipophilic Dyes in Water Using Stable Vesicles, Quatsomes, as Scaffolds and Their Use as Probes for Bioimaging

Antonio Ardizzone, Siarhei Kurhuzenkau, Sílvia Illa‐Tuset, Jordi Faraudo, Mykhailo Bondar, David Hagan, Eric W. Van Stryland, Anna Painelli, Cristina Sissa, Natalia Feiner, Lorenzo Albertazzi, Jaume Veciana, Nora Ventosa. DOI: 10.1002/smll.201703851

16.- Journal of Materials Chemistry A (10.733)

A CO_2 optical sensor based on self-assembled metal-organic framework nanoparticles

Blanca Chocarro-Ruiz, Javier Pérez-Carvajal, Civan Avci, Olalla Calvo-Lozano, Maria Isabel Alonso, Daniel Maspoch, Laura M. Lechuga. DOI: 10.1039/c8ta02767f

Defect tolerant perovskite solar cells from blade coated non-toxic solvents

Zhuoneng Bi, Xabier Rodríguez-Martínez, Clara Aranda, Enrique Pascual-San-José, Alejandro R. Goñi, Mariano Campoy-Quiles, Xueqing Xu, Antonio Guerrero
DOI: 10.1039/c8ta06771f

Passivation layers for nanostructured photoanodes: ultra-thin oxides on InGaN nanowires

P. Neuderth, P. Hille, J. Schörmann, A. Frank, C. Reitz, S. Martí-Sánchez, M. de la Mata, M. Coll, J. Arbiol, R. Marschallh, M. Eickhoff. DOI: 10.1039/c7ta08071a

Reactive laser synthesis of nitrogen-doped hybrid graphene-based electrodes for energy storage

Ángel Pérez del Pino, Andreu Martínez Villarroya, Alex Chuquitarqui, Constantin Logofatu, Dino Tonti, Enikö György. DOI: 10.1039/c8ta03830a

The nickel battery positive electrode revisited: stability and structure of the beta-NiOOH phase

Montse Casas-Cabanas, Maxwell D. Radin, Jongsik Kim, Clare P. Grey, Anton Van der Ven, M. Rosa Palacín. DOI: 10.1039/c8ta07460g

17.- Chemistry of Materials (10.15)

Electrochemical Intercalation of Calcium and Magnesium in TiS_2: Fundamental Studies Related to Multivalent Battery Applications

Deyana S. Tchitchekova, Alexandre Ponrouch, Roberta Verrelli, Thibault Broux, Carlos Frontera, Andrea Sorrentino, Fanny Bardé, Neven Biskup, M. Elena Arroyo-de Dompablo, M. Rosa Palacín. DOI: 10.1021/acs.chemmater.7b04406

Publications

MOST CITED ARTICLES OF 2018

The most cited articles published in 2018 (data from July 2019, Web of Science) are the following:

1.- Self-assembly of polyhedral metal-organic framework particles into three-dimensional ordered superstructures

Avci, Civan; Imaz, Inhar; Carne-Sanchez, Arnau; Angel Pariente, Jose; Tasios, Nikos; Perez-Carvajal, Javier; Isabel Alonso, Maria; Blanco, Alvaro; Dijkstra, Marjolein; Lopez, Cefe; Maspoch, Daniel. Nature Chemistry. DOI: 10.1038/NCHEM.2875

Total Citations: 33

2.- Topological distribution of reversible and non-reversible degradation in perovskite solar cells

Gomez, A.; Sanchez, S.; Campoy-Quiles, Mariano; Abate, A. Nano Energy
DOI: 10.1016/j.nanoen.2017.12.040

Total Citations: 16

3.- Electrochemical Intercalation of Calcium and Magnesium in TiS_2: Fundamental Studies Related to Multivalent Battery Applications

Tchitchekova, Deyana S.; Ponrouch, Alexandre; Verrelli, Roberta; Broux, Thibault; Frontera, Carlos; Sorrentino, Andrea; Barde, Fanny; Biskup, Neven; Elena Arroyo-de Dompablo, M.; Rosa Palacin, M. Chemistry of Materials
DOI: 10.1021/acs.chemmater.7b04406

Total Citations: 14

4.- On the road toward calcium-based batteries

Ponrouch, A.; Palacin, M. R. Current Opinion in Electrochemistry
DOI: 10.1016/j.coelec.2018.02.001

Total Citations: 13

5.- Emergent chirality in the electric polarization texture of titanate superlattices

Shafer, Padraic; Garcia-Fernandez, Pablo; Aguado-Puente, Pablo; Damodaran, Anoop R.; Yadav, Ajay K.; Nelson, Christopher T.; Hsu, Shang-Lin; Wojdel, Jacek C.; Iniguez, Jorge; Martin, Lane W.; Arenholz, Elke; Junquera, Javier; Ramesh, Ramamoorthy. Proceedings of the National Academy of Science of the United States of America
DOI: 10.1073/pnas.1711652115

Total Citations: 12

6.- Gold Nanoparticle Plasmonic Superlattices as Surface-Enhanced Raman Spectroscopy Substrates

Matricardi, Cristiano; Hanske, Christoph; Garcia-Pomar, Juan Luis; Langer, Judith; Mihi, Agustin; Liz-Marzan, Luis M. ACS Nano. DOI: 10.1021/acsnano.8b04073

Total Citations: 11

7.- Diglyme Based Electrolytes for Sodium-Ion Batteries

Westman, K.; Dugas, R.; Jankowski, P.; Wieczorek, W.; Gachot, G.; Morcrette, M.; Irisarri, E.; Ponrouch, A.; Palacin, M. R.; Tarascon, J. -M.; Johansson, P. ACS Applied Energy Materials. DOI: 10.1021/acsaem.8b00360

Total Citations: 11

8.- Hydroxypropyl cellulose photonic architectures by soft nanoimprinting lithography

Espinha, Andre; Dore, Camilla; Matricardi, Cristiano; Isabel Alonso, Maria; Goni, Alejandro R.; Mihi, Agustin. Nature Photonics. DOI: 10.1038/s41566-018-0152-1

Total Citations: 10

9.- Role of Polymorphism and Thin-Film Morphology in Organic Semiconductors Processed by Solution Shearing

Riera-Galindo, Sergi; Tamayo, Adrian; Mas-Torrent, Marta. ACS Omega.
DOI: 10.1021/acsomega.8b00043

Total Citations: 10

10.- Enhanced UV- and visible-light driven photocatalytic performances and recycling properties of graphene oxide/ZnO hybrid layers

Gyorgy, Eniko; Logofatu, Constantin; Perez del Pino, Angel; Datcu, Angela; Pascu, Oana; Ivan, Raluca. Ceramics International. DOI: 10.1016/j.ceramint.2017.10.117

Total Citations: 8

11.- Energetics of oxygen-octahedra rotations in perovskite oxides from first principles

Chen, Peng; Grisolia, Mathieu N.; Zhao, Hong Jian; Gonzalez-Vazquez, Otto E.; Bellaiche, L.; Bibes, Manuel; Liu, Bang-Gui; Iniguez, Jorge. Physical Review B
DOI: 10.1103/PhysRevB.97.024113

Total Citations: 8

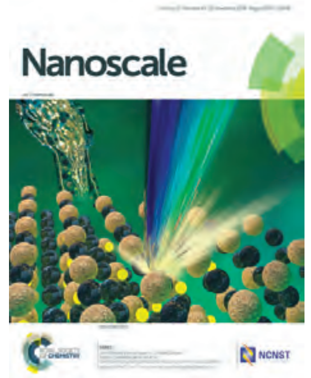
HIGHLY CITED PAPER

1.- Self-assembly of polyhedral metal-organic framework particles into three-dimensional ordered superstructures

Avci, Civan; Imaz, Inhar; Carne-Sanchez, Arnau; Angel Pariente, Jose; Tasios, Nikos; Perez-Carvajal, Javier; Isabel Alonso, Maria; Blanco, Alvaro; Dijkstra, Marjolein; Lopez, Cefe; Maspoch, Daniel. Nature Chemistry. DOI: 10.1038/NCHEM.2875

