Institut de Nanociència i Nanotecnologia

ACTIVITY REPORT 2017-18

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UNIVERSITAT DE BARCELONA

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i Nanotecnologia

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1. FOREWORD

FOREWORD

DR. GUILLEM AROMÍ BEDMAR
IN²UB Director

The Scientific Activity Report you have in your hands summarizes two years of intense and continued efforts by the dedicated group of scientists conforming the Institute of Nanoscience and Nanotechnology of the University of Barcelona (IN²UB). Created in 2006, the Institute aims to harness the multidisciplinary skills of the UB researchers interested in nanotechnology, with a view of favoring ambitious collaborative research. Thus, it integrates members from up to six Faculties of the University, namely Physics, Chemistry, Farmacy, Medicine, Biology and, most recently, Geology. As a Director, it has been to me a huge responsibility and a tremendous challenge to uphold the high standards set out by my predecessors, Prof. Amilcar Labarta and Prof. Jordi Borrell.

The IN²UB is devoted to serve society in three fronts; *i)* **frontier scientific research**, *ii)* **excellent teaching and education**, and *iii)* **technology transfer and outreach**. In the arena of scientific excellence, the period covered by this memoir has witnessed the production of more than **650 research articles**, of which, more than 82% belong to the first quartile. This impressive production of knowledge has been sustained by funds from local Catalan, Spanish or European competitive grants attracted by our researchers, amounting to about 7 MEur. During this period, the steering committee has reorganized the scientific domains of activity in order to better map out the nature of our research. The internal scientific committee has also been renewed and enlarged, while a prestigious external scientific advisory board has been recently put into place. With these actions we have provided the organization with a set of powerful tools and with considerable muscle to set solid scientific policies and strategies.

During the years covered by this memoir, the successful IN²UB program of **internal collaborative research grants (ART, transversal research actions)** has been provided with increased resources. The Institute is seeing already the fruits from these efforts in form of common interdisciplinary joint ventures among different groups from the organization. Meanwhile, the Institute has continued to contribute to the funding of **international conferences** organized by its members. Noteworthy, a regular program of **research seminars (IRS, International Research Seminars)** has been recently put into place by the IN²UB, which gives to our community the opportunity to listen every month to a prestigious expert in any of the domains of the nanotechnology world.

The mission of enhancing postgraduate education is facilitated to the IN²UB by the existence at our University of a **Masters' Program of Nanoscience and Nanotechnology** (taught entirely in English) and the **Doctorate of Nanoscience**. Both programs are not only coordinated by members of our Institute. Most of the Master courses are tough by IN²UB professors, while the research credits are mainly conducted at groups from the Institute as well as most of the PhD thesis of the Doctorate. The IN²UB has continued to use part of its structural funds to offer student fellowships to develop Masters' theses within the research groups of its members, while the University of Barcelona still yields to the research groups of the Unit a quota of its PhD fellowships, most of which feed the Doctorate of Nanoscience. The above-mentioned IRS program has been very useful for exposing the students from both programs to seminars by some of the best current scientist involved with Nanotechnology.

This report mirrors the commitment of IN²UB researchers with technology transfer, in form of patents and up to six active spin off companies. Along these lines, we have completed the process to participate, for the first time in the **Business Forum** taking place every year at the Chemistry and Physics Department of the UB.

The true devotion of the Institute to science outreach is illustrated by the very active participation of our scientists in very popular science fairs, addressed to the general public. These include the festival **10alamenos9**, **Festa de la Ciència**, **European Research Night**, etc. The current steering committee has formalized this genuine interest with the creation of a Permanent Commission of Outreach within our Institute, which has been extremely useful to increase, organize and expand the involvement of the IN²UB on this important facet.

I would like to finish this foreword by thanking all the members of the IN²UB for contributing with their talent and generous efforts to make this unit a better platform for the creation, transfer and outreach of knowledge, better serving the University community and society as a whole.

1. ACTIVITY REPORT 2017-18

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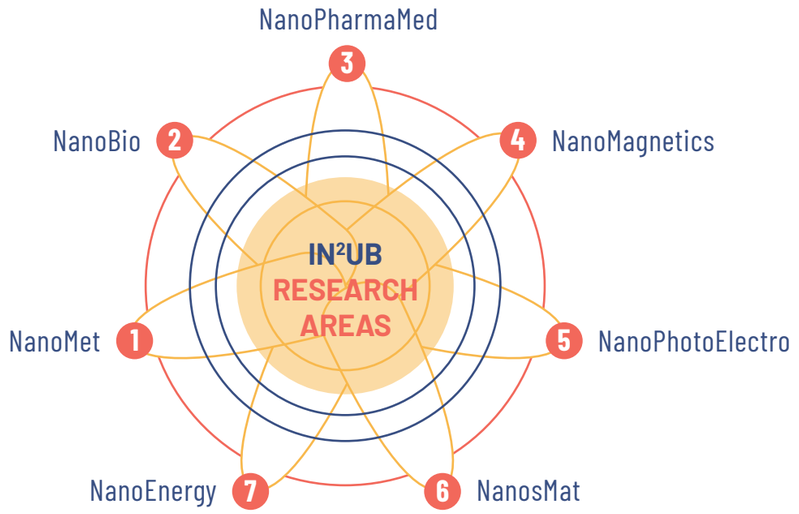
1. ABOUT IN²UB

1.1. PRESENTATION

The Institute of Nanoscience and Nanotechnology of the University of Barcelona (IN²UB) was created in 2006. Its main goal is to coordinate and enhance multidisciplinary research among research groups from the Faculties of Chemistry, Physics, Pharmacy and Food Sciences, Biology, Earth Sciences and Medicine and Health Sciences that work on the different phenomena occurring at the nanoscale. This collaborative spirit aims at integrating both, internally and internationally, interdisciplinary activities which integrate equally, basic and applied research.

The IN²UB wants to contribute to the progress of science, while spurring, at the same time, industrial excellence. In this sense, several spin-off companies are now led by IN²UB researchers. Finally, all members of the IN²UB are strongly involved in teaching duties, the most important program being the Master of Nanoscience and Nanotechnology and the Doctoral Program in Nanoscience and Nanotechnology. Research and education are our strong commitments with the society.



IN²UB gathers around 200 researchers (including permanent, postdoctoral researchers and PhD Students). They are organized in 49 research groups distributed among seven major research areas.

Research Areas:

1. Modeling, Simulation and Nanoscopic Methods (NanoMet)
2. Nanobioscience, Nanobiomechanics and BioNanotechnology (NanoBio)
3. Nanopharmaceutics and Nanomedicine (NanoPharmaMed)
4. Nanomagnetism and Spintronics (NanoMagnetics)
5. Nanoelectronics, Nano-optics and Nanophotonics (NanoPhotoElectro)
6. Nanostructured materials (NanosMat)
7. Nanoenergy: Production and Storage (NanoEnergy)

1.2. ORGANIZATION

Director: **Dr. Guillem Aromí Bedmar**

Secretary: **Dr. Albert Romano Rodríguez**

STEERING COMMITTEE

- Dr. Xavier Batlle Gelabert
- Dr. Enric Bertran Serra
- Dr. Gustavo Egea Guri
- Dr. Sònia Estradé Albiol
- Dr. Giancarlo Franzese
- Dr. M. José García Celma
- Dr. Blas Garrido Fernandez
- Dr. Frank Güell Vilà
- Dr. Narcís Homs Martí
- Dr. Sergi Hernández Márquez
- Dr. Jordi Ignés Mullol
- Dr. Francesca Peiró Martínez

RESEARCH AREAS COORDINATORS

1. NanoMet: Dr. Francesca Peiró
2. NanoBio: Dr. Gustavo Egea
3. NanoPharmaMed: Dr. M José García-Celma
4. NanoMagnetics: Dr. Xavier Batlle
5. NanoPhotoElectro: Dr. Blas Garrido
6. NanosMat: Dr. Enric Bertran
7. NanoEnergy: Dr. Narcis Homs

INTERNAL SCIENTIFIC BOARD

- Dr. Maria Pilar Vinardell Martinez Hidalgo (President)
- Dr. Ramon Farre Ventura
- Dr. Amílcar Labarta Rodríguez
- Dr. Francesc Sagués Mestre

SCIENTIFIC ADVISORY BOARD

- Dr. Ivan Schuller (UC San Diego) (President)
- Dr. Kenneth Dawson (UC Dublin)
- Dr. Katja Schenke-Layland (Eberhard Karls University Tübingen)
- Dr. Maria Jesús Vicent (Centro de Investigación Príncipe Felipe)

OUTREACH COMMISSION

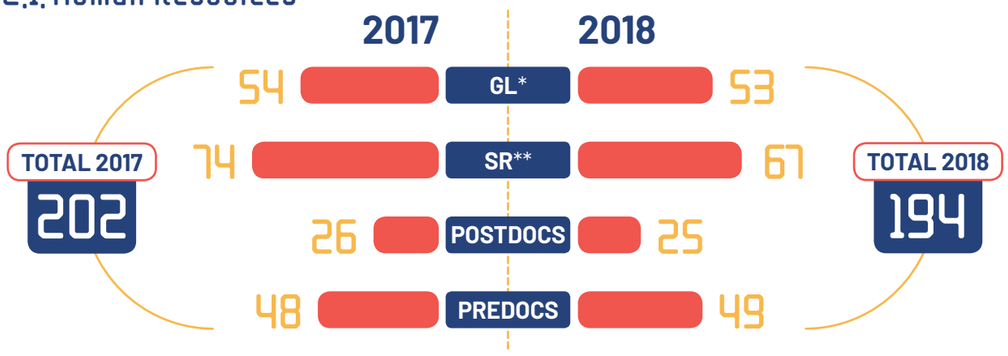
Dr. Sònia Estradé (Coordinator);
Dr. Xavier Batlle; Dr. Giancarlo Franzese;
Dr. M. Aranzazu Fraile; Dr. Blas Garrido;
Dr. Oscar Iglesias; Dra. Francesca Peiró;
Dr. Laura Rodríguez; Dr. M. Antònia Busquets;
Dr. Giancarlo Franzese; Mariona Escoda,
Elena Lopez; Dr. Jordi Díaz i Dra. Sonia Trigueros.

Contact: in2ub-divulga@ub.edu

RESEARCH MANAGEMENT

Dr. Ifigènia Saborit Villarroya

1.2.1. Human Resources

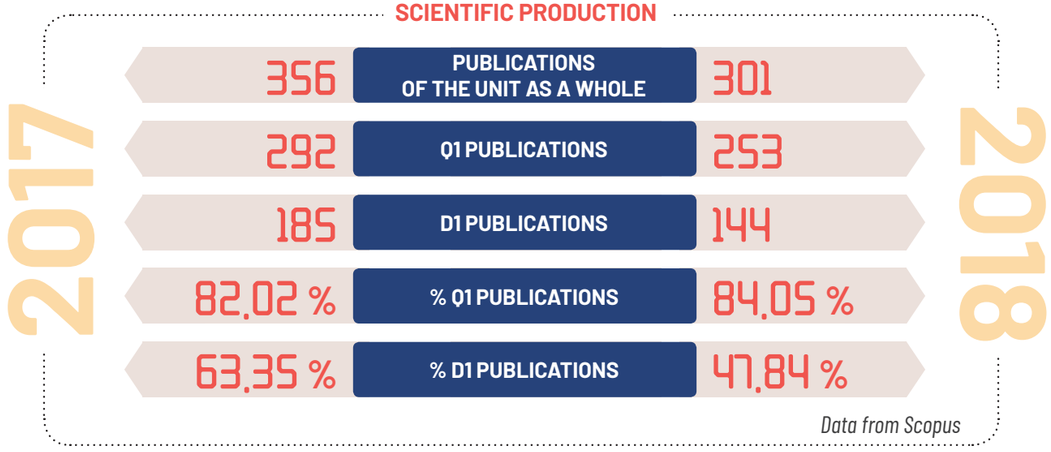


**GL: Group Leader, leading an independent research group at the unit*

***SR: Senior researcher, Investigator leading one or several projects in a research group, but not being GL*

1.3. RESEARCH OUTPUTS AND FUNDING SOURCES

The following major subject areas represent IN²UB scientific production: Chemistry, Physics and Astronomy and Material Science, Biochemistry, Genetics and Molecular Biology, Engineering, Medicine and Chemical Engineering, Pharmacology and Pharmacology, Toxicology and Pharmaceutics. The rest of IN²UB publications, are integrated in other related fields such as Mathematics, Energy and Environmental Science. So, it is to note that IN²UB is really a multidisciplinary research unit, mainly harvesting research in the field of Chemistry, Physics, Material Science, Pharmacology and Biology. The analysis of these areas during 2017-2018 period, represented 657 papers published in indexed journals in Scopus, with an average of 83.03% of this production at first quartile.



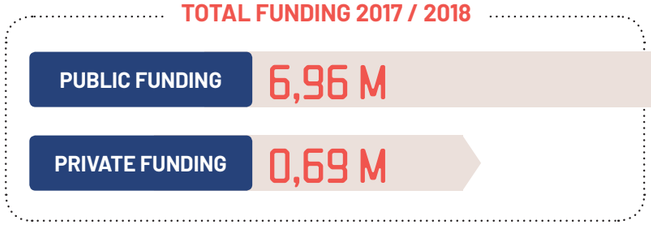
1.3.1. High Index Publications 2017-2018

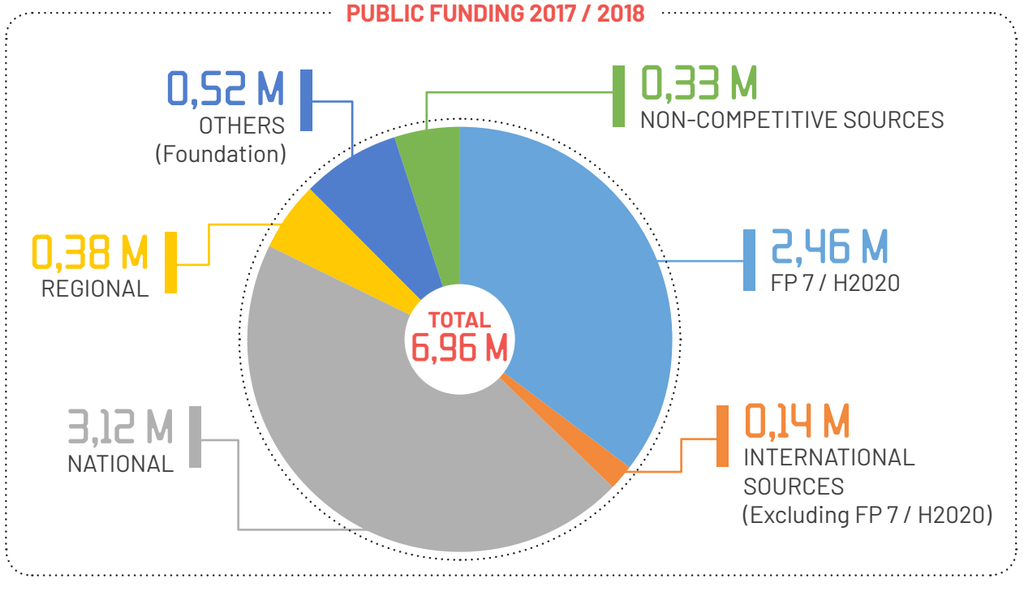
- *Experimental measurement of binding energy, selectivity, and allostery using fluctuation theorems.* Camunas-Soler J., Alemany A., Ritort F. *Science*. Vol. 355, Issue 6323, pp. 412-41. (2017)
- *Force Triggers YAP Nuclear Entry by Regulating Transport across Nuclear Pores.* Elosegui-Artola A., Andreu I., Beedle A.E.M., Lezamiz A., Uroz M., Kosmalska A.J., Oria R., Kechagia J.Z., Rico-Lastres P., Le Roux A.-L., Shanahan C.M., Trepat X., Navajas D., Garcia-Manyes S., Roca-Cusachs P. *Cell* , 171, (6), 1397-1410. (2017)
- *Taming active turbulence with patterned soft interfases*. Guillamat P., Ignés-Mullol J., Sagués F. *Nature Communications* volume 8, Article number: 564 (2017)
- *Single molecule high-throughput footprinting of small and large DNA ligands.* Manosas M., Camunas-Soler J., Croquette V., Ritort F. *Nature Communications* volume 8, Article number: 304 (2017)
- *A Magneto-optical Molecular Device: Interplay of Spin Crossover, Luminescence, Photomagnetism, and Photochromism.* Estrader M., Salinas Uber J., Barrios L.A., Garcia J., Lloyd-Williams P., Roubeau O., Teat S.J., Aromí G. Angewandte *Chemie - International* Edition vol: 56 (2017)
- *Lipid nanoparticles (SLN, NLC): Overcoming the anatomical and physiological barriers of the eye -Part II - Ocular drug-loaded lipid nanoparticles.* Sánchez-López E., Espina M., Doktorovova S., Souto E.B., García M.L. European *Journal of Pharmaceutics and Biopharmaceutics* 110, 58 (2017)
- *A multicaloric cooling cycle that exploits thermal hysteresis*. Gottschall T., Gràcia-Condal A., Fries M., Taubel A., Pfeuffer L., Mañosa L., Planes A., Skokov K.P., Gutfleisch O. *Nature Materials* 17, 929 (2018)

- *Anomalously low dielectric constant of confined wàter*. Fumagalli L., Esfandiar A., Fabregas R., Hu S., Ares P., Janardanan A., Yang Q., Radha B., Taniguchi T., Watanabe K., Gomila G., Novoselov K.S., Geim A.K. *Science* 360, 1339 (2018)
- *How small amounts of Ge modify the formation pathways and crystallization of kesterites*. Giraldo S., Saucedo E., Neuschitzer M., Oliva F., Placidi M., Alcobé X., Izquierdo-Roca V., Kim S., Tampo H., Shibata H., Pérez-Rodríguez A., Pistor P. *Energy and Environmental Science* 11, 582 (2018)
- *Giant intrinsic circular dichroism of prolinol-derived squaraine thin films*. Schulz M., Zablocki J., Abdullaeva O.S., Brück S., Balzer F., Lützen A., Arteaga O., Schiek M. *Nature Communications* volume 9, Article number: 2413 (2018)
- *3D Electrophoresis-Assisted Lithography (3DEAL): 3D printing functional molecules to create anisotropic hydrogels*. J.P. Aguilar, M. Lipka, G.A. Primo, E.E. Licon-Bernal, J.M. Fernández-Pradas, A. Yaroshchuk, F. Albericio, A. Mata. *Advanced Functional Materials* 28, 1703014-1/10 (2018)
- *Caloric response of Fe49Rh51 subjected to uniaxial load and magnetic field*. Gràcia-Condal A., Stern-Taulats E., Planes A., Mañosa L. *Phys. Rev. Materials* 2 (2018)

1.3.2. Inputs 2017/2018

The graphic and pies below show the amount available during 2017/2019.