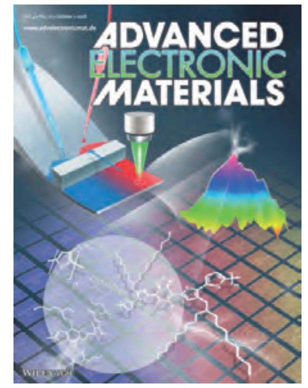
Publications

JOURNAL COVERS



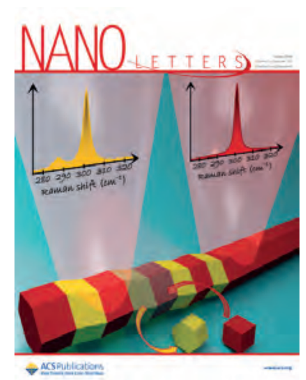
Direct and Converse Piezoelectric Responses at the Nanoscale from Epitaxial $BiFeO_3$ Thin Films Grown by Polymer Assisted Deposition

José M. Vila-Fungueiriño, Andres Gomez, Jordi Antoja-Lleonart, Jaume Gazquez, César Magén, Beatriz Noheda and Adrian Carretero-Genevrier
Nanoscale, 10, 20155-20161, 2018.
DOI:10.1039/C8NR05737K



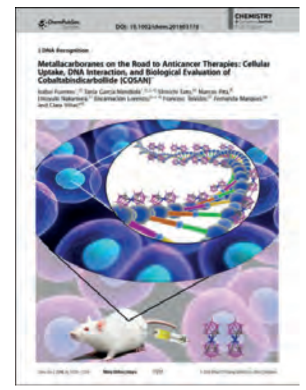
High-Throughput Multiparametric Screening of Solution Processed Bulk Heterojunction Solar Cells

Antonio Sánchez-Díaz, Xabier Rodríguez-Martínez, Laura Córcoles-Guija, Germán Mora-Martín and Mariano Campoy-Quiles. Advanced Electronic Materials, 4, 1700477, 2018. DOI: 10.1002/aelm.201700477



Crystalline, Phononic, and Electronic Properties of Heterostructured Polytypic Ge Nanowires by Raman Spectroscopy

Claudia Fasolato, Marta De Luca, Doriane Djomani, Laetitia Vincent, Charles Renard, Giulia Di Iorio, Vincent Paillard, Michele Amato, Riccardo Rurali, and Ilaria Zardo
Nano Letters, 18, 11, 7075-7084, 2018.
DOI: 10.1021/acs.nanolett.8b03073



Metallacarboranes on the Road to Anticancer Therapies: Cellular Uptake, DNA Interaction, and Biological Evaluation of Cobaltabisdicarbollide [COSAN]

Isabel Fuentes, Tania García Mendiola, Shinichi Sato, Marcos Pita, Hiroyuki Nakamura, Encarnación Lorenzo, Francesc Teixidor, Fernanda Marques, Clara Viñas
Chem. Eur. J., 24, 17239-17254, 2018

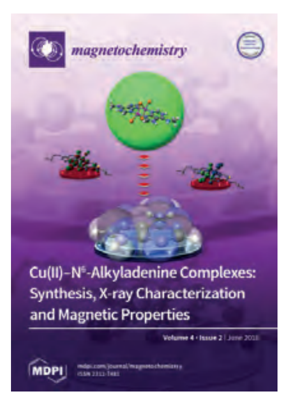
DOI: 10.1002/chem.201803178

Tailoring oxygen redox reactions in ionic liquid based Li/O_2 batteries by means of the Li+ dopant concentration

Laura Cecchetto, Alvaro Y. Tesio, Mara Olivares-Marín, Marc Guardiola Espinas, Fausto Croced and Dino Tonti. Sustainable Energy Fuels, 2, 118-124, 2018.
DOI: 10.1039/C7SE00389G

Discovery of Potent EGFR Inhibitors through the Incorporation of a 3D-Aromatic-Boron-Rich-Cluster into the 4-Anilinoquinazoline Scaffold: Potential Drugs for Glioma Treatment

Marcos Couto, María Fernanda García, Catalina Alamón, Mauricio Cabrera, Pablo Cabral, Alicia Merlino, Francesc Teixidor, Hugo Cerecetto, Clara Viñas
Chem. Eur. J., 24, 3122-3126, 2018. DOI: 10.1002/chem.201705181



Cu(II)–N^6-Alkyladenine Complexes: Synthesis, X-ray Characterization and Magnetic Properties

María Soledad Martínez, Antonio Bauzá, Amparo Caubet, Ángel García-Raso, Ángel Terrón, Juan J. Fiol, Elies Molins, Miquel Barceló-Oliver and Antonio Frontera
Magnetochemistry, 4(2), 24, 2018.
DOI: 10.3390/magnetochemistry4020024

Awards

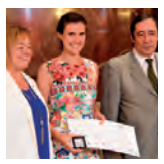
Staff

__Enric Canadell__ elected member of the Royal Academy of Sciences and Arts of Barcelona (RACAB)

__Sole Roig,__ PhD researcher at the NN group, finalist of the UAB contest "Tesi en 4 minuts"

***Judith Guasch, Arántzazu González and Ignasi Fina** awarded with a Ramón y Cajal grant*

__Roberta Verrelli__, winner of the 6th Early Career Scientist Presentation Contest of the World Materials Research Institute Forum



__Mariona Coll__ acknowledged by the CSIC for her L'Oréal-Unesco FWIS 2017 Research Award

*PhD Extraordinary award for three ICMAB graduates: **Justo Cabrera, María de la Mata Fernández and Manuel Souto***

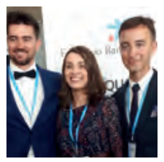
***Roberta Verrelli and Elzbieta Pach**, new Juan de la Cierva postdoctoral fellows at ICMAB*

__Martí Gich__ awarded with a 2018 ERC Consolidator Grant!

***Arnau Bertran:** Premi Sant Jordi 2018 from the SCQ-IEC for his bachelor's thesis*

***Five ICMAB graduates** in Materials Science received the PhD Extraordinary Award : Laura Cabana, Pedro López-Aranguren, Nerea Murillo, David Pesquera and Albert Queraltó*

__Arpita Saha__ receives the 3rd prize for the Oral Communication at the UAB Jornades Doctorals 2018



***José Jurado, Milena Cervo and Jan Grzelak** received their INPhINIT "la Caixa" fellowship at Caixaforum*

__Ana M. López-Periago__, second prize at the science monologues contest "Científiques a prop"

***Jaume Veciana:** Olivier Kahn Plenary Lecture speaker at the ICMM 2018*

__Nora Ventosa__ designated new numerary member of the IEC

***Judit Morlà-Folch and the NANOMOL group** awarded with a TECNIOspring Plus grant*

ICMAB

***The ICMAB** awarded with the Gender Equality Certificate by the CSIC*

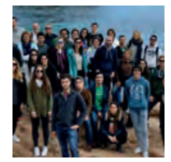
Research projects and groups

***MIT-Spain grant for ICMAB project:** new materials for photovoltaics*

*CIBER-ONC/CIBER-BBN grant for an ICMAB project on cancer immunotherapy: **ALYCIA***

*Comfuturo project granted to **Ignasi Fina** for his project on improving photovoltaic efficiency*

__NANBIOSIS__ renews its accreditation as ICTS



__NANOMOL__ group accredited with the TECNIO certification

***The project Greene3D**, awarded as best initiative of circular economy by the Generalitat and the PRUAB*

***A project to prevent infectious diseases with functionalized catheters** led by Imma Ratera awarded by La Marató de TV3*

Communication & outreach projects

__ICMAB__ received the Maker of Merit award at the Barcelona Maker Faire 2018

Achievements

*High interdisciplinarity and leadership within **ICMAB researchers** according to their h-index*

***The ICMAB** is the first center in the CSIC in terms of research outputs per capita, according to Nature Index*

***The ICMAB website:** the most visible of the CSIC*

***The ICMAB most cited article of all time** has more than 7400 citations!*

INSTITUTIONAL HIGHLIGHTS

Research Staff

Scientific staff is formed by the permanent research staff (61), postdoctoral fellows (58), and PhD researchers (113), giving a total of 232 researchers. 52 % of the postdocs and 47 % of the PhD fellows are from abroad.

The support staff (58) is formed by the technical staff (27), the administration staff, the library staff, the IT department and the maintenance and safety staff (31). From the support staff, 56 % have a permanent position and 43 % are female.

In addition, we have visiting researchers (6), undergraduate and master students (34), and the staff working also in spin-offs (6).

Of the total staff, 58 % are male (42 % female) and 30 % are from abroad, from a total of 26 countries. 41 % of the staff has less than 30 years old, and 16 % are more than 50.

External Funding

The Institute secured a total budget of 14.7 M€ in 2018. The competitive budget represents a 64 % (9.4 M€) and 36 % comes from the CSIC (5.3 M€). The budget from the European Union represents a 27 % of the total budget (4 M€), and 19 % of the total budget comes from the Ministry of Science, Innovation and Universities (2.8 M€). The budget from private sources (including contracts and services) represents a 5 % of the total budget (0.8 M€).

A 51.8 % of the budget devoted to the scientific projects carried out at the ICMAB comes from the European Union, a 35.9 % from the Ministry of Science, Innovation and Universities, a 10.3 % are Industry Contracts and a 2 % is funding from the Generalitat de Catalunya. The EU funding has been extraordinary high during 2017-2018.

Half of the ICMAB personnel are funded by the CSIC (50 %), while the other half are funded by projects (31 %), other fellowships (13 %), ICREA (4 %) and CIBER (2 %).

Scientific Services

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. Nine technical facilities run by specialized technicians form the Scientific Equipment Platforms, together with the Nanoquim Platform, a 10,000 Clean Room. These are open to external uses either from academia and industry, with conditions tailored to meet customer technology demands. During 2018, the Scientific Coordinator of the Services is Prof. M. Rosa Palacín, also Deputy Director of the Institute.

On 5 February 2018 we hosted the seminar entitled "Latest innovations in the Nanoquim Platform and ICMAB Scientific Services" to inform about the new released videos for the Nanoquim users and the new website, and to talk about some novelties in the rest of the services, especially in the Low Temperatures and Magnetomery Service and the X-ray diffraction (XRD) lab.

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

1. Nanoquim Platform

The Nanoquim Platform during 2018 performed a total of 1946 experiments, 3 % more respect to 2017. A total of 143 are active users, 119 from the ICMAB, 19 from the PRUAB, and 1 from an external company. During 2018 the platform acquired two new equipment, both located in Laboratory 1: a Plasma cleaner, and an Optical microscope. The Nanoquim Platform, on behalf of the ICMAB, participated in the Ramón Tobar Prize offered by the CSIC in the field of Health and Safety. In addition, the service receives multiple school visits (ESCOLAB, Bachelor and Master Students, summer schools) and from secondary school teachers. The new videos for the Nanoquim users and the new website was released.

2. Low Temperatures and Magnetometry Service

The laboratory has given service for a total of 10,037 hours, which are distributed quite equitably between the different equipment: 2,605 hours for PPMS (P2), 2,549 hours for PPMS (P3), 2,495 hours for MPMS XL-7 (S1), and 2,388 hours for MPMS XL-7 (S2). Nearly 50 % of the service is devoted to samples from the Superconducting and Large Scale Nanostructures (SUMAN) group, followed by the Advanced Characterization and Nanostructured Materials (ACNM) group (13.5 %) and external users (7.8 %), including the Institut Català de Nanociència i Nanotecnologia (ICN2) and the Universitat Autònoma de Barcelona (UAB). The users of the service belong to 22 PI (principal investigators). The laboratory has also given access to users within the NFFA Europe project (580 hours).
A recent feature of this lab is the new Helium liquefaction equipment, which allows recycling the Helium used to carry out the measurements at low temperatures. In total, during 2018, 63 % of the Helium used was recycled Helium, and only 37 % had to be bought.

The service has participated in many science education activities, including the 15th edition of the Argó programme, the ESCOLAB school visits, and the Kids' Day. The service has participated in many scientific publications.

3. X-ray diffraction (XRD) lab

The XRD lab has been used for a total of 4,927 hours in 2018, corresponding to 4,863 samples and 93 users from 32 PI. The equipment used are the diffractometers Siemens D-5000, GADDS and D8 Discover. The service has participated in many science education activities, including the 15th edition of the Argó programme, the ESCOLAB school visits, the Kids' day, and the activity "Converteix-te en un detectiu de minerals" for primary school students.

4. Thin Films Laboratory

The thin films laboratory has produced a total of 496 thin films deposits: 349 samples using Pulsed Laser Depositon (PLD) and 147 samples using Sputtering. 61 % of the samples are for the Laboratory of Multifunctional Thin Films and Complex Structures (MULFOX), 37 % for the Superconducting and Large Scale Nanostructures (SUMAN) group and 2 % for the Crystallography of Magnetic and Electronic Oxides and Surfaces (CMEOS) group. The laboratory has also given service to NFFA Europe users (59 samples). The service also participates in some outreach activities, especially school visits and secondary school teachers visits who love to see the PLD equipment.

5. Spectroscopic Techniques Laboratory

The Spectroscopic Techniques Laboratory includes the FT-IR equipment, the UV-Vis-NIR instrument, the optical microscopy and the EPR (Electron Paramagnetic Resonance) equipment. All the equipment have a high internal use. The external users represent the 5 % of the total users. Specifically, 26 PI have used the FT-IR service, 23 the UV-Vis-NIR service, 16 the optical microscopy and 8 the EPR. The UV-Vis-NIR service has been the most used, with a total of 727 hours.

6. Preparation and Characterization of Soft Materials (Soft Lab)

The Soft Lab counts with 50 % of external users, 33 % of the users come from the CIBER-BBN, and 17 % are internal users from the ICMAB (from 8 PI). The external users during 2018 include: Institut de Biotecnologia i Biomedicina (IBB), Vall d´Hebron Research Institute (VHRI), Universitat Autònoma de Barcelona (UAB), Instituto de Ciencias del Mar (ICM-CSIC), Institut d'Investigacions Biomèdicas de Barcelona (IIBB-CSIC), Universitat de Barcelona (UB), Institut Català de Nanociència i Nanotecnologia (ICN2), Universidad de Salamanca, Instituto de Ciencias Fotónicas (ICFO), Instituto de Investigaciones Biomedicas de Bellvitge (IDIBELL), Hospital de Salamanca, Centro Investigación Cáncer (CIC), Hospital de Sant Joan de Déu, Pragmatics Diagnostics, Nanomol Technologies, BCN-Peptide, Carburos Metálicos, Leitat and Spherium Biomed.

The service has participated in many science education activities, including the ESCOLAB school visits, and the Kids' Day, and has participated in many scientific publications (6 in 2018).

7. Scanning Probe Microscopy (SPM)

This service, which counts with two Atomic Force Microscopy (AFM) equipment, has given service to 63 users, giving a total of 4,770 images, corresponding to 12 PI. The service has also actively participated at the NFFA Europe project. The users of the NFFA Europe project and the SPM service have collaborated in many scientific projects.

The service has participated in many science education activities, including the ESCOLAB school visits, and the Kids' Day, and has participated in many scientific publications (7 in 2018).

8.Electron Microscopy (Transmission and Scanning Electron Microscopy)

The Electron Microscopy service is formed by the Transmission Electron Microscopy (TEM) and the Scanning Electron Microscopy (SEM), which are run by two technicians. The TEM in 2018 gave service for a total of 489.5 hours. 42 % of the hours were for the Nanoparticles and Nanocomposites group (206 hours), 28 % for the Solid State Chemistry Group, 11 % for the Inorganic Materials and Catalysis Laboratory, 6.3 % for the Superconducting Materials and Large Scale Nanostructures, and the rest distributed between the Crystallography, Functional Nanomaterials Surfaces, Advanced Characterization and Nanostructure Materials, Nanostructured Optoelectronic Materials, Molecular Nanoscience and Organic Materials, and only 9 hours for external users. During 2018, 15 publications of the Institute used the TEM service.

The service has participated in many science education activities, including the 15th edition of the Argó programme, the ESCOLAB school visits, the Kids' Day, the activity "Converteix-te en un detectiu de minerals" for primary school students, and Master Students visit from the UAB.

The SEM in 2018 gave service for a total of 1,181 hours, a 42.9 % with technician, and 57.1 % self user, with an average of 107.4 hours per month. Of these hours, 1,166 hours have been for internal users, and 21 hours for external users (Kostal and Carburos Metálicos) and users from the NFFA Europe Project. A total of 115 users have used the SEM, belonging to all the experimental groups at ICMAB: CMEOS, Crystallography, LMI, NN, FunNanoSurf, Nanomol, MULFOX (16.1 %), ACNM, Surfaces, Nanoptener (16.5 %), LASER, Solid State Chemistry (13.6 %) and SUMAN (23.5 %).

The service has participated in many science education activities, including the 15th edition of the Argó programme, the ESCOLAB school visits, and the Kids' Day.