1.3.3. Transfer Indicators

Another interesting indicator is the number of spin-off companies emerged from IN²UB. The Institute has 6 spin-offs currently active, which are described below:

- Impetux Optics, S.L., created in 2012 lead by Mario Montes. Impetux Optics focuses its activity on Design, Manufacturing and Marketing of optical force measurement systems for Optical Tweezers. The company makes available a patented technology that overcomes existing limitations, providing clear advantages when measuring optical forces. The systems developed, allow force measurements in experiments where trap stiffness calibration is difficult or impossible.
- Advanced Nanotechnologies, S.L., created in 2012 by Enric Bertran, Esther Pascual y José Luís Andújar. Advanced Nanotechnologies S.L. is devoted to materials and surface applications addressed to general consumers and to the business market. It supports R&D projects by developing specific processes and equipment for each application. The company offers innovative solutions based on nanotechnology adapted to specific developments of the costumers, related to the manufacturing of nanostructured materials. It offers also consultancy services.
- Smalle Technologies, S.L. (by Christophe Serre, Alejandro Pérez Rodríguez), created in 2012. Smalle Technologies is a company that develops new methods for maximizing the benefits from renewable and sustainable energy sources in order to address energy supply shortages of off-grid devices. Smalle Technologies develops generators that transform the energy contained in the waves into electricity to supply power to off-shore devices.
- EndoASIC, S.L. (2013) (Dieguez Barrientos, Angel; Alonso Casanovas, Oscar and Vila Arbones, Ana Maria members of the entrepreneurial group). This company develops, micro and nanotechnologies, autonomous minimally invasive systems for the substitution of gastrointestinal endoscopic systems.
- Enlighting Technologies, created in 2016 by Blas Garrido and Sergi Hernández. It aims at achieving a more comfortable and adaptable light to each need and situation. They have developed the FLEXILIGHT-UB technology, which is able to reproduce any spectrum of light accurately and imitate any kind of light.
- ColorSensing, S.L, created in 2018 by Daniel Prades, devoted to smart packaging for food processing efficiency, quality, and safety.

During this reference period, IN²UB had applied for 6 priority patents and 4 PCT/EUR/ USA patents.

2. RESEARCH AT IN²UB

2.1. RESEARCH LINES

1 MODELING, SIMULATION AND NANOSCOPIC METHODS (NANOMET)

This research area develop instrumentation and methodology (employing experimental and theoretical tools) to characterize nanostructures and nanosystems of any nature,

- **A.** NanobioInteractions: Interactions between biological and nanoscopic systems.
- **B.** Confinement-related phenomena: reactivity, magnetism, optoelectronics and quantum photonics.
- **C.** Transport and conduction.
- **D.** Surface effects.
- **E.** Electronic structure and excitations.
- **F.** Bose-Einstein condensates and quantum confined gases.
- **G.** Advanced Electronic Microscopy (EFM, TEM, STM, EELS, EDS)
- **H.** Instrumentation and Methodology Development in Electron Microscopy.

2 NANOBIOSCIENCE, NANOBIOMECHANICS AND BIONANOTECHNOLOGY (NANOBIO)

This research area studies the organizational patterns observable in the molecular structures that control and rule the biological systems both at the cellular and at the molecular scales. Its most relevant application is that of developing techniques and devices aimed at prevention and diagnose in nanomedicine.

- **A.** Functionalisation of surfaces.
- **B.** Cellular and molecular biomechanics
- **C.** Biomimetic structures and systems
- **D.** Nanofluidics and nanorobotics. Nanomotors.
- **E.** Diagnosis in nanomedicine: marking and molecular observation
- **F.** Nanobiosensors; DNA and Protein Chips; lab on chip.

3 NANOPHARMACEUTICS AND NANOMEDICINE (NANOPHARMAMED)

This area aims at developing nanostructured systems for controlled drug release and to the improvement of drug therapeutic efficiency when administered on targets to treat diseases.

- **A.** Nanostructured Systems for controlled drug release. Nanocapsules.
- **B.** Nanostructured systems interaction with biological structures.
- **C.** Bioavailability, toxicity and therapeutic efficiency of nanostructured systems.
- **D.** Non-viral vectors. Gene therapy. Pharmacogenomics and nutrigenomics.
- **E.** Molecular internalization, molecular marking and detoxification.

4 NANOMAGNETISM AND SPINTRONICS (NANOMAGNETICS)

The area aims at developing new systems for storage and processing of information at the nanoscopic scale for information processing. It is also devoted to the study of new phenomena appearing at the nanometric size for the implementation of innovative devices of application in healthcare, sustainable energy, environment, healthy food and security.

It is also involved with the preparation and study of multifunctional molecular nanomagnets for spintronics and quantum computing.

- **A.** Magnetic nanoparticles and single molecule magnets.
- **B.** Dynamic processes in nanomagnetism and interaction with microwaves.
- **C.** Magnetic electronics.
- **D.** Spin-based molecular quantum bits and quantum gates for quantum computing.

5 NANOELECTRONICS, NANO-OPTICS AND NANOPHOTONICS (NANOPHOTOELECTRO)

Study and exploitation at the nanoscale of the interaction of electric, magnetic and optical properties for the design of functional nanosystems.

- **A.** NEMS (Nanoelectromechanical Systems).
- **B.** Nanodevices, nanosensors and electronic nanosystems, optoelectronics and photonics. Photonic crystals.

6 NANOSTRUCTURED MATERIALS (NANOSMAT)

This research area aims at developing new nanostructured materials or improving the properties of existing materials. This line also includes knowledge-frontier research in characterization techniques and manipulation tools at the nanoscale (as electron and probe microscopies, surface analysis, or spectroscopic and magnetic characterization).

- **A.** Synthesis, nanomanufacturing and nanomanipulation.
- **B.** Thin layers, nanostructured multilayers and coatings.
- **C.** Nanoparticles, gels, nanofibers, nanorods, nanothreads and nanotubes.
- **D.** Nanoestructured metallic Oxydes.
- **E.** Mesoporous Materials and Nanopatterns.

7 NANOENERGY: PRODUCTION AND STORAGE (NANOENERGY)

The aim of this research line is the application of nanomaterials to energy production and storage to overcome efficiency and lifetime limits.

- **A.** Catalytic nanostructures for energy production. Fuel cells.
- **B.** Nanomaterials for solar cells and photocatalytic processes.
- **C.** Nanoestructured systems for energy storage.

2.2. GROUPS AT THE RESEARCH LINES

2.2.1. Bioelectrical Characterization at Nanoscale (NanoBio)

Department of Electronics and Biomedical Engineering, Faculty of Physics

Team

- **Gabriel Gomila Lluch (Full Professor)**

Research

The main goal of the group is to develop new experimental setups based on atomic force microscopy and new theoretical frameworks enabling the quantification of the electrical properties of biological systems at the nanoscale (including biomembranes, single viruses, single bacteria cells and eukaryotic cells).

Our main aim is to contribute to develop new label-free biological nanoscale characterization methods and new electronic biosensors.

During these years, the group has been involved in the investigation of the dielectric properties of water confined in nanostructures.

Selected Projects

- Microscopio de barrido de fuerzas eléctricas para medidas electrofisiológicas a la nanoescala. IP. Gabriel Gomila. TEC2016-79156-P. Ministerio de Economía y Competitividad (MCOC), 2016-2019.
- Gabriel Gomila. ICREA Academia. 2015-2019. Fundació Institució Catalana de Recerca i Estudis Avançats (ICREA).

SELECTED PAPERS

- *Direct mapping of the electric permittivity of heterogeneous non-planar thin films at gigahertz frequencies by scanning microwave microscopy.* Biagi M.C., Badino G., Fabregas R., Gramse G., Fumagalli L., Gomila G. *Physical Chemistry Chemical Physics.* Vol: 19. **2017**.
- *Regulation of ribonucleotide synthesis by the Pseudomonas aeruginosa two-component system AlgR in response to oxidative stress.* Crespo A., Pedraz L., Van Der Hofstadt M., Gomila G., Torrents E. *Scientific Reports.* Vol: 7. **2017**.
- Interdigitation in spin-coated lipid layers in air. Dols-Perez A., Fumagalli L., Gomila G. *Colloids and Surfaces B: Biointerfaces.* Vol: 172. **2018**.
- *Anomalously low dielectric constant of confined water.* Fumagalli L., Esfandiar A., Fabregas R., Hu S., Ares P., Janardanan A., Yang Q., Radha B., Taniguchi T., Watanabe K., Gomila G., Novoselov K.S., Geim A.K. *Science.* Vol: 360. **2018**.

2.2.2. Bio-Inorganic Chemistry (BIC) (NanoPharmaMed)

Department of Inorganic and Organic Chemistry, Faculty of Chemistry

Team

- **Patrick Gamez Enamorado (ICREA Researcher)**
- **Amparo Caubet Marín (Associate Professor)**
- **Ana Belén Caballero (Tenure-Track Lecturer)**

Research

The research carried out in **BIC** lies in the areas of cancer and Alzheimer's disease (AD). Great efforts have been/are dedicated to these two fields of investigations; hence, two very important approaches/ innovations recently developed by the group for these two topics can be highlighted.

- Cancer: photoactivatable compounds are receiving increasing attention in anticancer drug design. The **BIC** group has developed a new approach to generate photoswitchable metal complexes whose

biological activity can be changed through the photomodification of the ligand. The pioneering results achieved were published in *Angewandte Chemie* (**2015**, 54, 4561-4565) and *Inorganic Chemistry* (**2016**, 55, 5356-5364 and **2018**, 57, 4009-4022). The Angewandte paper was highlighted by an Associate Editor of ACS Chemical Biology (**2015**, 10, 911-913).

- Alzheimer's disease: amyloid-β is a peptide involved in AD that leads both to oxidative stress and to the formation of senile plaques. The **BIC** team is designing and producing tri- and tetrapeptides that show (i) anti-aggregation properties (thus impeding the formation of amyloid-β fibrils) and (ii) strong copper-binding properties, hence blocking its redox behaviour and therefore the generation of harmful oxidative species; the significant results obtained were published in *Chemistry: A European Journal* (**2016**, 22, 7268-7280 and **2018**, 24, 5153-5162).

The **BIC** group is currently using Fe_3O_4 and Au nanoparticles as nanocarriers and drug-releasing systems for the biologically active compounds described above.

Selected Projects

- GDRI — HC3A (Groupement de Recherche International of CNRS-France), *Hetero-elements and Coordination Chemistry: from Concepts to Applications*; 2015-2018.
- *Multitarget compounds with therapeutic potential against Alzheimer disease: Design and in vitro studies (CHELALZ).* 656820. Horizon 2020. IP: Gamez, Patrick. 2016 –2018.
- *Nanocarriers for drug delivery through thermal release.* CTQ2017-88446-R. Ministerio de Economía y Competitividad of Spain. IP1: Gamez, Patrick 2018 –2020.

Singular Equipment

- Horizontal and vertical gel electrophoresis (analysis of oligo- and polynucleotides)
- Microplate reader (aggregation studies of amyloids)
- Compact xenon light source (photochemistry/photoactivation of drugs)

International Collaborations

- Prof. Norah Barba-Behrens (Univ.Nacional Autónoma de México)
- Prof. Brian J. Frost (University of Nevada, Reno, USA)
- Dr Olga Iranzo (Institut des Sciences Moléculaires de Marseille, France)
- Dr Seiji Komeda (Suzuka University of Medical Science, Japan)
- Prof. Unchulee Chaveerach (Khon Kaen University, Thailand)
- Prof. Piero Mastrorilli (DICATECh, Politecnico di Bari, Italy)

SELECTED PAPERS

- *pH-Driven preparation of two related platinum(II) complexes exhibiting distinct cytotoxic properties*, Jordi Molas Saborit, Amparo Caubet, Rosa F. Brissos, Luís Korrodi-Gregório, Ricardo Pérez-Tomás, Manuel Martínez and Patrick Gamez *Dalton Trans.* **2017**, 46, 11214-11222.
- *Drastic effect of the peptide sequence on the copper-binding properties of tripeptides and the electrochemical behaviour of their copper(II) complexes*, Silvia Mena, Andrea Mirats, Ana B. Caballero, Gonzalo Guirado, Leoní A. Barrios, Simon J. Teat, Luis Rodriguez-Santiago, Mariona Sodupe and Patrick Gamez *Chem. Eur. J.* **2018**, 24, 5153-5162.
- *Photoactivation of the cytotoxic properties of platinum(II) complexes through ligand photoswitching*, Presa A., Vázquez G., Barrios L., Roubeau O., Korrodi-Gregório L., Perez-Tomas R., Gamez P. *Inorg. Chem.* **2018**, 57, 4009-4022.
- *Highly Cytotoxic Ruthenium(II)-Arene Complexes from Bulky 1-Pyrenylphosphane Ligands*, Rosa Brissos, Pau Clavero, Albert Gallen, Arnald Grabulosa, Leoní A. Barrios, Ana B. Caballero, Luís Korrodi-Gregório, Ricardo Perez-Tomas, Guillermo Muller, Vanessa Soto-Cerrato, Patrick Gamez *Inorg. Chem.* **2018**, 57, 14786-14797.
- *Antiproliferative properties of iron supramolecular cylinders*, Rosa F. Brissos, Luís Korrodi-Gregório, Ricardo Pérez-Tomás, Olivier Roubeau, Patrick Gamez *Chem. Sq.* **2018**, 2, 4.

2.2.3. Biomolecule and small-system physics: Small Biosystems Lab (NanoBio)

Department of Condensed Matter Physics, Faculty of Physics

Team

- **Fèlix Ritort Farran (Full Professor)**
- **Maria Mañosas (Postdoctoral Researcher Ramon y Cajal)**

Research

The main goal of the Small Biosystems Lab is to combine advanced experimental techniques and theoretical knowledge to address questions related to energy processes in the nano-scale. The main research lines are single-molecule biophysics and non-equilibrium physics. The research developed has spanned the study of intermolecular interactions (such as peptides and proteins binding to DNA), intramolecular interactions (DNA hybridization, DNA, RNA and protein folding) and fundamental research in nonequilibrium physics of molecular systems, where Brownian fluctuations rule energy, entropy and information flows. The group has also demonstrated the power of combining nonequilibrium physics theories and single molecule methods to extract ligand-DNA binding free energies and binding sites by mechanically footprinting DNA with unprecedented accuracy. Their research is now moving towards information-work energy conversion and how to define thermodynamic information in nonequilibrium processes under feedback control and mutational molecular ensembles.

Two recent developments will expand future research in the group. First, the optical tweezers with temperature controller that operates in the range 5-40ºC. This permits to measure enthalpy and entropy differences down to the single weak molecular bond accuracy (1kcal/mol) improving the knowledge of nucleic acids thermodynamics. Second, a new line of research based on electrical measurements of single molecule translocation across nanopores (using glass pipette nanochannels) is now available in the lab. The new electrical setup combined with optical tweezers allows for controlled molecular translocation through electrical and force measurements, offering a potentially useful tool for single molecule sequencing.