Scientific and Technical Services Staff

9. Thermal Analysis Lab

The Thermal Analysis Lab is formed by two equipment: the TGA (thermogravimetric analysis) and DSC (differential scanning calorimetry). Regarding the TGA, of a total of 225 samples (450 experiments, because each sample is done twice), 81 % of them belong to internal users from the ICMAB, and 19 % from external users. Among the internal users, the samples belong to 12 PI and 7 research groups, 30 % from the LMI group, 25 % from Solid State Chemistry, 23 % from the NN group, and the rest distributed between the Crystallography group, the FunNanoSurf, the MULFOX and the SUMAN group. The external users during 2018 were the ICN2, the Universidad del País Vasco, APPLUS, and the UAB.

The DSC equipment has been used to analyse 55 samples, 45 % belong to internal users and 55 % to external users. The internal samples correspond to 6 PI and 3 research groups: 52 % from the Nanomol group, 28 % from the Solid State Chemistry group and 20 % from the LMI group. The external users during 2018 were the ICN2, Laboratorios Maverick, APPLUS and the UAB.

The service has participated in the ESCOLAB school visits during the year.

10. Molecular Beam Epitaxy (MBE)

The MBE service in 2018 was stopped for some time due to a problem in the vacuum system. All its activity was related to one project: MAT2015-70859-P (HIBRI2) in particular on thermoelectric phenomena in type IV semiconductors (Si, Ge, and SiGe alloys) from 2 PI. The service is used by self-users since no technical personnel is associated to it. In 2018, two papers directly related to work done in the service were published.

Library

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 more than 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.

Alejandro Santos is the Librarian & Documentalist of the ICMAB Library "Manuel Cardona".

Library Activities 2018:

The library has 2,363 titles registered in the institution's collective catalogue, with 17 new acquisitions in 2018, and 77 open subscriptions to scientific journals. The library has registered 29 monograph loans from 25 active readers during the year.

The service for requesting documents counted with 79 external requests (42 from CSIC centres), including 68 for journal articles and 11 for monographs, according to the URICI statistics.

For several months, the library, in collaboration with the Communication and Outreach Officer, gave the "Essential Documentation Tools" course for young researchers. The training course included modules focused on documentation resources, such as "Document access", "Publication and Open Access" and "Databases", among others.

In March, after several specific training sessions, the integral library management system of the CSIC Library Network was changed from Aleph to ALMA in order to improve the management of information and the quality of the service to our users.

The library participated in face-to-face training courses in reference databases, Scopus and Web of Science, at the Research and Development Centre (CID) in Barcelona.

The library also carried out various bibliometric calculations for researchers and for the centre as a whole, such as, for example, the bibliometric report for the SAB evaluation of the Severo Ochoa project.

Maintenance Service

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.

The Maintenance Service was formed in 2018 by Toni Pons, Oriol Sabater, José Manuel Rodriguez, José Ángel Algar, Pere Fernández, Juan José Monis and Roberto Ibánez. In August 2018, Toni Pons, who was in charge of the Maintenance Service from its origins, retired. On 23 July 2018 we wished him good luck, with a nice breakfast and gifts from all the staff. Oriol Sabater, who worked hand in hand with Toni since the year 2000, became then the head of the Maintenance Service.

New laboratories and offices

In 2018 we inaugurated two new laboratories in the third floor of the MATGAS building: a new Cleanroom and a Chemistry Lab, corresponding to the ERC-Ultrasupertapes project.

On the ground floor, the plans were to begin the works for a new Chemistry Lab, corresponding to the ERC-Nest project, and a Chemistry and a Physics Lab, corresponding to the ERC-Tmol4Trans project. The works finally started in 2019.

Moreover, during 2018, more space was made, both at the MATGAS and ICMAB buildings, to allocate more tables for scientific, technical and support staff.

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.

Information Technology Department

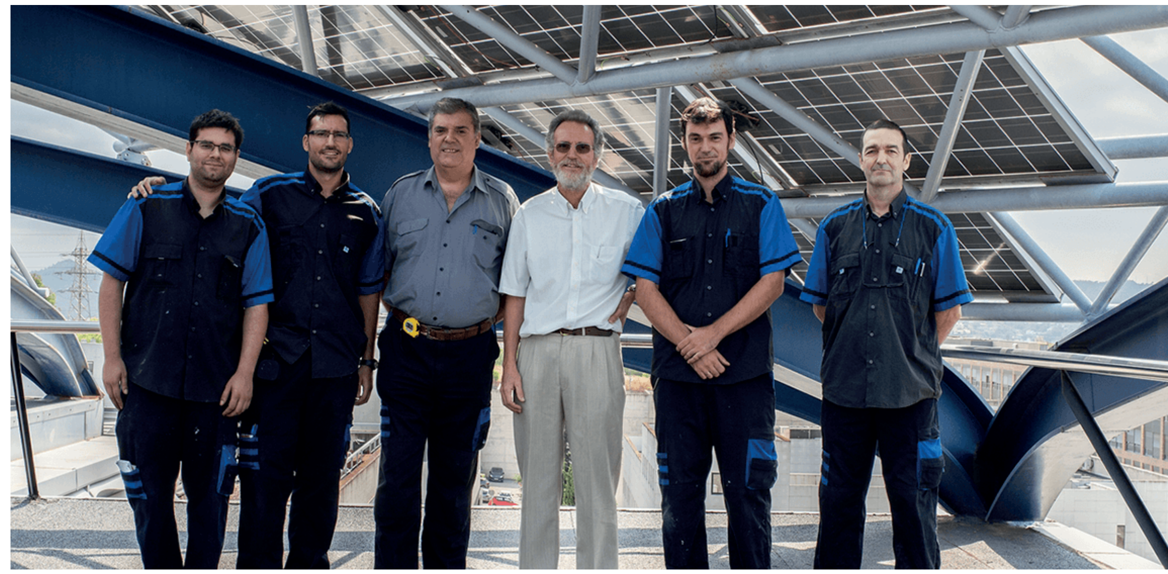
The IT Service, formed by Joan Figuerola, Ángel Elbaz, Javier Rubio, Albert Moreno and José Antonio Gómez, manages all the computer systems, the data network, internal software and the digital presence of the ICMAB, placing them at the service for the researchers and management staff.

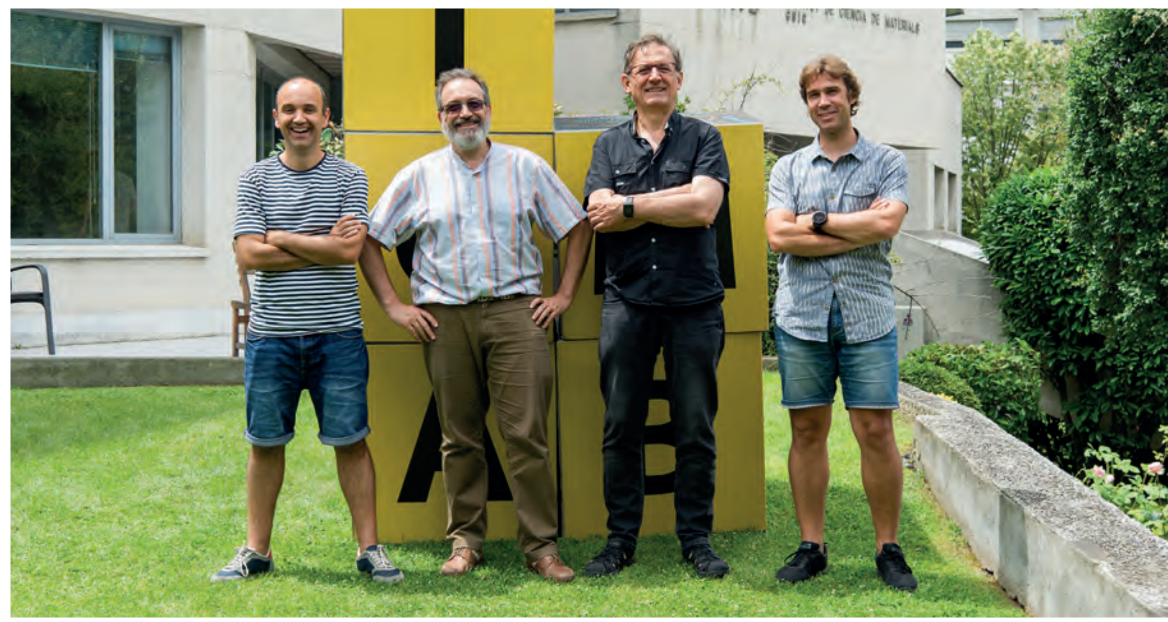
During 2018, the IT Service has carried out the following activities:

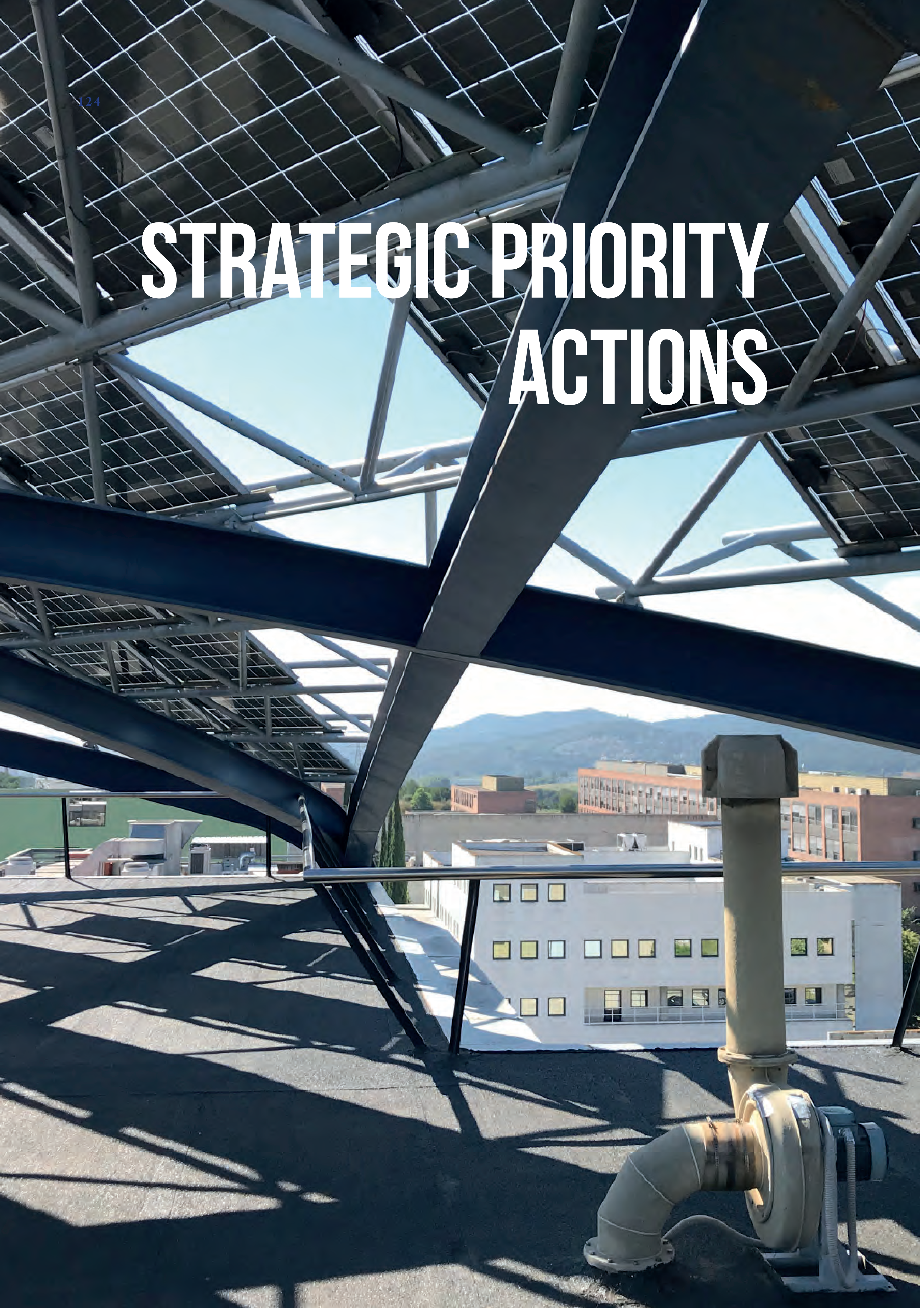
- Improvement of the ICMAB hardware and network: new WiFi infrastructure, incorporation of new audiovisual and conference call equipment in common spaces, maintenance and improvement of the network infrastructure, adaptation of the common spaces to HPC (high performance computing) equipment.
- Improvements in security measures: update of the website and servers with new security measures, maintenance of the websites (around 100), implementation of granular back up for file recovery, migration of equipment to an Active Directory domain, network implementation for replication of virtual machines. Update and securitization of the IP telephony server and full integration with SIP CSIC telephony system.
- Software development and improvement: development of conference websites (hpsp18) and department and projects websites, online system for personnel recruitment, maintenance and evolution of programs (purchases, invoices, booking experiments, personnel management, projects…)
- Improvements in the user's PC: extensions and improvements in user's PC, update of Windows 10 in all the computers.
- Infographics and design of all the websites and corporative material, including flyers, banners and posters, in coordination with the Communication and Outreach Office.

Administration


Library


Maintenance Service


Information and Technology Department



STRATEGIC PRIORITY ACTIONS

Frontier Interdisciplinary Projects (FIPs)

Continuing the Strategic Vision for the Severo Ochoa programme FUNMAT ("Smart FUNctional MATerials for social grand challenges"), the ICMAB opened in 2018 the call for the third edition of the Frontier Interdisciplinary Projects (FIP). Out of all the proposals submitted, 9 projects in different fields were granted.

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.

The researchers of the Institute are able to propose innovative and risky ideas with potential to end up in the market, "proof-of-concept" trials based on previously obtained results or novel ideas for radically new technologies. The projects run for 1 or 2 years, and can be individual or collaborative (between researchers of different research groups).

In 2016 we granted 6 projects with a total of 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 a total of 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. In 2018 we financed 9 projects with a total of 540,000 €, allowing to recruit 2 Master students, 5 PhD researchers and 3 postdoctoral fellows. From these 9 projects, 2 of them were individual, 6 collaborative and 1 proof-of-concept. In total, during the Severo Ochoa period, we financed 24 FIP projects: 6 for RL1, 2 for RL2, 7 for RL3, 2 for RL4 and 7 for RL5.

The granted FIP projects of this call 2018 are the following:

Individual FIP

- *José Vidal: Developing New Contrast Agents for Magnetic Resonance Imaging*
- *Xavier Torrelles: Oxide Surfaces with catalytic activity in switchable films by reversal ferroelectric polarization of the substrate*

Proof-of-concept

- *Joffre Gutiérrez: High field superconductors' technology for particle accelerators*

Collaborative FIP

- *José Giner and Concepción Domingo: Exploring the limits of the uniqueness of hierarchical hybrid adsorbents for energy applications*
- *Arántzazu González and Ana M. López-Periago: Preparation of bifunctional nanodevices for photodynamic therapy obtained from surface anchored Metal Organic Frameworks using sustainable CO_2 technology*
- *Anna Palau and Narcís Mestres: Reversible switching of superconductor-insulator transition for green electronic devices*
- *Florencio Sánchez and Ignasi Fina: HfO_2-based EPItaxial ferroelectric tunnel junction MEMories integrated with Si(001)*
- *Alberto Pomar and Benjamín Martínez: All-oxide heterostructures for pure spin currents generation and detection*
- *Jaume Veciana and Paula Mayorga: Higher efficient charge-transport induced by chiral perchlorotriphenylmethyl radical based*

Important outputs of the FIPs are already detected, including strong generation of internal synergy, high risk of ideas incentivized and enhanced competitiveness. Some of the outputs include 27 publications, 56 presentations in conferences, 15 training contracts, 12 new projects, 5 dissemination activities, 2 patents, 4 contracts with the industry and 6 new established collaborations.

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 especially focused on Master students, PhD and postdoc fellows, and permanent researchers. In total, during the Severo Ochoa period, 21 Master students, 61 PhD researchers, 24 postdoctoral fellows, 5 technicians and 6 tenured scientists have been recruited so far.

TOOLS & ACTIONS

MASTER STUDENTS ACTIONS

1 - 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 could 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, in 2017, 7 scholarships for 5 months and 5,000 € each, and in 2018 we granted 7 more scholarships for 5 months and 5,000 € each. A total of 21 scholarships for Master students have been granted in these three years.

2 – University of Barcelona Careers Fair (Fira d'Empreses)

On May 2018, the ICMAB was among the over 100 companies and research institutes to interact with students taking the first steps towards a career in science at the UB Physics Faculty. We explained the students our PhD program and opportunities to carry out research with us.

PREDOCTORAL ACTIONS

1 - Own doctoral programme COFUND MSCA DOC-FAM

With this MSCA COFUND DOCtoral training programme in Functional Advanced Materials (DOC-FAM) project, coordinated by the ICMAB and with 4 more partners (ALBA Synchrotron, IMB-CNM-CSIC, IREC, ICN2) we have incorporated 5 new PhD fellows in the first call in 2017 and 4 more will be incorporated in the 2018 call (financial assistance 33,000 €/year for 3 years). A total of 22 early stage researchers (ESR) will be part of this programme.