Selected Projects

- *Investigaciones de interacciones intermoleculares en ácidos nucleicos, proteínas y fármacos mediante ensayos de molécula única.* FIS2016-80458-P. IP: Félix Ritort Ministerio de Economia y Competitividad. 2017-2019
- PROtein SEQuencing using Optical single molecule real-time detection (PROSEQO). IP: Félix Ritort. European Union (Horizon 2020). 2016-2019
- ICREA ACADEMIA 2008, 2013, 2018. IP: Félix Ritort. Generalitat de Catalunya (2009-2023).

Singular Scientific Equipment

- Optical tweezers instruments (3 at room temperature, 1 with temperature controller), 1 magnetic tweezers, 1 instrumental setup for single molecule translocation also combined with optical tweezers.

SELECTED PAPERS

- *Force-Dependent Folding and Unfolding Kinetics in DNA Hairpins Reveals Transition State Displacements Along a Single Pathway.* A. Alemany and F. Ritort. *The Journal of Physical Chemistry Letters* Volume 8 895-900. **2017**.
- *Derivation of nearest-neighbor DNA parameters in magnesium from single-molecule experiments.* J. M. Huguet, M. Ribezzi-Crivellari, C. V. Bizarro and F. Ritort. *Nucleic Acids Research* Volume 45 12921-12931. **2017**.
- *Single molecule high-throughput footprinting of small and large DNA ligands.* M. Manosas, J. Camunas-Soler, V. Croquette and F. Ritort. *Nature Communications* Volume 8, 2041-1723. **2017**.
- *Experimental measurement of binding energy, selectivity, and allostery using fluctuation theorems.* J. Camunas-Soler, A. Alemany and F. Ritort. *Science* Volume 355, Issue 6323, 412-415. **2017**.
- *Experimental test of ensemble inequivalence and the fluctuation theorem in the force ensemble in DNA pulling experiments.* A.M. Monge, M. Manosas and F. Ritort. *Physical Review* E 98, 032146. **2018**.

International Collaborations

- Università degli Studi di Padova (Italy); B. Ibarra (IMDEA,Madrid); U. Keyser (U. Cambridge); U. Seifert (U. Stuttgart), P. Pietzonka (U. Cambridge), M. Baiesi and I. Di Terlizzi (U. Padova); A. Alemany (Hubrecht Inst.,Utrecht), J. Johansson and H. Linke (U. Lund), J. M. Parrondo (U. Autonoma Madrid) and M. Ribezzi (ESPCI, Paris), on information-energy conversion; A. Zaltron, G. Mistura, F. Seno (U. Padova), J. Sancho (U. Zaragoza) and S. Frutos (Parc científic, Barcelona) on protein folding; C. V. Bizarro (U. Porto Alegre) on RNA unzipping. G. Wuite (U. Vrije, Amsterdam) on red blood cell dynamics; V. Croquette (ENS, Paris) on helicase dynamics; F. Cleri (U. Lille, France) on simulations of hairpin folding kinetics; A. Crisanti (U. La Sapienza, Roma) and M. Picco (U. Paris VI, Paris) on fluctuation theorems in glassy systems; F. Westerlund (U. Chalmers, Gotheborg) on force spectroscopy of nucleic acids.

2.2.4. Biophysics and Bioengineering Unit (NanoBio)

Department of Biomedicine, Faculty of Medicine

Team

- **Daniel Navajas Navarro (Full Professor)**
- **Ramon Farré Ventura (Full Professor)**
- **Pere Roca Cusachs (Associate Professor)**

Research

The Unit of Biophysics and Bioengineering is largely specialized in applying the principles and methodologies of physics and engineering to the study of a variety of biological systems in normal and diseased conditions. The scope of this multidisciplinary research includes both basic and translational approaches, and is conducted in close collaboration with clinical research groups. The goal is to improve the diagnostic and treatment of human diseases. Most of the work applies to different length scales, including the molecular, cellular and tissue/organ level. The main areas of research include mechanobiology, respiratory and cardiovascular biophysics, and biomedical image processing.

Selected Projects

- *Mecanismos del aumento del crecimiento tumoral y metástasis inducido por hipoxia intermitente en modelo celular/animal de apnea del sueño. Papel del envejecimiento y la menopausia.* PI14/00004. IP: Farre Ventura, Ramon. Ministerio de Economia y Competitividad. 2015-2017
- *Impact of Obstructive sleep apnea in the evolution of Alzheimer Disease. Role of hypoxia and sleep fragmentation.* IP: Farre Ventura, Ramon. Fundació La Marató de TV3. 2015-2018.

SELECTED PAPERS 2.2.4.

- *Force loading explains spatial sensing of ligands by cells.* Oria R., Wiegand T., Escribano J., Elosegui-Artola A., Uriarte J.J., Moreno-Pulido C., Platzman I., Delcanale P., Albertazzi L., Navajas D., Trepat X., García-Aznar J.M., Cavalcanti-Adam E.A., Roca-Cusachs P. *Nature* **2017**. volume 552, pages219–224.

- *Role of cyclooxygenase-2 on intermittent hypoxia-induced lung tumor malignancy in a mouse model of sleep apnea.* Campillo N., Torres M., Vilaseca A., Nonaka P.N., Gozal D., Roca-Ferrer J., Picado C., Montserrat J.M., Farré R., Navajas D., Almendros I. *Scientific Reports*. **2017**. Mar 16;7:44693

- *Force Triggers YAP Nuclear Entry by Regulating Transport across Nuclear Pores.* Elosegui-Artola A., Andreu I., Beedle A.E.M., Lezamiz A., Uroz M., Kosmalska A.J., Oria R., Kechagia J.Z., Rico-Lastres P., Le Roux A.-L., Shanahan C.M., Trepat X., Navajas D., Garcia-Manyes S., Roca-Cusachs P. *Cell*. **2017**. Nov 30;171(6):1397-1410

- *A portable continuous positive airway pressure device that can perform optimally under strenuous conditions.* Villanueva J.A., Isetta V., Montserrat J.M., Navajas D., Farré R. *American Journal of Respiratory and Critical Care Medicine*. **2018**. Oct 1;198(7):956-958.

- *Control of Mechanotransduction by Molecular Clutch Dynamics.* Elosegui-Artola A., Trepat X., Roca-Cusachs P. *Trends Cell Biol*. **2018**. May;28(5):356-367

2.2.5. BiOPT: Optical Trapping Lab - Grup de Biofotonica (NanoBio)

Department of Applied Physics, Faculty of Physics

Team

- **Mario Montes Usategui (Associate Professor)**
- **Estela Martín Badosa (Associate Professor)**
- **Raul Bola Sampol (PhD Student)**
- **Dorian Treptow (PhD Student)**
- **Arnau Farré Flaquer (Collaborator)**
- **Ferran Marsà Samper (Collaborator)**
- **Antonio Marzoa (PhD Student)**

Research

The group, which has an increasingly interdisciplinary composition, develops photonic tools to address problems of biological interest. Specifically, the group explore the capabilities of optical tweezers technology for the study of living matter at the molecular and cellular scales.

The systems developed in the group combine fluorescence microscopy, holographic optical manipulation, force measurement and high speed imaging, allowing to reach inside cells and help study their inner processes.

Selected Projects

- Medida de fuerzas y reología en el interior de células vivas mediante 'laser tweezers'. Ministerio de Economia y Competitividad, FIS2014-60052-R. 2015-2017
- SCREAM: Super-fast Confocal Microscopy through Efficient Acusto-optic Modulation (LLAVOR, 2016LLAV00022). Agència de Gestió d'Ajuts Universitaris i de Recerca (AGAUR). 2017-2018
- Grup de Recerca en Enginyeria de Fronts d'Ona (EFO), 2017SGR607, Agència de Gestió d'Ajuts Universitaris i de Recerca (AGAUR). 2017-2019

Singular Scientific Equipment

The group has two complete optical tweezers setups mounted on vibration-isolated optical tables, and equipped with high power lasers (@1064 nm) and research microscopes (Nikon TE-2000E) for brightfield, phase-contrast, DIC and epifluoresence imaging. For the dynamic manipulation of samples the group has liquid crystal spatial light modulators (Hamamatsu X10468-03) for the creation of holographic trap patterns or, alternatively, acousto-optic deflectors (AA Optoelectronic DTSXY-400-1064) for time-sharing traps. It can be directly measure the forces exerted by the traps from changes in the light momentum (Impetux Optics LUNAM T40-i). Other equipment includes conventional CCD and fast and sensitive EMCCD cameras (Qimaging QICAM, Andor Ixon-860 EMCCD), precision optomechanical components, position-sensitive detectors (PSDs) and a piezo-electric positioning platform (Piezosystem Jena TRITOR 102 SG). The group also have a fully-equipped cell culture laboratory.

SELECTED PAPERS

- *Influence of experimental parameters on the laser heating of an optical trap.* F. Català, F. Marsà, M. Montes-Usategui, A. Farré, and E. Martín-Badosa, *Sci. Rep.* 7, 16052. **2017**.

- *Extending calibration-free force measurements to optically-trapped rod-shaped samples.* F. Català, F. Marsà, M. Montes-Usategui, A. Farré, and E. Martín-Badosa *Sci. Rep.* 7, 42960. **2017**.

- *Beyond the Hookean spring model: direct measurement of optical forces through light momentum changes.* A. Farré, F. Marsà, and M. Montes-Usategui, in *Optical Tweezers: Methods and Protocols, Methods in Molecular Biology* 1486, 41-76, Arne Gennerich (ed.), *Springer New York*. **2017**.

2.2.6. Cancer therapy group (NanoBio)

Department of Biochemistry and Physiology, Faculty of Pharmacy and Food Sciences

Team

- **Carlos Ciudad Gómez (Full professor)**
- **Verònica Noé Mata (Associate Professor)**
- **Alejandro Jiménez Félix (PhD Student)**
- **Eva Aubets Gil (PhD Student)**
- **Sonia Trigueros (External Collaborator-University of Oxford)**

Research

Our research is focused in the development of new applications for our technology of Polypurine reverse Hoogsteen hairpins (PPRHs) for gene silencing and gene editing.

PPRH hairpins are non-modified DNA molecules formed by two antiparallel polypurine strands linked by a pentathymidine loop that allows the formation of intramolecular reverse-Hoogsteen bonds between both strands. These PPRHs bind to polypyrimidine stretches in the DNA via Watson-Crick bonds, while maintaining the hairpin structure. Upon binding their polypyrimidine target in a dsDNA, PPRHs provoke strand displacement of the polypurine tract of the duplex, producing inhibition of transcription or altering splicing, thus causing specific gene silencing.

In addition to demonstrate the silencing effectiveness of PPRHs *in vitro*, two *in vivo* efficacy assays were conducted using two different routes of administration, either intratumoral or intravenous, in a subcutaneous xenograft tumor model of prostate cancer cells.

We have studied the ability of PPRHs to silence a variety of relevant cancer-related genes in several human cell lines. All PPRHs were effective in decreasing cell survival and mRNA levels and increasing apoptosis in cancer cells. In the context of tumor immunology, we designed PPRHs to silence both CD47/SIRPα and PD1/PDL-1 pathways with the aim to eliminate tumor cells by macrophages in co-culture experiments.

Stability experiments revealed that the half-life of PPRHs is much longer than that of siRNAs. Regarding the innate immune response, different determinations indicated that PPRHs, unlike siRNAs, do not activate the innate inflammatory response. More recently, we have performed a pharmacogenomics study that indicated that unspecific PPRHs did not originate differentially expressed genes, thus demonstrating the lack of off-target effects.

Correction of point mutations that lead to aberrant transcripts, often with pathological consequences, has been the focus of considerable research. We explored the possibility of repairing a point mutation in mammalian cells using PPRHs as tools. These Repair-PPRHs contain a hairpin core bearing an extension sequence at one end, homologous to the DNA strand to be repaired but containing the wild type nucleotide instead of the mutation. We demonstrated *in vitro* that PPRHs bind specifically to their polypyrimidine target sequence, opening the two strands of the dsDNA, and allowing the binding of a given repair oligonucleotide to the displaced strand of the DNA. Then, different Repair-PPRHs were designed to correct

SELECTED PAPERS

- *Polypurine Reverse Hoogsteen Hairpins as a Gene Silencing Tool for Cancer.* Ciudad CJ, Rodríguez L, Villalobos X, Félix AJ, Noé V. *Curr Med Chem.* **2017**. 24(26):2809-2826. Review.
- *Silencing of Foxp3 enhances the antitumor efficacy of GM-CSF genetically modified tumor cell vaccine against B16 melanoma.* Miguel A, Sendra L, Noé V, Ciudad CJ, Dasí F, Hervas D, Herrero MJ, Aliño SF. *Onco Targets Ther.* **2017**. Jan 23;10:503-514
- *Polypurine reverse-Hoogsteen (PPRH) oligonucleotides can form triplexes with their target sequences even under conditions where they fold into G-quadruplexes.* Solé A, Delagoutte E, Ciudad CJ, Noé V, Alberti P. *Sci Rep.* **2017**. Jan 9;7:39898.
- *Cancer immunotherapy using PolyPurine Reverse Hoogsteen hairpins targeting the PD-1/PD-L1 pathway in human tumor cells.* Medina Enríquez MM, Félix AJ, Ciudad CJ, Noé V. *PLoS One.* **2018**. Nov 6;13(11):e0206818.
- *Functional pharmacogenomics and toxicity of PolyPurine Reverse Hoogsteen hairpins directed against survivin in human cells.* Félix AJ, Ciudad CJ, Noé V. *Biochem Pharmacol.* **2018**. Sep;155:8-20.

insertions, deletions, substitutions present in a collection of mutants at the endogenous locus of the aprt gene. Surviving colonies were analyzed by DNA sequencing, and by mRNA and enzymatic measurements, confirming that all the aprt mutants had been corrected.

Selected Projects

- Terapia génica mediada por pprhs: vehiculizacion, silenciamiento, reparacion y aproximaciones *in vivo*
  Institution: Ministerio de Ciencia, Innovación y Universidades
  Principal Investigator: Verónica Noé Mata/ Carlos Ciudad Gomez, UB
  Reference: RTI2018-093901-B-I00, 2019-2021
- PPRHs. Diseño avanzado, vehiculización, ómica y aplicaciones terapéuticas en linfomas, inmunoterapia y reparación génica.
  Institution: Ministerio de Economía, Industria y Competitividad
  Principal Investigator: Verónica Noé Mata/ Carlos Ciudad Gomez, UB
  Reference: SAF2014-51825-R, 2015-2017

International Collaborations

- Dr Alejandra Bruna from the Cancer Research UK Cambridge Institute, University of Cambridge, UK, who has developed a breast cancer PDTX biobank, to perform in vivo approaches in order to evaluate the effectiveness of PPRHs.
- Dr. Sonia Trigueros, Co-Director of the Oxford Martin Programe on Nanotechnology, Institute of Nanoscience for Medicine, Department of Physics, University of Oxford, to test an innovative system of transfection for PPRHs using gold nanoparticles.
- Dr. Lawrence Chasin, Department of Biological Sciences, Columbia University, NY, on the repair of dhfr and aprt mutant cell lines.

2.2.7. Catalysis and Advanced Inorganic Materials (MATCAT) (NanoEnergy)

Department of Inorganic and Organic Chemistry, Faculty of Chemistry

Team

- **Narcis Homs Martí (Full professor)**
- **Pilar Ramírez de la Piscina (Full professor)**
- **Paulina Raquel Martinez Alanis (Adjunct Lecturer-Postdoc)**
- **Arturo Pajares Rojas (PhD Student)**
- **Yan Wang (PhD Student)**

Research

The research activities of the group focus on the preparation of tailored, nanostructured catalytic materials for energy conversion and chemical storage. The main goal of the research is to reach a high level of preparative abilities of nanostructured materials and the understanding of their characteristics. Then, this strategy is applied to two main domains: i) H_2 production from bioresources (mainly bioalcohols) using catalytic reforming and photocatalytic processes and ii) the chemical recycling of CO_2 trough catalytic conversion and photoreduction to chemicals and liquid fuels. Two PhD and four Master Thesis on these subjects have been achieved in the last period (2017-18).

Selected Projects and activities

- Desarrollo de nuevos catalizadores para la reducción selectiva de CO_2 y su transformación mediante procesos integrados a combustibles líquidos oxigenados MAT2014-52416-P. IP: Homs Martí, Narcís. Ministerio de Economia y Competitividad. 2015-2017.

- Diseño de catalizadores basados en carburos de metales de transicion eficientes en procesos de producción de H2 y para la activacion selectiva de CO_2. MAT2017-87500-P. IP: Homs Martí, Narcís. Ministerio de Economia y Competitividad. 2018-2020.
- Generalitat de Catalunya, 2017SGR1086

The MATCAT organized (Pilar Ramirez de la Piscina and Paulina Raquel Martinez-Alanis, Chair and Secretary, respectively of the organizing committee and Narcis Homs, President of the scientific committee) the HYCELTEC 2019 symposium, devoted to H_2 and related technologies, fuel cells and advanced batteries, held in Barcelona 1-3 July 2019.

Singular Scientific Equipment

- Microwave and ultrasonic facilities for synthesis and reaction
- TG-DSC-microcalorimetry coupled to MS
- TPR/TPO/TPD analysis coupled to MS
- In-situ DRIFTS coupled to MS facility
- Thermal and photocatalytic reactors with on-line GC-MS analysis

International Collaborations

- Dr. Marcelo Maciel Pereira, UFRJ, Brazil
- Dr. Elisabete Assaf, IQSC, USP, Brazil
- Dr. Jamil Toyir, Fez, Morocco
- Dr. Weijie Cai, Dalian, China

2.2.8. Cellular Responses to Xenobiotics (NanoPharmaMed)

Department of Biochemistry and Physiology, Faculty of Pharmacy and Food Sciences

Team

- **Maria Pilar Vinardell Martínez-Hidalgo (Full professor)**
- **Montserrrat Mitjans Arnal (Associate Professor)**
- **M del Carmen Moran Bádenas (Associate Professor)**
- **Wawan Kurniawan (PhD Student)**
- **Michele Ferrari (External Collaborator-CNR-ICMATE Italy)**

Research

The Celular Responses to Xenobiotics Group (CEREX) develops its research in the Physiolgy section of Department of Biochemistry and Physiology (Faculty of Pharmacy and Food Sciences).

The group focus its research in the development of *in vitro* methods to evaluate the potential cytotoxicity of nanoparticles and nanovesicles for drug delivery. The increase use of nanomaterials supposes a potential risk to the human health and it is necessary to ensure the safety of these materials before marketing.

SELECTED PAPERS

- *Effective and Highly Selective CO Generation from CO_2 Using a Polycrystalline α-Mo_2C Catalyst.* Liu, Xianyun; Kunkel, Christian; Ramirez de la Piscina, Pilar; Homs, Narcis; Vines, Francesc; Illas, Francesc, *ACS Catalysis.* **2017**. 7(7).
- *CO_2 reduction over Cu-ZnGaMO (M = Al, Zr) catalysts prepared by a sol-gel method: Unique performance for the RWGS reaction.* Liu, Xianyun; Ramirez de la Piscina, Pilar; Toyir, Jamil; Homs, Narcis. *Catalysis Today*. **2017**. 296, 181-186.
- *Promoter effect of Ga in Pt/Ga-TiO_2 catalysts for the photo-production of H_2 from aqueous solutions of ethanol.* Sola, A. C.; Broch Gosser, M.; Ramirez de la Piscina, P.; Homs, N. *Catalysis Today* . **2017**. 287, 85-90.
- *Study of Ni/CeO_2-ZnO catalysts in the production of H2 from acetone steam reforming.* Elias, K. F. M.; Bednarczuk, L.; Assaf, E. M.; Ramirez de la Piscina, P.; Homs, N., *International Journal of Hydrogen Energy*. **2018**.
- *Understanding bifunctional behavior of Ni/HZSM5 catalyst under isobutane atmosphere.* Maia, Aline Junqueira; Pereira, Evandro Brum; Sola, Alberto C.; Homs, Narcis; de la Piscina, Pilar Ramirez; Louis, Benoit; Pereira, Marcelo Maciel. *Molecular Catalysis*. **2018**. 458 (Part B).

There is an especial interest in the adaptation of the present methods to study the cytotoxicity of small particles given that their toxicity is affected by the exposition area. The potential interference of these particles with the classical cytotoxicity endpoints makes necessary the search of new endpoints. The present activity of the group is the search of assessment of the irritant and/or sensitization capacity of nanoparticles developed for transdermal drug delivery. The group obtain particles with higher loading efficiency and loading capacity and high biocompatibility as promising DNA vehicles to be used as non-viral gene delivery systems.

Another area of interest is the study of nanoparticle interactions with erythrocytes and plasma proteins and the coagulation process. The potential photoprotective effect of nanovesicles are also studied.

The very slow progress in the therapeutic efficacy of the treatment of severe diseases has suggested the use of a growing need for a multidisciplinary approach to the delivery of therapeutics to targets tissues. There has been increasing effort in the design of stimuli-responsive nanomaterials that they will be developed into effective drug delivery vehicles. Most commonly, effective drug delivery is associated with nanomaterial-facilitated accumulation and/or cellular internalization. Ongoing research is focused on building up stimulus triggered devices for the effective delivery of gene/drugs.

Selected Projects

- CIBER-BBN 2016-2017 Proyectos Intramurales: BIOFILM-ATTACK: New highly positively charged nanovesicular structures for the treatment of biofilm formation in lower extremity ulcers. Ministerio de Economia y Competitividad
- CIBER-BBN 2016-2017 Proyectos Intramurales: FUNCTIOLENSES: Novel functionalized contact lenses with antiantimicrobial properties for the prevention of keratitis. Ministerio de Economia y Competitividad
- CTQ2017-88948-P: Lipoaminoacidos y liquidos ionicos biocompatibles para el desarrollo de nuevas estrategias de control antimicrobiano y eliminacion de biofilms. Ministerio de Economía, Industria y Competitividad.

International Collaborations

- Michele Ferrari. Instituto di Chimica della Materia Condensata e di Tecnologie per l'Energia (ICMATE-CNR). Genova, Italy. Codi GREC 18407- Framework Cooperation Agreement (2018/2021). Faculty of Pharmacy and Food Science (UB)- Institute for Chemistry of Condensed Matter and Technologies for Energy (ICMATE-CNR).
- Clarice M B Rolim. Department of Industrial Pharmacy, Universida de Federal de Santa Maria, Av. Roraima 1000, 97105-900 Santa Maria, RS, Brazil.
- Emanuela Corsini. Dipartimento di scienze farmacologiche e biomolecolari. Università degli Studi di Milano, Milan, Italy.

SELECTED PAPERS

- *Efficient encapsulation and release of RNA molecules from gelatin-based nanoparticles.* M.C. Morán, I. Forniés, G. Ruano, M.A. Busquets, M.P. Vinardell. *Colloids Surf.* A 516. **2017**. 226–237.
- *In vitro comparative skin irritation induced by micro and nano zinc.* Vinardell, M.P.; Llanas, H.; Marics, L.; Mitjans, M. *Nanomaterials*, 7. **2017**.
- *Dual responsive gelatin-based nanoparticles for enhanced 5-fluorouracil efficiency.* M. C. Morán, J. Carazo, M. A. Busquets. Colloids Surf. B 172. **2018**. 646–654.
- *Nanotoxicity in vitro: Limitations of the main cytotoxicity assays. In Nanotoxicology: Toxicity evaluation, risk assessment and management.* Mitjans, M.; Vinardell, M.P.; Nogueira-Librelotto, D.R. *CRC Press*, Taylor and Francis Group Ed. pp 171-192. **2018**.
- *Metal/Metal Oxide Nanoparticles for Cancer Therapy. In Nanooncology: engineering nanomaterials for cancer therapy and diagnosis.* Vinardell, MP; Mitjans, M. Edited by: Goncalves, G; Tobias, G. *Book Series: Nanomedicine and Nanotoxicology.* Pages: 341-364.

2.2.9. Colloids (NanoPharmaMed)

Department of Pharmacy and Pharmaceutical Technology and Physical-Chemical, Faculty of Pharmacy and Food Sciences

Team

- **Joan Estelrich Latràs (Full Professor)**
- **M. Antonia Busquets Viñas (Associate Professor)**

Research

Since laser-induced photothermal ablation has shown satisfactory results for the removal of tumors, the group Colloidal Group is working on the development of new generation of nanoparticles (NP) aimed for photothermal therapy (PTT). These NP are light-absorbing materials, namely photothermal agents (PA) that can convert absorbed light into heat. The result proves the ablation of malignant areas noninvasively by heating the tissue locally above 42 °C while keeping the temperature of the surrounding tissue at a normal level. In laser ablation, the spectral ranges of the used wavelengths are located in the Near Infrared region, the so called biological windows, where tissues become partially transparent as a result of a simultaneous reduction in both absorption and scattering. The researchers have designed and developed PA that generate heat after irradiation at the second biological window which offers improved light penetration, lower background signal, and higher maximum permission exposure compared to the traditional first window. The developed nanoparticles will also be designed to be directed by an external magnetic field or to be used as image probe, therefore as theranostic agents.

2.2.10. Conformational Diseases Group (NanoPharmaMed)

Department of Pharmacy and Pharmaceutical Technology and Physical-Chemical, Faculty of Pharmacy and Food Sciences

Team

- **Raimon Sabaté Lagunas (Associate Professor)**
- **Alba Espargaró Colomé (Tenure-Track Lecturer)**

Research

Conformational Diseases Group is interested in studying bacterial inclusion bodies as a model to treat amyloid aggregation based human disorders, such as Alzheimer or Parkinson's diseases.

Selected Projects

- Nanocarriers for drug delivery through thermal release. CTQ2017-88446-R. IP2: Sabaté, Raimon. Ministerio de Economía y Competitividad of Spain. 2018 –2020.

SELECTED PAPERS 2.2.9.

- *Magnetic nanoemulsions: Comparison between nanoemulsions formed by ultrasonication and by spontaneous emulsification.* Rodríguez-Burneo N., Busquets M.A., Estelrich J. *Nanomaterials.* Vol: 7. **2017**.
- *Evidence of protein adsorption in pegylated liposomes: Influence of liposomal decoration.* Sangrà M., Estelrich J., Sabaté R., Espargaró A., Busquets M.A. *Nanomaterials.* Vol: 7. **2017**.
- *Iron oxide nanoparticles in photothermal therapy.* Estelrich J., Antònia Busquets M. *Molecules.* Vol: 23. **2017**.

SELECTED PAPERS 2.2.10.

- *Combined in Vitro Cell-Based/in Silico Screening of Naturally Occurring Flavonoids and Phenolic Compounds as Potential Anti-Alzheimer Drugs.* Espargaró A., Ginex T., Vadell M.D.M., Busquets M.A., Estelrich J., Muñoz-Torrero D., Luque F.J., Sabate R. *Journal of Natural Products.* Vol 80. **2017**.
- *Regioselective synthesis of 7-O-esters of the flavonolignan silibinin and SARs lead to compounds with overadditive neuroprotective effects.* Schramm S., Huang G., Gunesch S., Lang F., Roa J., Högger P., Sabaté R., Maher P., Decker M. *European Journal of Medicinal Chemistry.* **2018**.
- *Design, Synthesis, and Biological Evaluation of 1-Benzylamino-2-hydroxyalkyl Derivatives as New Potential Disease-Modifying Multifunctional Anti-Alzheimer's Agents.* Panek D., Więckowska A., Jończyk J., Godyń J., Bajda M., Wichur T., Pasieka A., Knez D., Pišlar A., Korabecny J., Soukup O., Sepsova V., Sabaté R., Kos J., Gobec S., Malawska B. *ACS Chemical Neuroscience.* **2018**.

2.2.11. Design and Improvement of Processes and Materials (DIOPMA) (NanoEnergy)

Department of Materials Science and Physical Chemistry, Faculty of Chemistry

Team

- **Mercè Segarra Rubí (Associate Professor)**
- **Elena Xuriguera Martín (Tenure-Track Lecturer)**
- **Joan Formosa Mitjans (Associate Professor)**
- **Jaume Calvo de la Rosa (PhD Student)**
- **Jordi Díaz Marcos (Adjunct Lecture)**

Research

DIOPMA's research activity in the field of nanotechnology is divided into two areas:

1. Synthesis of nanostructured materials used for the manufacture of components (electrolyte and electrodes) of solid oxide fuel cells (SOFC) and superconductors by the method of combustion using polyacrylamide gels. In addition, synthesis of nanoparticles conventionally, by reduction in aqueous media using surfactant, and characterization of these nanoparticles by Transmission Electron Microscopy (TEM). Synthesis of Ni nanoparticles by magnetic separation is also performed. Synthesis of $CuFe_2O_4$ nanoparticles were prepared by means of two chemical methods: polymer-assisted sol-gel method and co-precipitations
2. Nanomechanical characterization, by nanoindentation technique, of various SOFC electrolytes, such as LSGM (perovskite lanthanum, strontium, gallium and magnesium). Furthermore, nanomechanical characterization of welding copper alloys, magnesium phosphate cements, steel oxide layers... Moreover, Mechanical properties (Young's modulus (E), hardness (H) and fracture toughness (KIC)) as well as the different fracture mechanisms activated during the indentation process, using both the Nanoindentation techniques and Atomic Force Microscopy (AFM).

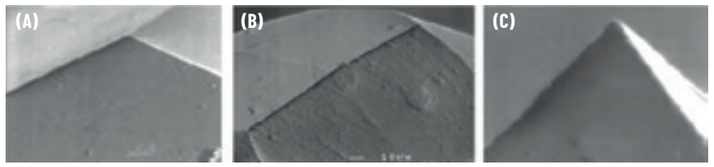


Figure1. SEM images of (A) Berkovich, (B) Knoop, and (C) cube-corner indenters.

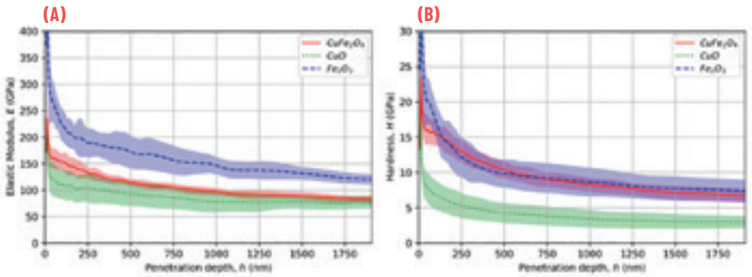


Figure2. Penetration Department of h dependence of the (A) elastic modulus (E), and (B) hardness (H) of the three different chemical composition pellets sintered during 6 hours at 1000 ºC. Solid lines represent the mean values, while the shadowed areas represent the standard deviation.

SELECTED PAPERS

- *Considerations for the use of metal alloys as phase change materials for high temperature applications.* Fernández A.I., Barreneche C., Belusko M., Segarra M., Bruno F., Cabeza L.F. *Solar Energy Materials and Solar Cells.* Vol: 171. **2017**.
- *Epitaxial Growth of SrTiO3 Films on Cube-Textured Cu-Clad Substrates by PLD at Low Temperature Under Reducing Atmosphere.* Padilla J.A., Xuriguera E., Rodríguez L., Vannozzi A., Segarra M., Celentano G., Varela M. *Nanoscale Research Letters.* Vol: 12. **2017**.
- *A eutectic salt high temperature phase change material: Thermal stability and corrosion of SS316 with respect to thermal cycling.* Liu M., Bell S., Segarra M., Steven Tay N.H., Will G., Saman W., Bruno F. *Solar Energy Materials and Solar Cells.* Vol: 170. **2017**.
- *High temperature systems using solid particles as TES and HTF material: A review.* Calderón A., Palacios A., Barreneche C., Segarra M., Prieto C., Rodriguez-Sanchez A., Fernández A.I. *Applied Energy.* Vol: 213. **2018**.
- *Corrosion of AISI316 as containment material for latent heat thermal energy storage systems based on carbonates.* Gallardo-González J., Martínez M., Barreneche C., Fernández A.I., Liu M., Tay N.H.S., Bruno F., Segarra M. Solar *Energy Materials and Solar Cells.* Vol: 186. **2018**.

Selected Projects

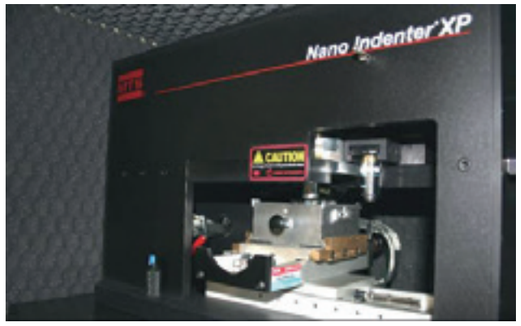
- Nuevas tecnologías para la impresión 3D de materiales avanzados. DPI2016-80119-C3-3-R. IP: Xuriguera Martin, M. Elena. Ministerio de Economia y Competitividad. 2016-2019.
- PhD on Innovation Pathways for TES (INPATH-TES). Segarra Rubi, Merce HORIZON 2020. PILLAR 3-SOCIETAL CHALLENGES. SC3-ENERGY. Secure, Clean and Efficient Energy. 2015-2018.