2- COFUND MSCA INPhINIT

We also participate in the COFUND MSCA INPhINIT coordinated by "la Caixa" Foundation, hosting 3 PhD fellows in the 2017 call, and 1 PhD fellow will start within the 2018 call (financial assistance 34,800 €/year for 3 years).

3- Spanish Ministry of Science, Innovation and Universities Program

We also host PhD fellows from the National Programme for the Promotion of Talent and its Employability (Spanish Ministry of Science, Innovation and Universities). Some of the predoctoral researchers have a Severo Ochoa Fellowship: 6 fellows from 2016, 4 fellows from 2017 and 4 fellows from 2018 (financial assistance 18,000-20,600 € for 4 years); 5 fellows have a FPU (Training of University Teachers), and 8 fellows a FPI (Training of Research Personnel).

4 – Generalitat Program

We host 3 fellows with a PhD grant from the Generalitat de Catalunya.

5 – China Scholarship Program

In 2018, we have a total of 23 PhD fellows from China carrying out their PhD at the ICMAB thanks to the China Scholarship Program grants.

POSTDOCTORAL ACTIONS

1 – COFUND MSCA P-SPHERE

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).

2 – MSCA Individual Fellowships (IF)

We support researchers in the preparation of proposals to MSCA-IF. In 2016, 3 proposals were awarded, in 2017, 1 proposal was awarded, and in 2018, 2 proposals were awarded. These fellowships are for 2 years of postdoctoral research at the ICMAB.

3 - National and regional calls (JdC, RyC, BdP)

We support the already existing calls for pre-doc and postdoc researchers, including the Juan de la Cierva (10 researchers currently), Beatriu de Pinós and Technio (5 researchers), Ramón y Cajal (4 researchers), and Jóvenes Investigadores (1 researcher).

PERMANENT RESEARCHERS

1 - Start-up package for new permanent researchers

We support the new permanent researchers with 25,000 € so that they can begin new projects, thanks to the Severo Ochoa project. In total, 1 CSIC permanent researcher was incorporated in 2016, 2 in 2017 and 3 in 2018.

TECHNICIANS

From the 5 technicians recruited during the Severo Ochoa period, 3 are PTA cofounded with the CSIC and 2 have Severo Ochoa contracts.

Mobility Actions, Training and Internationalization

PHD THESES 2018

In total, by the end of 2018 the ICMAB graduates amounted 254, and 113 PhD fellows were carrying out their thesis. During 2018, 14 PhD theses were defended, 5 women (36 %) and 9 men (64 %), and of the 25 supervisors of the graduated fellows, 15 were women (60 %) and 10 men (40 %).

SEMINARS

The types of seminars are organized within the ICMAB.
The first and more known ones are the ICMAB Periodical Lectures, organized by the Seminars and Training committee. These biweekly seminars are talks of general interest for the material science community. The invited speakers are selected by the committee among a pool of candidates nominated by scientists of the institute. The goal of these seminars is two-fold: (i) provide a general introduction to a non-specialized audience in that particular topic (speakers are requested to devote at least one third of their presentation to a broad introduction of the field); (ii) stimulate the collaboration with ICMAB researchers or reinforcing them, if already existing.

The second type of seminars are the Invited Seminars: invited researchers that come to the ICMAB to present their research and collaborate with some of our researchers, participate in a conference in the area, etc. This are hosted whenever the invited researcher is available, although most of them are on Mondays.

The third type of seminars are special seminars to commemorate a special day, such as the International Day of Women and Girls in Science or Christmas, for example. An invited speaker expert in a field (not necessarily Materials Science) is proposed by either the staff or the Communication and Outreach committee and invited to give a one-hour lecture for all our staff.

We hosted many seminars during 2018:

- 17 ICMAB Periodical Lectures
- 26 Invited Seminars, of which
  * One seminar on "Mileva Maric" for the International Day of Women and Girls in Science (11 February)
  * One seminar to show the "Latest innovations in the Nanoquim Platform and ICMAB Scientific Services"
  * Two seminars to celebrate the Feynman Year at ICMAB
  * One seminar on science dissemination 2.0 to celebrate Christmas at ICMAB

CONFERENCES AND MEETINGS

ICMAB researchers have presented their results in more than 139 international meetings and 17 national meetings. Of the communications, 53 were Invited Conferences, 75 Oral Communications, 3 Plenary Talks and 25 Poster Presentations. The conferences are of a broad range of topics: superconductivity, phosphorus, boron and silicon, nanocomposites, materials science, coordination chemistry, nanoparticles' applications, lithium batteries, organic and hybrid thermoelectrics, cellulose, solid state physics, paramagnetic materials, nanoscience and nanotechnology, low temperature electronics, synthetic metals, molecule-based magnets, medicinal chemistry, semiconductors, etc.

In addition, the researchres organized 3 international conferences, co-organized many symposiums in international conferences and participated in the scientific committees and as chair members, and participated in the SOMMa 100xciencia.3 meeting.

12-14 March:
COST TO-BE Spring Meeting "Towards Oxide Electronics" organized by RL3 ICMAB researchers in Sant Feliu de Guíxols

23-27 July:
International Conference and Workshop on High Pressure Semiconductors & Superconductors Physics in CosmoCaixa (Barcelona) organized by RL1 ICMAB researchers

15 November:
#100xCiencia.3 Meeting: Bridging Science and Society in CNIO (Madrid) with the participation and collaboration of ICMAB researchers

10-12 December: International Conference on Phosphorus, Boron and Silicon (PBSi 2018) organized in Barcelona by RL5 ICMAB researchers

COURSES AND WORKSHOPS

Workshops and Summer schools

Each RL organizes a workshop and/or a summer school per year. Workshops are small conferences that typically last two days and feature international invited speakers. It also gives ICMAB students and young postdocs an opportunity for visibility of their research activity and exposes them to a stimulating international environment. Summer schools are weekly long schools that include lectures and hands-on sessions with international professors and networking activities. In 2018, the RL1 and RL2 organized the summer school "Materials for Energy" (MATENER) on 17-20 September 2018. More than 40 students participated in the event. In addition, the RL3 organized the summer school in the framework of the EU COST action "TO-BE" on Oxide Electronics. The RL5 organized the one-day workshop "Nanomaterials and plants" in collaboration with the CRAG (Center for Research in Agricultural Genomics), and the RL3 co-organized a workshop on Atomic Layer Deposition. ICMAB researchers also collaborated in the organization of two other summer schools: the ICFO school on emerging photovoltaics (in collaboration with ICFO), and the summer school in nanoscience (organized by the UIMP)

Complementary skills courses and workshops

At the ICMAB we also make an effort to offer transversal knowledge to our researchers: skills on scientific presentations, use bibliographic tools, project management or how to protect knowledge through patent filling are essential. Researchers also learn scientific writing and results communication.

Support the participation in international conferences

We financially support the attendance to international conferences for our researchers (especially PhD fellows), so that they can present their research outside the walls of the ICMAB. In the two calls that we opened we were able to support the travels of 14 PhD students, all of them delivering an oral presentation at flagship conferences about materials science.

Networking activity during the "Materials for Energy" Summer school (MATENER)

Technology and Knowledge Transfer

The mission of the Knowledge Transfer Unit (KTU) at ICMAB is to translate the ICMAB research into social use via technology and knowledge transfer through a process that provides social and economic benefits to the ICMAB, the Industry and the society

We are approaching a quality improvement of our technology transfer processes, especially for new marketing opportunities of our research results. For this reason, in 2018 we have completed the project "Review of technology transfer practices at ICMAB: assessing the technology transfer potentials along selected value chains" commissioned by the Fraunhofer-IMW.

Following the KTU improvement plan, we have increased our Human Resources by incorporating one new expert with strategic capabilities, especially in IP issues.

To date we have filed and licensed a significant number of patents, and we are responsible of advising our researchers in IPR related matters.