Singular Scientific Equipment

- Nanoindentaitor Nano Indenter XP (MTS) with CSM (Continuous Stiffness Measurement)

International Collaborations

- CIEFMA - Centro de Integridad Estructural y Fiabilidad de los Materiales (UPC)
- GLT – Georgea Tech Lorraine, Metz (France)
- FEMAN - Grupo de Física e Ingeniería de Materiales Amorfos y Nanoestructuras (UB)



2.2.12. Drug Design and Response-evaluation within Pharmaceutical Nanostructured and self-ordered Systems Group (NanoPharmaMed)

Department of Pharmacy and Pharmaceutical Technology and Physical-Chemical, Faculty of Pharmacy and Food Sciences

Team

- **Elvira Escribano Ferrer (Associate Professor)**
- **Josep Queralt Regué (Emeritus Lecturer)**
- **Jacinto Lauroba Viladrosa (Associate Professor)**
- **Francesc Xavier García Sala (Adjunct Lecturer)**

Research

The main research lines lead by the group is the study of pharmacokinetic and biodistribution of drugs. Mainly:

- Biodistribution of nanostructured system, mainly magnetic nanoparticles in mice models, as well as the effect of application of a magnetic field during the administration of the particle. The aim is to achieve a selective distribution, increasing the efficiency and minimizing g non-desired side effects
- Transdermal delivery studies of nanostructured systems are being developed in order to improve the permeation through the skin of anti-inflammatory drugs or other.

SELECTED PAPERS

- *Chitosan and hyaluronan coated liposomes for pulmonary administration of curcumin.* Manconi M., Manca M.L., Valenti D., Escribano E., Hillaireau H., Fadda A.M., Fattal E. *International Journal of Pharmaceutics.* Vol: 525. **2017**.
- *Thymus essential oil extraction, characterization and incorporation in phospholipid vesicles for the antioxidant/antibacterial treatment of oral cavity diseases.* Manconi M., Petretto G., D'hallewin G., Escribano E., Milia E., Pinna R., Palmieri A., Firoznezhad M., Peris J.E., Usach I., Fadda A.M., Caddeo C., Manca M.L. *Colloids and Surfaces B: Biointerfaces.* Vol: 171. **2018**.
- *NLCs as a potential carrier system for transdermal delivery of forskolin.* Lason E., Sikora E., Miastkowska M., Escribano E., Garcia-Celma M.J., Solans C., Llinas M., Ogonowski J. *Acta Biochimica Polonica.* Vol: 65. **2018**.

2.2.13. Engineering of colloidal systems (NanosMat)

Department of Chemical Engineering and Analytical Chemistry, Faculty of Chemistry

Team

- **José Maria Gutiérrez González (Associate Professor)**
- **Alicia Maestro Garriga (Associate Professor)**

Research

The research developed by the group aims, from one hand, at the preparation of nanoemulsions and nanoparticles and from the other, to prepare mesoporous materials for food technology application.

SELECTED PAPERS 2.2.13.

- *Ion exchange columns for the synthesis of ordered mesoporous materials.* SantaMaria E., Méndez C., Maestro A., Gutiérrez J.M., González C. *Journal of Porous Materials.* Vol: 24 (2017). **2017**.

2.2.14. Genomics, Proteomics and Plant Metabolomics (NanoBio)

Department of Biology, Healthcare and the Environment and Department of Biochemistry and Physiology, Faculty of Pharmacy and Food Sciences

Team

- **Antonio Fernàndez Tiburcio (Full Professor)**
- **Jaume Bastida Armengol (Full Professor)**
- **Francesc Viladomat Meya (Full Professor)**
- **Montserrat Arró Plans (Associate Professor)**
- **Laura Torras Claveria (Adjunct Lecturer)**

Research

The group aims at investigating the potential application of natural products derived from plants as sources of drugs to treat diseases such as Alzheimer.

Selected Projects

- La Biodiversidad Iberoamericana como fuente de recursos naturales para su explotación sostenible. Bastida Armengol, Jaume. CYTED. 2016 - 2019.

SELECTED PAPERS 2.2.14.

- *Trichomonicidal and parasite membrane damaging activity of bidesmosic saponins from Manilkara rufula.* De Brum Vieira P., Silva N.L.F., Menezes C.B., Da Silva M.V., Silva D.B., Lopes N.P., Macedo A.J., Bastida J., Tasca T. *PLoS ONE.* Vol 12. **2017**.
- *Metabolic Flexibility Underpins Growth Capabilities of the Fastest Growing Alga.* Treves H., Murik O., Kedem I., Eisenstadt D., Meir S., Rogachev I., Szymanski J., Keren N., Orf I., Tiburcio A.F., Alcázar R., Aharoni A., Kopka J., Kaplan A. *Current Biology.* Vol 27. **2017**.
- *Polyamine oxidase 5 loss-of-function mutations in Arabidopsis thaliana trigger metabolic and transcriptional reprogramming and promote salt stress tolerance. Plant Cell and Environment.* Vol. 40. **2017**.
- *Cholinesterase-inhibitory effect and in silico analysis of alkaloids from bulbs of Hieronymiella species.* Ortiz J.E., Garro A., Pigni N.B., Agüero M.B., Roitman G., Slanis A., Enriz R.D., Feresin G.E., Bastida J., Tapia A. *Phytomedicine.* Vol 39. **2018**.
- *N-oxide alkaloids from crinum amabile (amaryllidaceae).* Tallini L.R., Torras-Claveria L., Borges W.D.S., Kaiser M., Viladomat F., Zuanazzi J.A.S., Bastida J. *Molecules.* Vol 23. **2018**.

2.2.15. Group of Magnetic Nanomaterials (NanoMet, NanoMagnetics, NanoPharmaMed, NanoPhotoElectro)

Department of Condensed Matter Physics, Faculty of Physics

Team

- **Amílcar Labarta Rodríguez (Full Professor)**
- **Xavier Batlle Gelabert (Full Professor)**
- **Òscar Iglesias Clotas (Associate Professor)**
- **Montserrat García del Muro Solans (Associate Professor)**
- **Arantxa Fraile Rodríguez (Associate Professor)**
- **Carlos Moya Alvarez (Postdocotoral Researcher)**
- **Ana Conde Rubio (PhD Student)**
- **Mariona Escoda Torroella (PhD Student)**

Research

The research of the group is mainly twofold. On the one hand, we focus on the study of the intimate correlation between the nanostructure and the physical properties (magnetic, electronic...) of a variety of nanostructures. On the other, on how these properties depend on finite-size, surface, proximity and interphase effects, together with inter-particle interactions and quantum phenomena, among others.

Our main goal is the understanding of the fundamental properties in a wide variety of nanosystems, such as, thin films and heterostructures, nanoparticles and nanocomposites, and ordered arrays of nanoelements. The group also works in the potential applications of magnetic nanoparticles in biomedicine and plasmonic arrays in sensing, enhanced spectroscopies and perfect absorbers.

During 2017-2018 our efforts have been devoted to:

1. Obtaining theranostic materials based on multifunctional iron oxide (for magnetic resonance imaging) and gold (for its plasmonic properties and used for thermal ablation) nanoparticles (NP).
2. Cobalt Ferrite NP: By modulating its crystallinity - changing only the amount of one reagent – we produce a huge effect on the magnetic properties. We can obtain from soft materials of low anisotropy, useful for MRI, to hard materials of high anisotropy, which can be used for hyperthermia.
3. Multifunctional nanoparticles of iron oxide and bismuth (III) sulfide. Bismuth has a high absorption of X-rays in the high-energy range especially, which makes it suitable for contrast agent in computed tomography. The combination with magnetic nanoparticles allows obtaining improved contrast in different diagnostic techniques.
4. Inspired by geometrically frustrated magnetic systems, hexagonal lattices of plasmonic nanoelements have been fabricated by electron beam lithography, studied by FTIR and characterized by simulations. The main goal is to find an analogue frustrated behavior in the optical properties. Considering the slow dynamics of the lattices and the occurrence of non-localized enhanced electric fields over large areas, these systems may be of interest as enhancers for applications related to light absorption or enhanced spectroscopies.
5. Plasmonic arrays of gold nanostructures for enhanced spectroscopies. Au nanoelement matrices with plasmonic properties are an ideal substrate for surface enhanced Raman spectroscopy, which can be used for the detection of biomolecules. We have focused on determining the biodetection limit and the study of monolayers. Currently, we are working on the detection and separation of enantiomers of molecules of biological interest.

SELECTED PAPERS

- *Deviation from bulk in the pressure-temperature phase diagram of V2 03 thin films.* Valmianski, I.; Ramirez, J. G.; Urban, C.; Batlle, X.; and Schuller, I. K. *Phys. Rev.* B 95. **2017**.
- *Geometric frustration in a hexagonal lattice of plasmonic nanoelements.* Conde-Rubio, A.; Fraile Rodríguez, A.; Borrisé, X.; Perez-Murano, F.; Batlle, X.; and Labarta, A. *Opt. Express* 26, 20211. **2018**.
- *Change in the magnetic configurations of tubular nanostructures by tuning dipolar interactions.* Salinas, H. D.; Restrepo, J.; and Iglesias, Ò. *Sci. Rep.* 8, 10275. **2018**.
- *Magnetization Ratchet in Cylindrical Nanowires.* Bran, C.; Berganza, E.; Fernandez-Roldan, J. A.; Palmero, E. M.; Meier, J.; Calle, E.; Jaafar, M.; Foerster, M.; Aballe, L.; Fraile Rodriguez, A.; del Real, R. P.; Asenjo, A.; Chubykalo-Fesenko, O.; Vazquez, M., *ACS Nano* 12, 5932–5939. **2018**.
- *Probing the variability in oxidation states of magnetite nanoparticles by single-particle spectroscopy.* Fraile Rodríguez, A.; Moya, C.; Escoda-Torroella, M.; Romero, A.; Labarta, A.; and Batlle, X. J. *Mater. Chem.* C 6, 875–882. **2018**.

Selected Projects

- *Nanoparticles and multifunctional nanoelements: magnetic and plasmonic properties*. (MAT2015- 68772-P; Spanish MINECO), PI: Xavier Batlle and A. Fraile-Rodríguez (2016-2018).
- *Groups of Excellence (Generalitat de Catalunya): Group of Magnetic Nanomaterials*, PI Amílcar Labarta, 2017SGR598 (2017-2019).
- *Multifunctional Nanoparticles for Magnetic Hyperthermia and Indirect Radiaion Therapy*, COST TD1402 Action RADIOMAG; Coordinator: Simo Spassov (Belgium), PI UB: Òscar Iglesias (21 European countries). (2015 -).
- *Large Scale Facilities.* Synchrotron radiation projects at BESSY (Germany), ALS-LBNL (USA), SLS-PSI (Switzerland) and ALBA (Spain). PI: A. Fraile. Average of 2-3 beam time projects per year.

Singular Scientific Equipment

- Fully equipped lab specialized in the preparation of particles and thin films by chemical and physical routes. We have a Glovebox and a Schenk line to work under controlled inert atmosphere. In addition, we use suitable set-ups and temperature controllers to have a full control of the particle reaction profile. The lab follows the current legislation in terms of storage of reactants, solvents, separation and management of residues.
- Atomic Force Microscope (AFM) equipped with a variety of operating modes: Magnetic Force Microscopy (MFM), torsion MFM, Piezo Force Microscopy, Electric Field Microscopy, conductive-AFM.
- Regular access time to synchrotron radiation facilities: BESSY (Germany), ALS-LBNL (USA), SLS-PSI (Switzerland) and ALBA (Spain).
- Physical properties lab: resistance, magnetoresistance and conductance, as functions of temperature and magnetic field (4.2 K, 5 T).
- Others: rf magnetron sputtering equipped with 3 guns for thin film deposition and arc furnace for bulk alloy synthesis; differential scanning calorimeter to study magneto-structural phase transition, for bulk materials as a function of temperature and magnetic field (4.2 K, 5 T).

International Collaborations

- Prof. I. K. Schuller, Physics Department, University of California San Diego (CA, USA)
- Dr. Andreas Scholl, Advanced Light Source, LBNL (USA)
- Dr. J. G. Ramírez, Universidad de Los Andes, Bogotá, Colombia
- Dr. F. Kronast, Helmholtz-Zentrum Berlin
- Dr. Cinthia Piamonteze, Swiss Light Source, Paul Scherrer Institut (Switzerland).
- Dr. Armin Kleibert and Prof. Frithjof Nolting; Paul Scherrer Institut (Switzerland).

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- Dr. Claudio Sangregorio and César de Julián, CNR Firenze-Parma (Italy)
- Prof. Harald Giessen, Physics Institute, University of Stuttgart.
- Drs. Nuno J. O. Silva and V. Amaral, Univ. Porto and CICECO (Aveiro, Portugal)
- Profs. Hari Srikanth and Manh-Huong Phan, Univ. South Florida (USF, EEUU)
- Dr. Johans Restrepo, Univ. Antioquia (Medellín, Colombia)
- Prof. Saurav Giri, Indian Association for the Cultivation of Science (IACS), Kolkata (India)
- Prof. Hamid Kachkachi, Université de Perpignan, Perpignan (France)
- Dr. Dimitris Kechrakos (ASPETE, Atenas), Greece

2.2.16. Instrumentation Systems and Communications (SIC) (NanoPhotoElectro, NanoEnergy)

Department of Electronics and Biomedical Engineering, Faculty of Physics

Team

- **Anna Vilà Arbonés (Associate Professor)**
- **Mauricio Moreno Sereno (Associate Professor)**
- **Christophe Serre (Associate Professor)**

Research

In the frame of Nanostructured Materials, we work since 2006 in printed electronics, developing our own inks to print conductors, semiconductors and isolants, mainly in the form of metal-oxides and polymers. The nanostructured films and devices obtained from our ecofriendly processes are nowadays focused on biocompatible optoelectronics and sensing applications.

The obtained experimental results are assessed by means of Quantum Mechanics calculations via Density Functional Theory and Molecular Dynamics. The polynucleation, degradation and decomposition processes of some of our inks have been described, bringing explanation of the physical changes observed and of the final materials obtained.

Another main research line of the group refers to harvesting and scavenging energy for low-power applications and self-powered devices. We work in the development of smart sensors and structural health monitoring, as well as in sustainable exploitation of marine renewable energy sources respectful with the environment.

Finally, bringing the limits of microelectronic technology the group is developping single-photon avalanche diode (SPAD) detectors for radiation and biomedical applications. Entirely-configurable easily-scalable low-cost fluorescence measurement systems aim to carry out fast diagnostic tests within a sort time span, allowing personalized medicine.

SELECTED PAPERS

- *Readout electronics for LGAD sensors.* O. Alonso, N. Franch, J. Canals, F. Palacio, M. López, A. Vilà, A. Diéguez, M. Carulla, D. Flores, S. Hidalgo, A. Merlos, G. Pellegrini and D. Quirion. *Journal of Instrumentation. Institute of Physics (IOP).* **2017**.
- *A low cost fluorescence lifetime measurement system based on SPAD detectors and FPGA processing.* N. Franch, O. Alonso, J. Canals, A. Vilà and A. Dieguez. *Journal of Instrumentation. Institute of Physics (IOP).* **2017**.12. C02070.
- *The role of Ethanolamine on the Stability of a Sol-Gel ZnO ink.* A. Gómez-Núñez, S. Alonso-Gil, C. López, P. Roura and A. Vilà. Journal of Physical Chemistry C. *American Chemical Society*. 121, 23839-23846. **2017**.

Selected Projects

- Diseño y fabricación de chips HV-CMOS para el upgrade del LHC. FPA2017-89138-R
  IP: O. Alonso, A. Dieguez. 2018-2019
- CMOS design of an array of LED drivers. Industrial project n. 309583 FBG
  IP: A. Dieguez. 2017-2018
- Overcoming the Limits of Diffraction with Superresolution Lighting on a Chip (ChipScope). FET-OPEN 737089
  IP: A. Diéguez. 2017-2020

Collaborations

We collaborate with the Universitat de Girona (UdG), the Instituto de Microelectrónica de Barcelona-Centro Nacional de Microelectrónica (IMB-CNM), the LAAS-CNRS from Toulouse (France) and the College of Engineering, Mathematics and Physical Sciences from Exeter (UK).