The 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:

- **FORTISSIMO** on computationally intensive simulations.
- **COMMON SENSE** responds to requests for integrated and effective data acquisition systems by developing innovative sensors that will contribute to our understanding of how the marine environment functions.
- **SEA-ON-A-CHIP** deals with the real time monitoring of SEA contaminants by an autonomous Lab-on-a-chip biosensor.
- **NAIADES** with the aim of develop and demonstrate the ambient Na-ion battery under realistic conditions as an effective alternative to the Li-ion battery for stationary Electric Energy Storage (EES) application.
- **SMART-4-FABRY** deals with the reduction on the Fabry disease tratment cost and a substantial improvement in the life-quality of Fabry disease patients.
- **FASTGRID** with the aim of enhancing the technical and economical attractiveness of high-temperature superconductor (HTS) coated conductors (REBCO conductors) for their application in SuperConducting Fault Current Limiters (SCFCL).
- **KARDIATOOL** translates a laboratory proven concept of a saliva biosensor to the clinical practice for addressing the priority needs in personalized HF diagnostics and therapy monitoring at the point of care.
- **E-MAGIC** aim is on practical Rechargeable Magnesium Batteries (RMB) as a cutting-edge high-risk / high-reward research and innovation that aim to demonstrate a new technological paradigm.

In 2018, particularly, we signed contracts with the following companies and institutions:

- Pharmaceutical companies: Grifols, Interquim, Mohes and Medichem
- Energy storage and batteries: Repsol
- Spin-offs: Nanomol Technologies, Oxolutia
- Technological centers: Fundació Eureca
- Global Institutions:
    - CEA-Comissariat à l'énergie atomique et aux énergies alternatives
    - SRON-ESA
    - ISG Global and USAID
    - Max Planck
    - WWSC

We also participated in industrial national projects called "Retos colaboración", which are led by the following companies: Pharma Mar and Almirall.

In 2018, the ICMAB has applied for 6 patents:

1. A post-functionalizable, sustainable and cost-effective graphene aerogel. A. López-Periago
2. Flexible graphene oxide electrodes by laser radiation. A. Pérez.
3. Quantum rods obtained in water with enhanced fluorescence intensity. F. Teixidor.
4. Quantum rings obtained in water with enhanced fluorescence intensity. F. Teixidor.
5. Mineral ice nucleation in sprays at high temperatures. A. Verdaguer
6. Superconducting material and process for producing the same. T. Puig

Some of our patents are in co-ownership with companies:

1. Insect repulsion and/or barrier arrangement and method for repelling insects. E. Molins, with Biogent
2. Mineral ice nucleation in sprays at high temperatures. A. Verdaguer, with Technoalpin
3. Superconducting material and process for producing the same. T. Puig, with Oxolutia

And we have licensed the following patent:

- Mineral ice nucleation in sprays at high temperatures. A. Verdaguer. Company: Technoalpin

Communication & Outreach

The ICMAB Communication & Outreach Office offers a range of services to effectively disseminate the knowledge generated at the Institute. Its goal is to maximise impact across all key stakeholder groups. Its actions are aimed at finding the most effective way to engage a range of audiences, from the internal community to industry and schools.
Among its responsibilities are:

• Internal communication: encourage collaboration, act as an information and consultation point, welcome protocol, organize events, communication plan
• Corporative image: institutional image, visual identity, logos, templates, posters, graphic design, ensure the quality of internal and external texts
• Protocol and public relations: visits, international days, conferences, celebrations
• External communication: management of the ICMAB website, social networks, newsletter, mailing lists
• Relationship with the press: press releases, science websites, coordination with the CSIC Communication Department
• Public engagement and science education activities and school visits: joint activities with BNC-b cluster and CSIC, prepare proposals for funding (FECYT, FGCSIC), promotional videos, contests and exhibitions
• Scientific events: coordinate summer schools, scientific meetings and seminars organized by ICMAB researchers

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.

A couple of news reports appeared in La Vanguardia and El Periódico, in which our researchers were stars, and we were also on the radio and TV:

- Els materials que canviaran el món (La Vanguardia, 19 August 2018)
- El repte de ser científiques i mares (El Periódico, 23 September 2018)
- Superconducting materials and levitation of magnets with Teresa Puig in "Els Matins de TV3"

SCIENCE EDUCATION ACTIVITIES

MATHEROES: Supermaterials, the heroes of the future

This is a project with FECYT and Severo Ochoa funding, in collaboration with Esciencia (Zaragoza), and with the participation of many ICMAB researchers.

A researcher in your classroom (12 sessions in 2018)

In this programme, an ICMAB researcher gives a talk in an educational center, usually a highschool or primary school.

Student stays at ICMAB during July 2018:

The students who join us, spend some weeks doing a research project within one of our research groups.

- Joves i Ciència (Fundació Catalunya La Pedrera) (7 students for one month)
- Programa Argó UAB (4 students for 3 weeks)

Students from the Societat Catalana de Química (2 students for 2 weeks)

ESCOLAB – School visits at our center (7 visits in 2018)

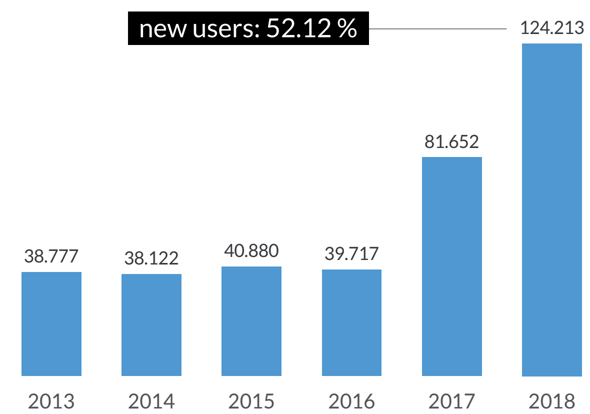
This programme allows us to receive the visit of highschool students who spend a morning with us for a science talk and visit to some of our laboratories.

Dramatised Reading "Madame Châtelet and her Instagram Followers "

This dramatized reading, prepared by a group of women from the ICMAB, explains the life and discoveries of some wise women of our history, to visibilize the role of women in science and encourage scientific vocations.

Other courses and visits:

- Seminari Permanent Física i Química
- "Dissabtes de la Física"
- Students visit from the Festival Nanoscience and Nanotechnology 10alamenos9
- XXX Chemistry Debate Bojos per la física - Mad for physics
- The FUB+GRAN nanotechnology students from Manresa visit the ICMAB
- «From quantum physics to nanotechnology»
- The ICFO School on Emerging Photovoltaics visits the ICMAB research labs
- Little scientists for a day: great Kids' Day at ICMAB 2018!
- Talk "Els nanomaterials per a la transició energètica" by Xavier Obradors at the RACAB
- "Converteix-te en un detectiu de materials" brings more than 100 students at ICMAB for the Science Week!



Website visitors 2018

WEBSITE AND SOCIAL NETWORKS

There is a 53 % increase in the number of users of our website, compared to 2017, and a 23 % increase in the number of sessions. Moreover, we have more users between 25 and 35 years old than what we used to have.

We are happy to announce that the ICMAB website was the most visible CSIC website in 2018, according to the "Research centers websites ranking", and rose from the fourth place to the second place in the total score, out of a total of 138 CSIC institutes websites.

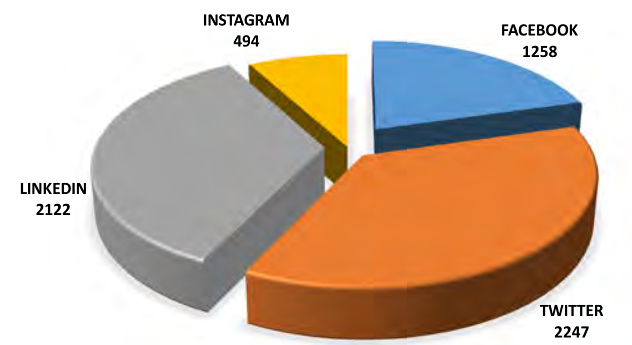
In addition, a 30% increase in followers has been observed in our main social networks, Twitter (>2200), Facebook (>1200), a 14 % increase in LinkedIn (>2100) and an 86 % increase in Instagram (>490), in the same period.

MAILING & INTRANET

The new weekly newsletter has nearly 500 subscribers. In every newsletter we send the latest news from our website, plus the forthcoming events and seminars at the ICMAB or BNC-b cluster, job offers and conferences and meetings organized by our researchers. We have another mailing list only for our staff, and another one for students and young people who might be interested in starting out their research career with us.