Singular Scientific Equipment:

- Materials inkjet printer DIMATIX 2831

2.2.17. Laboratory of connective tissue signaling and genetic diseases (CTS-GD) (NanoBio)

Department of Biomedicine, Faculty of Medicine

Team

- **Gustavo Egea Guri (Full Professor)**

Research

The research group is interested on genetic diseases of connective tissue, especially on Marfan syndrome, which is a rare genetic disease of the connective tissue (1:5,000 people) that affects the cardiovascular (the ascending aorta and the heart), respiratory (alveoli), skeletal (muscle, long

SELECTED PAPERS

- *Differences in the Thoracic Aorta by Region and Sex in a Murine Model of Marfan Syndrome.* F. Jimenez-Altayo, A.M. Siegert, F. Bonorino, T. Meirelles, L. Barbera, A. Paula Dantas, E. Vila and G. Egea. *Front. Physiol.* **2017**. Nov 15; 8:933.
- *High resolution morphological approach to analyse elastic laminae injuries of the ascending aorta in a murine model of Marfan syndrome.* López-Guimet J, Andilla J, Loza-Alvarez P and Egea G. *Scientific Reports.* 7(1):1505. **2017**.
- *Redox stress in Marfan syndrome: dissecting the role of the NADPH oxidase NOX4 in aortic aneurysm.* F. Jiménez-Altayó, T. Meirelles, E. Crosas-Molist, M.A. Sorolla, D. Gorbenko del Blanco, J. López-Luque, A. Mas-Stachurska, A.M. Siegert, F. Bonorino, L. Barberà, C. García, E. Condom, M. Sitges, F. Rodríguez-Pascual, F. Laurindo, K. Schröder, J. Ros, I. Fabregat and G. Egea. *Free Radic Biol Med*. **2018**. Apr; 118:44-58.
- *MicroCT imaging reveals differential micro-scale remodelling of the murine aorta in ageing and Marfan syndrome.* J. López-Guimet, L. Peña Pérez, R.S. Bradley, P. García-Canadilla, C. Disney, H. Geng, A.J. Bodey Philip J. Withers, B. Bijnens, M.J. Sherratt, G. Egea. *Theranostics*. **2018**. 8(21): 6038-6052.
- *Altered TGF-β endocytic trafficking contributes to the increased signaling in Marfan syndrome.* A.M. Siegert, C. Serra-Peinado, E. Gutiérrez-Martínez, F. Rodríguez-Pascual, I. Fabregat and G. Egea. *Biochim Biophys Acta Mol Basis Dis*. **2018**.Feb; 1864(2): 554-562.

bones and ribs), and ocular (crystalline) systems. This syndrome is caused by mutations in the gene that codifies for fibrillin-1 (FBN1), which is an essential component of elastic fibers. The main critical clinical problem is the formation of aortic aneurysm (abnormal dilatation) that usually leads to the dissection and rupture of the vessel. It is crucial a correct diagnosis of the disease and do it on time, and to follow-up the appearance and progression of aneurysm to subject the aorta to reparatory surgery at due time. Nowadays, there are pharmacological therapies that help to slow-down the formation of the aneurysm, but unfortunately, they do not prevent it. The research group assay alternative therapies using a murine model of the disease, as well as we investigate several physiopathological processes that seems to be involved in the progress of the disease: membrane trafficking of TGF-beta receptors, and TGF-beta signaling and mechano-transduction. At the same time, the group is highly interested to know what is the impact of smoking, the physical exercise and sleep apneas in the formation/progression of the aortic aneurysm.

Selected Projects

- Impacto fisiopatológico de un péptido anti-TGF-beta, del ejercicio físico y del humo de los cigarrillos en la formación del aneurisma aórtico en el síndrome de Marfan. SAF2017-83039-R. IP: Egea Guri, Gustavo. Ministerio de Economia y Competitividad. 2018-2020

2.2.18. LASER- Micro and Nanotechnology and nanoscopies for Electronic and Electrophotonic devices (MIND) (NanoPhotoElectro)

Department of Applied Physics, Faculty of Physics

Team

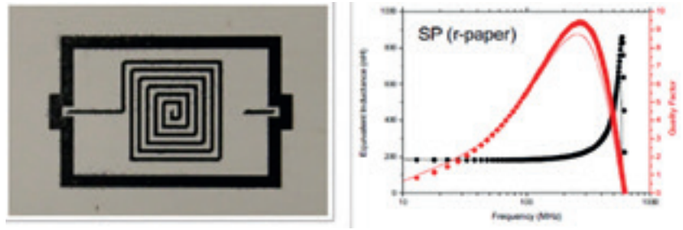
- **Pere Serra Coromina (Full Professor)**
- **Juan Marcos Fernández Pradas (Associate Professor)**
- **José Luís Morenza Gil (Emeritus Lecturer)**
- **Martí Duocastella Solà (Tenure-Track Lecturer-Serra Húnter)**
- **Francesc Caballero Lucas (PhD Student)**
- **Pol Sopeña Martinez (PhD Student)**

Research

In this period we have focused our activity on two main research lines. The first is the laser printing of conductive inks on cellulose paper substrates for paper electronics applications. We have proved the feasibility of laser-induced forward transfer (LIFT) for making interconnects and devices with screen-printing inks on regular paper. The impact of this result is twofold remarkable. First, because it makes possible to print high solid content inks in a digital fashion, something that could not be attained with other digital techniques, like inkjet printing, for example (the high solid content allows obtaining the low sheet resistances demanded by the printed electronics industry). Second, because thanks to the high viscosity of those inks it is feasible to print them on raw paper without

SELECTED PAPERS

- *Laser-induced forward transfer of low viscosity inks.* Sopeña P., Fernández-Pradas J.M., Serra P. *Applied Surface Science.* Vol 418. **2017**.
- *Low-Cost Fabrication of Printed Electronics Devices through Continuous Wave Laser-Induced Forward Transfer.* Sopeña P., Arrese J., González-Torres S., Fernández-Pradas J.M., Cirera A., Serra P. *ACS Applied Materials and Interfaces.* Vol 9. **2017**.
- *Spraying dynamics in continuous wave laser printing of conductive inks.* P. Sopeña, S. González-Torres, J.M. Fernández-Pradas, P. Serra. *Scientific Reports* 8, 7999-1/12. **2018**.
- *3D Electrophoresis-Assisted Lithography (3DEAL): 3D printing functional molecules to create anisotropic hydrogels.* J.P. Aguilar, M. Lipka, G.A. Primo, E.E. Licon-Bernal, J.M. Fernández-Pradas, A. Yaroshchuk, F. Albericio, A. Mata. *Advanced Functional Materials* 28, 1703014-1/10. **2018**.



High frequency inductor printed on paper with LIFT and corresponding electrical response

significant leaking in the interstices between the cellulose fibers, and therefore to avoid any surface treatment which ultimately makes the process less cost-effective and environmentally friendly. As a proof-of-concept, and in collaboration with the Radio Frequency Group (GRAF) of the Department of Electronics and Biomedical Engineering, we have printed a device (a high frequency inductor) entirely with LIFT with performances identical to those printed with conventional techniques.
The second research line is devoted to photothermal therapy activated with laser radiation in combination with smart nanomaterials. This research line emerges from the collaboration with the Colloids Group and the Cellular Responses to Xenobiotics Group, both in the Faculty of Pharmacy and Food Sciences. The main objective of this collaboration is to develop a strategy for treating cancer tumors in a less invasive way and with less side effects than actual therapies. The collaboration has received the thrust of the IN²UB by granting a related project in the ART2019 call.

Selected Projects

- *Impresión con láser para aplicaciones de electrónica basada en papel.* TEC2017-83301-P. IP: Pere Serra Coromina. Ministerio de Economía, Industria y Competitividad. 2018-2020.
- *Hacia una imprenta digital láser.* TEC2015- 72425-EXP IP: Pere Serra Coromina. Ministerio de Economía, Industria y Competitividad. 2017-2020.

International Collaborations

- Research Center: Naval Research Laboratory.
  Group leader: A. Piqué
  City: Washington DC (USA)
- Research Center: Université Aix-Marseille/CNRS.
  Group leader: P. Delaporte
  City: Marsella (França)
- Research Center: Istituto Italiano di Tecnologia.
  Group leader: M. Duocastella
  City: Gènova (Itàlia)

2.2.19. Laboratory of Electron Nanoscopies (LENS)- Micro and Nanotechnology and nanoscopies for Electronic and Electrophotonic devices (MIND) (NanoMet)

Department of Electronics and Biomedical Engineering, Faculty of Physics

Team

- **Francisca Peiró Martínez (Full professor)**
- **Sònia Estradé Albiol (Tenured Associate Professor)**
- **Josep Manel Rebled Corselles (Adjunct Lecturer)**
- **Pau Torruella Besa (PhD student)**
- **Catalina Coll (PhD student)**
- **Javier Blanco Portals (PhD student)**
- **Luís López Conesa (Collaborator)**
- **Gemma Martin Malpartida (Collaborator)**

Research

The main objective of LENS is the development of instrumental methods as well as data treatment for advanced scientific problems in nanomaterials using Transmission Electron Microscopy and related techniques. LENS pursues challenging objectives in cutting-edge methodologies as the combination of electron tomography (ET), precession (EP) and electron energy loss spectroscopy (EELS), with machine learning and DFT simulation tools for data analysis.

After the participation in the national consortium of a Consolider project (CSD2009-20016 Imagine, Microscopy at sub-Angstrom resolution) and in the Network of Excellence in Microscopy (MAT2016-81720-REDC), LENS has significantly contributed to the incorporation of the Unit of Transmission Electron Microscopy Applied to Materials of the Scientific and Technological Centers of the University of Barcelona (CCiT) as a new node of ELECMI, the Singular Scientific and Technological Infrastructure (ICTS) devoted to the Electron Microscopy of Materials.

In this period, the active research lines of LENS have been: i) from the instrumental point of view, the development of innovative protocols of electron beam alignment for quasi-parallel scanning transmission electron beam precession assisted modes *[Ultramicroscopy 193, 39-51 (2018)]*; ii) from the methodological side, we have applied machine learning algorithms to quantitatively exploit electron energy loss spectroscopy datasets *[Ultramicroscopy 185, 42–48 (2018)]* and ab-initio simulations for the understanding of oxygen vacancies or structural phase related signature in experimental EELS of functional oxides *[Journal of Physical Chemistry C 121, 24809-24815 (2017)]*;

SELECTED PAPERS

- *Tuning branching in ceria nanocrystals.* Berestok, T.; Guardia, P.; Blanco J.; López-Conesa, L.; Estradé, S.; Ibañez, M.; Nafria, R.; Luo, Z.; Kovalenko, M.V.; Peiró F. and Cabot, A. *Chemistry of Materials* 29, 4418-4424. **2017**.
- *Seeded growth synthesis of Au-Fe_3O_4 heterodimers: rational design and mechanistic insights.* E. Fantechi, A. G. Roca, B. Sépulveda, P. Torruella, S. Estradé, F. Peiró, N.G. Bastús, J. Nogués, V. Puntes. *Chemistry of Materials* 29, 4022-4035. **2017**.
- *Engineering Transport in Manganites by Tuning Local Nonstoichiometry in Grain Boundaries.* Chiabrera, F.; Garbayo, I.; López-Conesa, L.; Martín, G.; Ruiz-Caridad, A.; Walls, M.; Ruiz-González, L.; Kordatos, A.; Núñez, M.; Morata, A.; Estradé, S.; Chroneos, A.; Peiró, F.; and Tarancón, A. *Adv. Mater.*, 1805360 (1-8pp). **2018**.
- *Atomic-Scale Determination of Cation Inversion in Spinel-Based Oxide Nanoparticles.* Torruella, P.; Ruiz-Caridad, A.; Walls, M.; Roca, A.G.; Lopez-Ortega, A.; Blanco-Portals, J.; Lopez-Conesa, L.; Nogues, J.; Peiro, F.; Estrade, S. *Nano Letters* 18 (9), 5854-5861. **2018**.
- *Gradual Transformation of Ag2S to Au2S Nanoparticles by Sequential Cation Exchange Reactions: Binary, Ternary, and Hybrid Compositions.* Dalmases, M.; Torruella, P.; Blanco-Portals, J.; Vidal, A.; Lopez-Haro, M.; Calvino, J.J.; Estradé, S.; Peiró, F.; Figuerola, A. *Chemistry of Materials* 30, 6893–6902. **2018**.

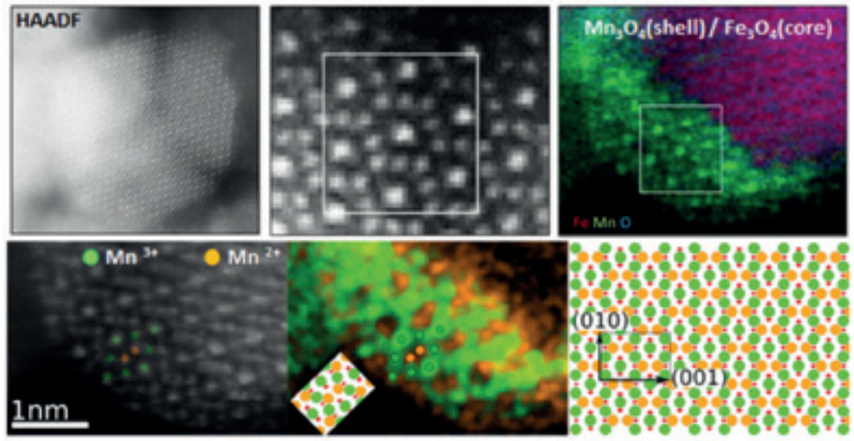


Figure 1. Atomic resolution maps of the Mn oxidation state in tetrahedral and octahedral coordination sites in Fe_3O_4/Mn_3O_4 core-shell nanoparticles

iii) the combination of all these procedures to advanced nanomaterials has allowed us to successfully tackle: the local measurement of the inversion parameter in Fe_3O_4/Mn_3O_4 spinel structure core/shell nanoparticles at atomic resolution by direct mapping of the Mn^{2+}/Mn^{3+} ions in the shell and the Fe^{2+}/Fe^{3+} in the core at the tetrahedral and octahedral coordination sites (figure 1) *[Nano Letters 18 (9), 5854-5861 (2018)]*; the elucidation of local non-stoichiometries at the grain boundaries of $La_{0.8}Sr_{0.2}MnO_{3\pm\delta}$ (LSM) thin films and the control of this grain boundary effect as a new and powerful tool for controlling electronic and mass transport properties of metal oxide thin films useful for solid state devices *[Adv. Mater., 1805360 (1-8pp)(2018)]* (figure 2); the characterization of critical steps in cation exchange reactions during the synthesis of binary, ternary, and hybrid compounds from Ag_2S to Au_2S nanoparticles *[Chem. Mater. 30, 6893–6902 (2018)]* and the elucidation of branching mechanisms in CeO_2 nanocrystals through electron tomography and high resolution STEM and HREM simulations (figure 3) *[Chemistry of Materials 29, 4418-4424 (2017)]*; iv) last but not least, we have consolidated the application of in-situ TEM electrical measurements for disentangling the conductive mechanisms in memristor devices *[Appl. Phys. Express 11, 014101 (2018)]*.

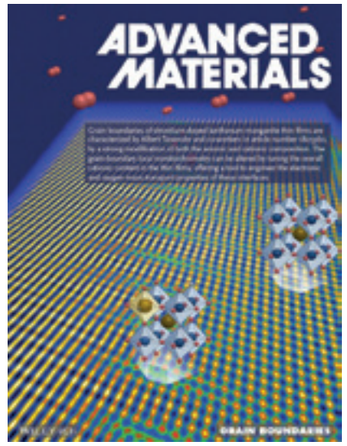


Figure 2. Cover letter of Advanced Materials, related to the work of local non-stoichiometry at $La_{0.8}Sr_{0.2}MnO3_{\pm\delta}$ (LSM) grain boundaries assessed by EELS.

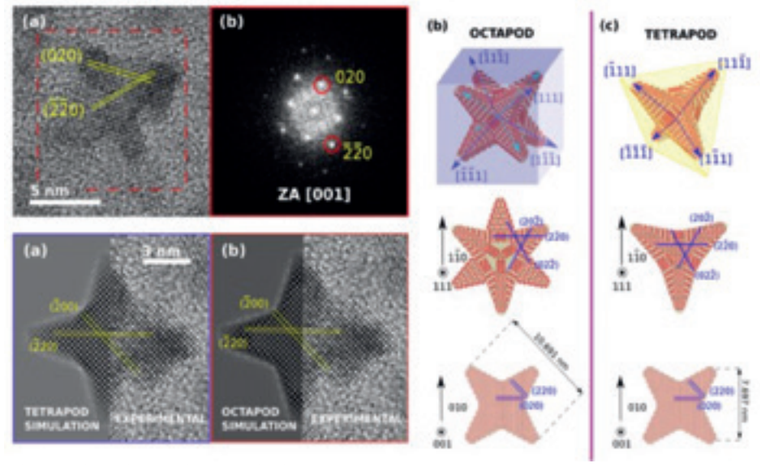


Figure 3. Simulations of high resolution images of octapod and tetrapod branched CeO_2 nanoparticles.