OUTREACH ACTIVITIES

- Nanoscience and Nanotechnology Festival 10alamenos9
- Feynman Total
- Participation in the CSIC project "Las Científicas Cuentan"
- YoMo - Youth Mobile Festival
- "Espai Ciència al Saló de l'Ensenyament"
- Exporecerca
- Festival Barcelona Ciència
- Pint of Science Festival
- Barcelona Maker Faire
- European Researchers' Night
- Expominer
- Science Tech Girls Vallès
- Setmana de la ciència - Science week



CELEBRATIONS

This year we have organized:

- Book exchange for Sant Jordi
- The Institute's Anniversary Party
- FOTICMAB photo contest for our staf. The "Photonic leaf" was the winner of the contest, by Cristiano Matricardi
- The Christmas party with a talk by Xavier Lasauca
- The Kids' Day with more than 80 kids from our staff
- Toni Pons retirement

CORPORATIVE 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. We continue with our welcome pack for our staff (old-timers and newcomers) consisting of a mug and a bag. This year, the new merchandising includes black and blue pens, USBs and folders for our conferences and meetings.

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 2018 the Unit was formed by Montse Salas, and Laura Cabana, who substituted Jorge Pérez

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 2018 we continued with a high success in international grant attraction: 3.8 M€ were from European H2020 projects, and 2.6 M€ from National projects. In total, we had 34 EU ongoing projects, 4 of them started in 2018: a new ERC Consolidator grant was awarded, a new FET-Proactive project, as well as two MSCA IF projects.

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 were incorporated during the second semester of 2018. 5 of them stated at the ICMAB their PhD.

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 finish in 2020. During 2018, ICMAB has participated in the following way: we have received 16 users to our facilities, from France, Italy, India, Switzerland, Russia, Germany and China.

The installations used in 2018: scanning electron microscopy (SEM), atomic force microscopy (AFM), X-ray diffraction (XRD), electron paramagnetic resonance (EPR), magnetometry by Superconducting Quantum Interference Devices (SQUID), Raman Spectroscopy, Pulsed Laser Deposition (PLD) and lithography. We also hosted one researcher who came to the ICMAB to learn the Raman spectroscopy technique with Alejandro Goñi for one week.

Two articles were published as a result of the NFFA exchange programme:

- ***Direct and Converse Piezoelectric Responses at the Nanoscale from Epitaxial BiFeO3 Thin Films Grown by Polymer Assisted Deposition.***
José M. Vila-Fungueiriño, Andres Gomez, Jordi Antoja-Lleonart, Jaume Gazquez, César Magén, Beatriz Noheda and Adrian Carretero-Genevrier. Nanoscale, 2018, 10, 20155-20161. DOI:10.1039/C8NR05737K

- ***Epitaxial La0.7Sr0.3MnO3 thin films on silicon with excellent magnetic and electric properties by combining physical and chemical methods.***
José Manuel Vila-Fungueiriño, Jaume Gázquez, César Magén, Guillaume Saint-Girons, Romain Bachelet, Adrián Carretero-Genevrier. Science and Technology of Advanced Materials, 2018, 19, 1, 702-710- DOI: 10.1080/14686996.2018.1520590

Anna May (Communication & Outreach), Laura Cabana (Strategic Managing Unit), Xavier Obradors (ICMAB's Director) and Montse Salas (Strategic Managing Unit)

Responsible Research and Innovation (RRI)

At the ICMAB we are clearly aware that any activity carried out at the ICMAB should be conducted by adhering to Responsible Research and Innovation (RRI) principles, namely:

1.- Governance to prevent harmful or unethical developments of our research and innovation.
2.- Open Access to research results and publications to boost innovation and increase the use of scientific results.
3.- Ethics to respect ethical standards and fundamental rights in response to societal challenges.
4.- Gender equality, and in a wider sense, diversity in research teams and topics.
5.- Public Engagement of all societal actors (researchers, industry, policy makers, civil society) for a reflective research process.
6.- Science Education to enhance current education processes and to better equip future researchers and society as a whole, with the necessary competences.

ETHICS

On 16 March 2018, with the aim of introducing this concept to the research community at ICMAB, and in collaboration with the Marie-Curie Initial Training Network (ITN) i-Switch, a workshop on "Ethics and Responsible Research & Innovation in Research" (RRI2018) was organized.
The workshop gathered several experts from the field that provided us with some insights on how to deal with some of the aspects included in RRI, from ethics and gender aspects in research to integrity and scientific misconduct. Two practical workshops focusing on the promotion of RRI and the available methods to implement it, by Rosina Malagrida (IrSiCaixa), were also included.

OPEN ACCESS

At the ICMAB we encourage the Golden Route to open access publications by the systematic use of CSIC's open access publication support agreements (RSC, ACS, Frontiers, PNAS, Springer Open), and we optimize the self-archiving (Green Route), by uploading the postprints to the Digital CSIC institutional repository with the help of our Librarian & Documentalist. Giving open access to our scientific results is essential to boost the benefits of the public investment in research and increase knowledge dissemination, following European and National policies.

We are planning to implement a system for the progressive increase of datasets associated to the published articles deposition and to offer specific training for our research staff on open access, open science and RRI issues From October 22 to October 28, we celebrated the International Open Access Week 2018, organized by the SPARC* (Scholarly Publishing and Academic Resources Coalition), with the slogan "Setting the Default to Open". The idea was to share the idea that Open Access is the most effective way to disseminate research!
ICMAB authors published in 2018 a total of 226 articles indexed in the Web of Science, from which 128 are currently open access: 52 are Gold Open Access, and 92 are found in the Digital CSIC Institutional repository, some already in open access and others still with the embargo.

GENDER EQUALITY

In 2018, the ICMAB was awarded by the CSIC with the Gender Equality Certificate (Distintivo de Acreditación en Igualdad de Género), in its first edition. This certificate was promoted by the CSIC President, Rosa Menéndez, following an explicit commitment to offer equal opportunities for men and women in their workplaces. The objective of the call was to promote gender perspective in all the CSIC institutes, and to promote measures to eliminate the barriers that women may encounter during their career. The Gender Equality Committee was engaged to organize the activities to celebrate the International Day of Women and Girls in Science. During the second and third weeks of February, the ICMAB celebrated the International Day of Women and Girls in Science, which was declared in 2016 by the United Nations to be on February, 11.
The slideshow and twitter campaign "I became a scientist" showed how and why did the women at ICMAB became researchers, and what did they want to do when they were kids.

In the framework of "11defebrero" and "A researhcer in your classroom", researcher Ana M. López gave a talk to secondary school students at La Ferreria (Montcada), Stefania Sandoval at La Guineueta (Barcelona), and Esther Barrena at Institut Provençana (Hospitalet de Llobregat). Anna Roig brought the play "Madame Châtelet and her Instagram followers" at Escola Can Periquet (Palau-solità i Plegamans).
To raise awareness about gender issues also among our staff, we hang some posters with some quizzes prepared by the Gender Equality Committee about curious facts on women in science and gender issues.
Anna May, Communication & Outreach Officer, and Mariona Coll, researcher at the Superconducting Materials Groups, participated on February 6 at a roundtable on "Women and Science: Breaking Stereotypes", at Ateneu Barcelonès (Barcelona). The event was organized by EspaiNANO, the Gender Committee of the Physics Department at UB, and the Nanoscience and Nanotechnology Festival "10 a la menos 9".
The dramatized reading "Madame Châtelet and her Instagram followers" was represented for a highschool in Barcelona (13 February 2018) and at the ICMAB (9 March 2018).

The Châtelet team from ICMAB went to congratulate Margarita Salas, now Doctor honoris causa by the UAB

ACKNOWLEDGEMENTS

MINISTERIO DE CIENCIA, INNOVACIÓN Y UNIVERSIDADES

erc

investing in your future
European Regional Development Fund
European Union

Agència de Gestió d'Ajuts Universitaris i de Recerca

ICREA

UAB
Universitat Autònoma de Barcelona

EXCELENCIA SEVERO OCHOA

SOMM EXCELLENCE ALLIANCE

UAB CEI
CAMPUS OF INTERNATIONAL EXCELLENCE

tecnio catalonia
Fins a 31/12/2019
ACCIÓ
Generalitat de Catalunya

CSIC IRTA UAB
Parc de Recerca UAB

bnc-b
BARCELONA NANOTECHNOLOGY CLUSTER-BELLATERRA

ciber-bbn
Centro de Investigación Biomédica en Red
Bioingeniería, Biomateriales y Nanomedicina

nanbiosis
Infrastructure of Production and Characterization
of Nanomaterials, Biomaterials and Biomedical Systems

Annual Report 2018

We are sure that you have felt the ICMAB environment and enthusiasm all through this report. If you want to still have more information about the ICMAB activities you can access the website version of our report at resources.icmab.es/annualreport2018

INSTITUT DE CIÈNCIA DE MATERIALS DE BARCELONA - ICMAB-CSIC   ANNUAL REPORT 2018

Cover Image: "Photonic Leaf" by Cristiano Matricardi