Selected Projects

- TEMPTATION: *Desarrollo de métodos de Precesión Electrónica, Tomografía y Técnicas Analíticas en el TEM para la elucidación de materiales avanzados*. MAT2016-79455-P.
  IP: Francisca Peiró Martínez / Sònia Estradé. Ministerio de Economia y Competitividad. 2016-2019.
- *RED de Excelencia IMAGINE*
  Program: ACCIONES DE DINAMIZACIÓN "REDES DE EXCELENCIA
  Coordinator: Jose Maria González Calbet (UCM)
  IP UB: Francisca Peiro Martinez
  MAT2016-81720-REDC
  Ministerio de Economia y Competitividad. 2017-2019
- *Formación Avanzada en Microscopía Electrónica en una Red Abierta*
  Call: Convocatoria 2017 de acciones de carácter internacional "europa investigación".
  EUIN2017-88579. IP: Sònia Estradé Albiol. 01/01/2018-31/12/2018
- Participation at: Erasmus+ Project: *Diversity in the cultures of physics*
  Coordinator: Freie Universität de Berlin. 2016-1-DE01-KA203-002918. Participants: Universitat de Barcelona, Universitat Autònoma de Barcelona (UAB), Uppsala Universitet (UU), University of Manchester (UoM) y University of Sheffield. 2017-2019

International Collaborations

- Electron Microscopy Center (EMZ-DA) at TU Darmstadt), Prof. Ute Kolb, optimization of 3D reconstruction of reciprocal space through electron beam precession assisted electron tomography.
- CCEM - Canadian Center of Electron Microscopy, Mc Master University, Canada (Prof. Gianluigi Botton), plasmonic hybrid nanomaterials and DFT simulations of advanced materials.
- Westfälische Wilhelms-Universität Münster, (Prof. Helmut Kohl, Alemania), theoretical modelling of beam precession.
- Structure Research and Electron Microscopy, Institut für Physik, Humboldt-Universität zu Berlin, con Robert S. Pennington y Christoph T. Koch, DFT simulations of structure factors.

2.2.20. Magnetic Interactions and Molecular Magnetism (NanoMagnetics)

Department of Inorganic and Organic Chemistry, Faculty of Chemistry

Team

- **Ramón Vicente Castillo (Full Professor)**
- **Albert Escuer Fité (Full Professor)**
- **Montserrat Corbella Cordomí (Associate Professor)**
- **Carmen Díaz Gasa (Associate Professor)**
- **Mohamed Salah El Fallah (Associate Professor)**
- **Júlia Mayans Ayats (Postdoctoral Researcher)**
- **Saskia Speed (Postdoctoral Researcher)**

SELECTED PAPERS

- *Transition Metal Single-Molecule Magnets: A {Mn31} Nanosized Cluster with a Large Energy Barrier of ~60 K and Magnetic Hysteresis at ~5 K*. Abbasi P., Quinn K., Alexandropoulos D.I., Damjanović M., Wernsdorfer W., Escuer A., Mayans J., Pilkington M., Stamatatos T.C. *Journal of the American Chemical Society*: 139, 15644-15647. **2017**.

Research

The Magnetic Interactions and Molecular Magnetism research group is dedicated to the Chemistry of Coordination of polynuclear compounds, whether they are discrete aggregates or monodimensional, two-dimensional or three-dimensional species, making their synthesis, structural characterization and magnetic studies (measures of magnetic susceptibility , magnetization and paramagnetic resonance spectroscopy).

At present, special attention is paid to the complexes built from enantiomerically pure chiral ligands that allows the direct synthesis of chiral coordination compounds that can be useful in the search of multifunctional systems in which optical or emissive properties could be combined with its magnetic response.

The objectives of the research are: 1) to find magnetic-structural relationships based on the magnetic and structural data of the new complexes in order to expand the field of these relationships and to predict and synthesize new polynuclear species with predetermined magnetic properties; 2) to reach the formation of new molecular magnets (SIM or SMM), either from discrete species of high nuclearity through the use of ions with strong anisotropy (Mn (III) or lanthanides) that can give rise to the formation of complexes in a fundamental state of high spin and/or large anisotropy; 3) to study the effect of the enantiopure systems in supramolecular chirality; 4) study mixed valence manganese species that behave as models of bioinorganic processes.

Selected Projects

- Nuevos materiales multifuncionales: clústers magnéticos quirales y/o luminiscentes de cationes de los bloques d y f. Aplicaciones como antioxidant. IP: tes y agentes de contraste. CTQ2015-63614-P. Escuer Fite, Albert. Ministerio de Economia y Competitividad. 2016-2018.

- *Influence of the Disposition of the Anisotropy Axes into the Magnetic Properties of MnIII Dinuclear Compounds with Benzoato Derivative Bridges.* Garcia-Cirera, B.; Gómez-Coca, S.; Font-Bardia, M.; Ruiz, E.; Corbella, M. *Inorganic Chemistry*, 56, 8135-8146. **2017**.
- *Triple halide bridges in chiral $Mn^{II}_2Mn^{III}_6Na^{I}_2$ cages. Structural and magnetic characterization.* Mayans, J.; Font-Bardia, M.; Escuer, A. *Inorganic Chemistry*, 57, 926-929. **2018**.
- *Chiral $[Mn^{II}Mn^{III}_3M']$ (M'=Na^{I}, Ca^{II}, Mn^{II}) and $[Mn^{II}Mn^{III}_6Na^{I}_2]$ Clusters Built from an Enantiomerically Pure Schiff Base: Synthetic, Chiroptical, and Magnetic Properties.* Mayans J., Font-Bardia M., Di Bari L., Górecki M., Escuer A. *Chemistry - A European Journal*. 24, 18705-18717. **2018**.
- *From Mesocates to Helicates: Nickel(II) Supramolecular Assemblies Derived from Chiral Tetradentate Schiff Bases. Structural, Magnetic and Chiro-Optical Studies.* Mayans, J.; Font-Bardia, M.; Di Bari, L.; Arrico, L.; Zinna, F.; Pescitelli, G.; Escuer, A. *Chemistry-A European Journal*, 24, 7653-7663. **2018**.

2.2.21. Magnetic Soft Matter Group (NanoBio)

Department of Condensed Matter Physics, Faculty of Physics

Team

- **Pietro Tierno (Associate Professor and ERC Starting Grant)**
- **Antonio Ortiz-Ambriz (Associate Professor)**
- **José Manuel García Torres (Collaborator)**

Research

The research group is interested in Soft matter systems like colloids, polymers or liquid crystals, with special emphasis on out equilibrium conditions, when external field or forces act over the systems. In particular, at the present we are working on the following topics:

- Artificial colloidal ice.
- Propulsion in viscous fluids.
- Ratchet transport.
- Realization of shape-anisotropic field responsive particles.
- Colloids in periodic potentials.

Selected Projects

- ENgineeringFRustrated states in Colloidal artificial ices: thermalization, *manipulation and 3D states (ENFoRCe).* From MEC: ACCIONES DE DINAMIZACIÓN «EUROPA EXCELENCIA» - CONVOCATORIA 2018, Proj. ERC2018-092827. PI: Pietro Tierno (2018 – 2019)
- Dynamics and assemblies of colloidal particles under Magnetic and Optical forces (DynaMO)" ERC Starting Grant from European Research. Council (Proj. num 335040); (2014 – 2018)
  PI: Pietro Tierno
- Magnetically Actuated BIO-inspired metaMATERials (abiomater) (Proj. 665440, Call H2020-FETOPEN-2014-2015-RIA "Future and Emerging Technologies:FETOPEN")
  PI: Spanish node with F. Sagués and I. Pagonabarraga. Coordinator: Feodor Ogrin (UK) (2016 – 2018)

International Collaborations

- Andrejs Cebers (Uni. Latvaia, Latvia), Piotr Garstecki (IPC, Poland), Thomas M. Fischer, and Matthias Schmidt (Uni. Bayreuth, Germany), Christian Pichot (CNRS, France), Ramin Golestanian, Fanlong Meng (MPI Gottingen, Germany), Tom H Johansen (Uni. Oslo, Norway), Michael Kasha and Michael Roper (Florida State, USA), Andras Libal (Uni. Babes-Bolyai, Romania), Charles Mingotaud (CNRS, France), Peter Reimann (Uni.Bielefeld, Germany), Igor M. Sokolov, Lutz Schimansky-Geier and Arthur Straube (Uni Humboldt, Germany), D. B. Weibel (Uni.Wisconsin, USA), George M. Whitesides (Harward Uni., USA), A. Soba (COCINET, Argentina), H. Lowen (Uni Dusserdolf), Leticia Cugliandolo (Université Pierre et Marie Curie, France), Philipp Mass (Uni Osnabrueck), Yair Shokef (Tel aviv University), Charle Reichhardt and Cristiano Nisoli (Los alamos National Lab, USA).

SELECTED PAPERS

- *Mixed-order phase transition in a colloidal crystal.* Ricard Alert Zenon, Pietro Tierno and Jaume Casademunt. *Proc. Natl. Acad. Sci.* USA 114 12906-12909. **2017**.
- *Active apolar doping determines novel routes to colloidal clusters and gels.* H. Massana-Cid, J. Codina, I. Pagonabarraga, P. Tierno, *Proc. Natl. Acad. Sci.* USA 115 10618-10623. **2018**.
- *Ice Rule Fragility via Topological Charge Transfer in Artificial Colloidal Ice.* A. Libal, D. Yun Lee, A. Ortiz-Ambriz, C. Reichhardt, C. J. O. Reichhardt, P. Tierno, C. Nisoli. *Nature Comm.* 9 4146. **2018**.
- *Magnetically tunable bidirectional locomotion of a self-assembled nanorod-sphere propeller.* Jose Garcia-Torres, Carles Calero, Francesc Sagués, Ignacio Pagonabarraga and Pietro Tierno. *Nature Comm.* 9 1663. **2018**.
- *Emergent Hydrodynamic Bound States Between Magnetically Powered Micropropellers.* Fernando Martinez-Pedrero, Eloy Navarro-Argemi, Antonio Ortiz-Ambriz, Ignacio Pagonabarraga, Pietro Tierno. *Science advances* Vol. 4, no. 1, eaap9379. **2018**.

2.2.22. Magnetism (NanoMagnetics)

Department of Condensed Matter Physics, Faculty of Physics

Team

- **Javier Tejada Palacios (Full Professor)**
- **Antoni García Santiago (Associate Professor)**
- **Joan Manel Hernández Ferràs (Associate Professor)**
- **Ferran Macià Bros (Postdoctoral Researcher Ramon y Cajal)**

Research

The research developed by the group explores the intersection field between the static and rotating magnetic fields, the low and ultra low temperatures and the interaction with radiation of microwaves in magnetic and superconducting materials. Among the main lines of research are quantum magnetic deflagration, the effect of acoustic waves on the magnetic behavior of various systems, the rotational Doppler effect on magnetic resonance, commensurability phenomena in nanostructured type II superconductors, intermediate status in type-I superconductors and the measurement of properties of hybrid systems formed by alternate layers of magnetic and superconducting materials.

Selected Projects

- Control magneto-mecánico de la magnetización en sistemas nanométricos mediante ondas acústicas.
  IP: Joan Manel Hernandez Ferras MAT2015-69144-P.
  Ministerio de Economia y Competitividad. 2016-2018

Singular Scientific Equipment

- RF SQUID Magnetometer. Temperature: from 1.8 K to 300 K. Magnetic field: from -5 T to 5 T
- DC SQUID Magnetometer. Temperature: from 50 mK to 4.2 K. Magnetic field: from -5 T to 5 T
- E4448A PSA Series Spectrum Analyzer, 3 Hz - 50 GHz
- 8565E Portable Spectrum Analyzer, 9 kHz to 50 GHz
- 8510C Vector Network Analyzer
- E8361A PNA Network Analyzer, 10 MHz to 67 GHz
- PNA Millimeter-Wave Network Analyzer, 10 MHz to 110 GHz

International Collaborations

- Prof. Eugene M. Chudnovsky (The City University of New York)
- Prof. Jaume Veciana (ICMAB)
- Prof. Victor Moshchalkov (KU LEUVEN)

SELECTED PAPERS

- *Multiphase magnetic deflagrations in a Nd5Ge3 single crystal.* Villuendas D., Vélez S., Tsutaoka T., Hernandez J.M. *New Journal of Physics.* Vol: 19. **2017**.
- *Long-range proximity effect in Nb-based heterostructures induced by a magnetically inhomogeneous permalloy layer.* Cirillo C., Voltan S., Ilyina E.A., Hernández J.M., Garca-Santiago A., Aarts J., Attanasio C. *New Journal of Physics.* Vol: 19. **2017**.
- *High Electrocatalytic Response of a Mechanically Enhanced NbC Nanocomposite Electrode Toward Hydrogen Evolution Reaction.* Coy E., Yate L., Valencia D.P., Aperador W., Siuzdak K., Torruella P., Azanza E., Estrade S., Iatsunskyi I., Peiro F., Zhang X., Tejada J., Ziolo R.F. *ACS Applied Materials and Interfaces.* Vol: 19. **2017**.
- *Generation and stability of dynamical skyrmions and droplet solitons.* Statuto N., Hernandez J.M., Kent A.D., Macia F. *Nanotechnology.* Vol: 29. **2018**.
- *Ex vivo assessment and in vivo validation of non-invasive stent monitoring techniques based on microwave spectrometry.* Gálvez-Montón C., Arauz-Garofalo G., Rodriguez-Leor O., Soler-Botija C., Amorós García de Valdecasas S., Gerez-Britos F.D., Bayes-Genis A., O'Callaghan J.M., Macià F., Tejada J. *Scientific Reports.* Vol: 8. **2018**.

2.2.23. Magnetism and Functional Molecules Group (GMMF) (NanoMagnetics, NanosMat)

Department of Inorganic and Organic Chemistry, Faculty of Chemistry

Team

- **Guillem Aromí Bedmar (Full Professor)**
- **Eva Carolina Sañudo (Associate Professor)**
- **Albert Figuerola Silvestre (Associate Professor)**
- **David Aguilà Avilés (Postdoctoral Researcher Juan de la Cierva)**
- **Leoni A. Barrios Moreno (Postdoctoral Researcher)**
- **Verónica Velasco Amigó (Adjunct Lecturer)**
- **Rosa Diego Creixenti (PhD Student)**
- **Lidia Rosado (PhD Student)**

Research

- Functional Molecules: Synthesis and characterization

  At GMMF we pursue the design and preparation of molecular materials with multifunctional properties. We focus mainly on the combination of magnetic properties (single molecule magnets -SMMs-, spin crossover -SCO- molecules or molecular quantum bits and quantum gates) with optical properties like fluorescent emission or reversible photoswitching by using the right combination of ligands and metals. For the former optical properties, we work with imine ligands with fluorescent markers or azo groups and we combine these with anisotropic transition metals or lanthanide ions. For the photoswitching, we incorporate dithienylethene moieties into ligands capable to assemble functional coordination complexes.

  SCO supramolecular helicates capable to encapsulate functional guests are prepared and studied in the group.

- Molecular Based Quantum Computing

  Molecular quantum bits (qubits) and quantum gates (qugates) that use the electronic spin as elementary unit of quantum information are prepared with transition metals and lanthanides. Quantum gates assemble two or three qubits entangled and not equivalent for individual addressing. The quantum coherent properties of these systems is investigated and the molecules are incorporated (in the context of a consortium) into quantum electrodynamic devices with the aim to build hybrid quantum processors.

- Crystal Engineering

  SCO crystals capable to exchange small molecules with the environment are studied as chemosensors. Crystallographic phase transitions coupled to magnetic transitions (reversible or irreversible) involfing metastable states, are studied with these materials.

SELECTED PAPERS

- *Double-decker luminescent ytterbium and erbium SMMs with symmetric and asymmetric Schiff base ligands.* S. Gholizadeh Dogaheh, H. Khanmohammadi and E. C. Sañudo, *New J. Chem.* **2017**. 41, 10101–10111.
- *Hybrid molecular-inorganic materials: a heterometallic [Ni4Tb] complex grafted on superparamagnetic iron oxide nanoparticles.* L. Rosado Piquer, E. Jiménez, Y. Lan, W. Wernsdorfer, G. Aromi and E. C. Sañudo, *Inorg. Chem. Front.* **2017**, 4, 595–603.
- *A Magneto-optical Molecular Device: Interplay of Spin Crossover, Luminescence, Photomagnetism, and Photochromism.* M. Estrader, J. S. Uber, L. A. Barrios, J. Garcia, P. Lloyd-Williams, O. Roubeau, S. J. Teat, G. Aromí, Angewandte. *Chemie, International Edition.* **2017**, 56, 15622-15627.
- *Guest-tuned spin crossover in flexible supramolecular assemblies templated by a halide (Cl–, Br– or I–).* M. D. Darawsheh, L. A. Barrios, O. Roubeau, S. J. Teat and G. Aromí. *Chem. Commun.* **2017**, 53, 569-572.
- *Encapsulation of a Cr(III) Single-Ion Magnet within an Fe(II) Spin-Crossover Supramolecular Host.* M. Darawsheh, L. A. Barrios, O. Roubeau, S. J. Teat, G. Aromí, Angewandte. *Chemie, International Edition.* **2018**. 57, 13509 –13513.

- Molecular Nanoscience

  Once interesting molecules have been made and characterized, we deal with the nanostructuration of these molecules, mainly SMMs on surfaces. It is a key factor to understand the molecule-surface interaction in order to implement applications such as molecular spintronics, information storage or information processing with SMMs. We have devoted the last 4 years to prepare hybrid systems using nanoparticles and complex coordination complexes that are SMMs. Magnetic characterization of these systems has been a challenge that we tackle using synchrotron radiation to perform X-ray magnetic circular dichroism, XMCD, an element sensitive technique. We have also used our expertise to prepare water soluble iron oxide nanoparticles for biomedical applications.

Selected Projects

- Scaling Up quantum computation with MOlecular spins. Reference: EU H2020 ERA-NET Consortium (QuantERA); Acronym, SUMO. Coordinator: Fernando Luis. PI Working Package 1 (PCI2018-093106): Guillem Aromí. Extension: 2018-2020
- *Materiales funcionales moleculares y nanoestructurados para aplicaciones nanotecnológicas.* Reference: CTQ2015-68370-P. IP: Guillem Aromí. Ministerio de Economía y Competitividad. Extension: 2016-2018
- *Prize ICREA Academia.* IP: Guillem Aromí. Institució Catalana de Recerca i Estudis Avançats. 2014-2018

Singular Scientific Equipment

Bruker apexii qazar single crystal x-ray diffractometer

International Collaborations

- Liu, Chun Sen (Zhenzhou Light Industry University, P.R. China): synthesis of MOFs
- Jan Dreiser (Paul Scherrer Institute, SLS, Switzerland): XAS and XMCD

QUANTERA Consortium:

- Consejo Superior de Investigaciones Científicas (CSIC); F. Luis
- University of Manchester (UMAN); R. Winpenny
- Consorzio Interuniversitario Nazionale per la Scienza e Tecnologia dei Materiali (INSTM); S. Carretta
- Universität Stuttgart/ Institut für Funktionelle Materie und Quantentechnologien (FMQ) ; S. Loth
- TU Wien/Atom Institut (TUWIEN) ; J. Majer

2.2.24. Materials for Energy, Photonics and Catalysis, ENPHOCAMAT (NanosMat)

Department of Applied Physics, Faculty of Physics

Team

- **Enric Bertran Serra (Full Professor)**
- **José Luis Andújar Bella (Associate Professor)**
- **Adolf Canillas Biosca (Associate Professor)**
- **Esther Pascual Miralles (Associate Professor)**
- **Franc Güell Vilà (Associate Professor)**

- **Oriol Arteaga Barriel (Postdoctoral Researcher Ramon y Cajal)**
- **Roger Amade Rovira (Tenure-Track Lecturer)**
- **Arevik Musheghyan Avetisyan (PhD Student)**
- **Luis Fernando Pantoja Suárez (PhD Student)**
- **Islam Alshaikh (PhD Student)**
- **Joan Martí González (PhD Student)**

Research

During this last period 2017-2018, the group 'Materials for Energy Photonics and Catalysis' (ENPHOCAMAT) focuses its activity on the search of advanced materials through the production, treatment, structural and compositional characterization, physical-chemical functionality, photonic characterization of materials in general and of nanometric structures. All these activities are aimed at catalysis, photonics and energy applications, as well as the formation and diffusion of knowledge. The group has the necessary infrastructure for the production of materials through technologies in the steam phase (CVD and PVD), mechanical, chemical, electrochemical and laser treatment for the production of nanostructures and for their functionalization. In addition, the group is made up of a team of researchers who are experts in the structural and compositional characterization, optics and photonics, and in surface and analysis techniques, to carry out the study of the properties of materials and nanomaterials in the face of its applications. The research of the Catalytic Materials Group is centred on the preparation and characterization of new materials with catalytic properties. The environmental impact of the current use of fossil fuels could be diminished if biomass-derived resources were considered as an alternative feedstock for hydrogen and syngas production. The production of hydrogen from biomass-derived substrates could contribute in the medium term to the implementation of the use of H2 as an energy vector through the use of fuel cells. The use of photo-assisted catalytic processes could decrease the energy necessary for the process. Over recent years, we have developed new multicomponent materials, which effectively catalyse the steam reforming of C1-C4 bio-alcohols. Special attention has been paid to the selectivity and stability of catalysts, which is related to their characteristics. The use of renewable substrates such as bio-ethanol as platform molecules has also been envisaged through their transformation by selective catalytic processes.

Recently, we considered the transformation of biosubstrates assisted by photocatalysis as a new research topic. Moreover, we are developing new materials for the chemical recycling of CO2 and contemplating its transformation to hydrocarbons, DME or higher alcohols. The characterization of materials before and after the catalytic processes is of major importance in order to establish the relationship between their catalytic behaviour, stability and the characteristics of the catalysts.

SELECTED PAPERS

- *Laser-driven coating of vertically aligned carbon nanotubes with manganese oxide from metal organic precursors for energy storage.* A. Pérez del Pino; E. György; I. Alshaikh; F. Pantoja-Suárez; J.L. Andújar; E. Pascual; R. Amade; E. Bertran-Serra. *Nanotechnology.* 28. **2017**. 1-9.
- *Partially coherent light propagation in stratified media containing an optically thick anisotropic layer.* Nichols, S.M.; Arteaga, O.; Martin, A. T.; Kahr, B. *Applied Surface Science.* **2017**.
- *Plasma synthesis of polyaniline enrobed carbon nanotubes for electrochemical applications.* Hussain, S.; Kovacevic, E.; Amade, R.; Berndt, J.; Pattyn, C.; Dias, A.; Boulmer-Leborgne, Ch.; Ammar, M.-R.; Bertran-Serra, E. *Electrochimica Acta, 268.* **2018**. 218-225.
- *Field Enhancement of Multiphoton Induced Luminescence Processes in ZnO Nanorods.* Hyyti, J.; Perestjuk, M.; Mahler, F.; Grunwald, R.; Güell, F.; Gray, C.; McGlynn, E; Steinmeyer, G., *J. of Physics D-Appl. Phys.* 51. **2018**. 105306.
- *Easily reduced bis- pincer (NS2) 2molybdenum(IV) to (NHS2) 2Mo(II) by alcohols vs. redox- inert (NS2) (NHS2) iron(III) complexes.* Robles-Marin, Elvis; Mondragon, Alexander; Martinez-Alanis, Paulina R.; Aullon, Gabriel; Flores-Alamo, Marcos; Castillo, Ivan. *Dalton Transactions, 47.* **2018**. 10932 10940.

Lines and activities of the Group ENPHOCAMAT:

- New nanostructured materials
- Nanostructured carbon supercapacitors
- Optical characterization: polarimetry and generalized ellipsometry
- Photonic Materials
- Preparation and characterization of new materials with catalytic properties
- Studies of the relationship between the catalytic behavior and the characteristics of materials;
- The application of new materials as catalysts in:
  - Chemical recycling of CO_2
  - Transformation of biomass-derived resources into chemicals and energy carriers.

Highlights:

- Characterization of depolarizing media based on Mueller matrix
- Graphene deposition by ICP-CVD
- Carbon nanotube based electrodes for supercapacitor applications
- Structure-catalytic behavior relationship
- Catalysis by metals and oxides
- Tailored catalysts
- Bioalcohols for hydrogen production
- CO_2 conversion
- Nanostructured materials
- Hydrogen production;
- Photo-assisted hydrogen production
- C1 chemistry

Selected Projects

- NANOTUBE, Carbon hybrid and metal oxides nanocomposites for application in supercapacitors ENE2014-56109-C3-1-R Enric Bertran Serra (IP), Esther Pascual Miralles (Co-IP). State Program R+D+I RETOS, MCOC - Ministerio de Economia y Competitividad. 2015-2017
- ADHES, Synthesis of CNS (VACNTs and GNWs) in flexible metal tapes and study of their electrochemical properties after functionalization with metal oxide composites, ENE2017-89210-C2-2-R. Enric Bertran Serra (IP), Esther Pascual Miralles (Co-IP). State Program R+D+I RETOS, MCOC - Ministerio de Economia y Competitividad . 2018 -2020

Singular Scientific Equipment

- Catalysis laboratory: http://www.qi.ub.es/matcat/eng%20laboratori.htm
- Spectral and Generalized Ellipsometer (UV-VIS)
- Mueller Matrix Polarimeter
- PECVD-PVD CNTs reactor
- ICP-CVD Graphene reactor

- Magnetron Sputtering PVD system
- Langmuir Blodgett, for 2D coloidal crystalls deposition

International Collaborations

- Group of Prof. Pagona Papakonstantinou del NIBEC, University of Ulster, Belfast, Northern, Ireland (UK).
- Group of Prof. David Mariotti del NIBEC, University of Ulster, Belfast, Northern Ireland (UK).
- Group of Prof. MPY Desmulliez and Dr. José Marques-Hueso of Institute of Sensors, Signals & Systems, School of Engineering & Physical Sciences, Institute of Mechanical, Process & Energy Engineering, Energy Academy, Heriot-Watt University.
- Departamento de Materiales, Facultad de Ingeniería Mecánica, Escuela Politécnica Nacional, Quito (Ecuador).
- Group of Dr. Adrian Boyd and Dr. Shahzad Hussain of the NIBEC, Jordanstown, Ulster University, Norther Ireland, UK.
- Group of Prof. Thomas Bechtold and Dr. Noemi Aguiló Aguayo of Research Institute of Textile Chemistry and Textile Physics, University of Innsbruck, Austria.
- Group of Prof A. Dimoulas y Dr. S. Chaitoglou of Laboratory of Epitaxy and Surface Science, Institute of Nanoscience and Nanotechnology, NCSR Demokritos , Greece.

2.2.25. Materials: Phase transitions (NanoMet)

Department of Condensed Matter Physics, Faculty of Physics

Team

- **Antoni Planes Vila (Full Professor)**
- **Lluís Mañosa Carrera (Full Professor)**
- **Teresa Castán Vidal (Full Professor)**
- **Michela Romanini (Postdoctoral Researcher Juan de la Cierva)**
- **Marcel Porta Tena (Adjunct Lecturer)**

Research

Research activity of our group has the following three main objectives. The first two are experimental and aim at,

- The development and characterization of new materials with giant caloric response, which is a class of materials potentially interesting for environmentally friendly solid state refrigeration and energy harvesting applications. The giant response is a consequence of a remarkable coupling between an external field (either mechanic, electric or magnetic) and the corresponding degrees of freedom inherent to these materials that allows highly-amplified functional effects to be realized. We are interested in developing novel routes aimed at designing and optimizing materials that display cross response to multiple fields, and thus show multicaloric effects. The interest of multicaloric materials is twofold. On the one hand, it is expected that the caloric response can be enhanced by the application of multiple fields and, on the other hand, to show that it is possible to tune the temperature operation range, and consequently to improve the reproducibility of the caloric response during cycling.
- The study of externally driven materials that respond intermittently through a sequence of avalanches. This occurs, for instance, associated with structural transitions, magnetization processes or the compression of nanoporous materials, and show strong analogies with Earth seismicity. The interest of these studies is that often avalanches occur with absence of time and length scales, a behaviour that defines the so-called avalanche criticality. In these processes the dynamics is characterised by power law distributions of the avalanche size, duration and energy. Usually avalanches stem from sudden changes of the internal strain field and can thus be detected using high-resolution (microseconds in time and nanometers in space) acoustic emission techniques. In our group we are essentially interested in the study of the dependence of the distributions of energy and duration of acoustic emission avalanches in materials with tailored microstructures with the aim of gaining understanding on the influence of heterogeneities on their dynamics.

The third objective is devoted to:

- Phase field modelling and numerical simulation of microstructural pattern formation in materials with multiple degrees of freedom that undergo structural transitions. This is applied to the study of the caloric and multicaloric response of these systems and the occurrence intermittent dynamic processes and its influence on hysteresis effects in this class of materials.

Selected Projects

- Materiales con respuesta activa para refrigeración limpia y eficiente. MAT2016-75823-R. Antoni Planes Vila (Co-IP). Ministerio de Economia y Competitividad. 2016-2020

Singular Scientific Equipment

- DSC calorimeter with applied magnetic field and stress
- Acoustic emission detection systems in he frequency range of MHz.
- High resolution infra-red camera.

International Collaborations

- Prof. E.K.H. Salje, Department of Earth Sciences, University of Cambridge, U.K.
- Prof. Mehmet Acet, Physics Department, Universität Duisburg-Essen, Germany
- Profs. N. D. Mathur and X. Moya, Department of Materials Science, University of Cambridge, U.K.
- Dr. Avadh Saxena, Theoretical Division, Los Alamos National Lab., U.S.A.
- Dr. Oliver Gutfleisch, Technische Universität Darmstad., Germany

SELECTED PAPERS

- *Materials with giant mechanocaloric effects: Cooling by strength.* L. Mañosa and A. Planes. *Adv. Mater.*, 29, 1603607. **2017**.
- *Giant barocaloric effects over a wide temperature range in the superionic conductor AgI.* A. Aznar, P. Lloveras, M. Romanini, M. Barrio, J. L. Tamarit, C. Cazorla, D. Errandonea, N. D. Mathur, A. Planes , X. Moya, L. Mañosa. *Nature Comm.*, 8, 1851. **2017**.
- *A novel multicaloric cooling cycle that exploits thermal hysteresis.* T. Gottschall, A. Gràcia-Condal, M. Fries, A. Taubel, L. Pfeuffer; L. Mañosa, A. Planes, K. Skokov, and O. Gutfleisch. *Nature Mater.*, 17, 929. **2018**.
- *Experimental evidence of accelerated seismic release without of critical failure in the acoustic emission of compressed nanoporous materials.* J. Baró, K. A. Dahmen, J. Davidsen, A. Planes, P. O. Castillo, G. F. Nataf, E. K. H. Salje, and E. Vives. *Phys. Rev. Lett.*, 120, 245501. **2018**.
- *Intermittent dynamics in externally driven ferroelastics and strain glasses.* M. Porta, T. Castán, P. Lloveras, A. Saxena, and A. Planes. *Phys. Rev.* E, 98, 032143. **2018**.

2.2.26. Microbian Enzymes for Industrial Applications Group (NanoBio)

Department of Genetics, Microbiology and Statistics, Faculty of Biology

Team

- **Francisco I. Javier Pastor Blasco (Full Professor)**
- **Pilar Díaz Lucea (Full Professor)**
- **Josefina Martínez Martínez (Associate Professor)**
- **Susana Valenzuela Mayorga (Adjunct Lecturer)**
- **Carolina Buruaga (PhD Student)**
- **Lourdes Verónica Cabañas (PhD Student)**

Research

The group of Microbial Enzymes for Industrial and Environmental Applications works on the biotransformation of natural polymers, including the development of enzymes that catalyze their modification, hydrolysis, and/or synthesis. In addition, we are exploring the potential of bacterial nanocellulose and other nanocellulosic materials, as sources of new biomaterials, suitable for high added value applications.

We have deep experience in the study of molecular biology of carbohydratases and esterases, and the identification and design of enzymes for biotechnological application in pulp bleaching and paper recycling, production of biofuels, synthesis of new compounds from wastes, improvement of textile fibers, food industry, and development of new materials based on lignocellulose and lipids. With different approaches, we have expanded the toolbox of new enzymes, or their improvement by protein-engineering strategies, available for the community. We aim at combining basic research with applied studies and innovation.

Figure 1. Surface analysis of cellulosic substrates developed in our lab. Optical microscopy (1st row) and Field Emission Scanning Electron Microscopy (2nd and 3rd rows) of Bacterial cellulose (A), Avicel (B), 75% Phosphoric acid swollen cellulose (C), 76% Phosphoric acid swollen cellulose (D), Regenerated amorphous cellulose (E), and 78% Phosphoric acid swollen cellulose (F). (1), Bacterial cellulose FESEM image was taken with 8000X instead of 4500X

In the past years, we have been exploring sustainable ways to generate bio-nanoparticles produced from cellulosic sources. The development of these materials displays exceptional physicochemical properties, such as an ultrafine reticulated structure, high crystallinity, high tensile strength, high hydrophilicity and biocompatibility. These unique properties are allowing us to develop new biocomposites and to evaluate their properties.

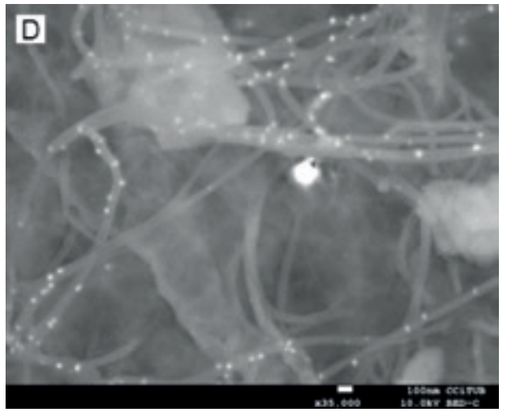
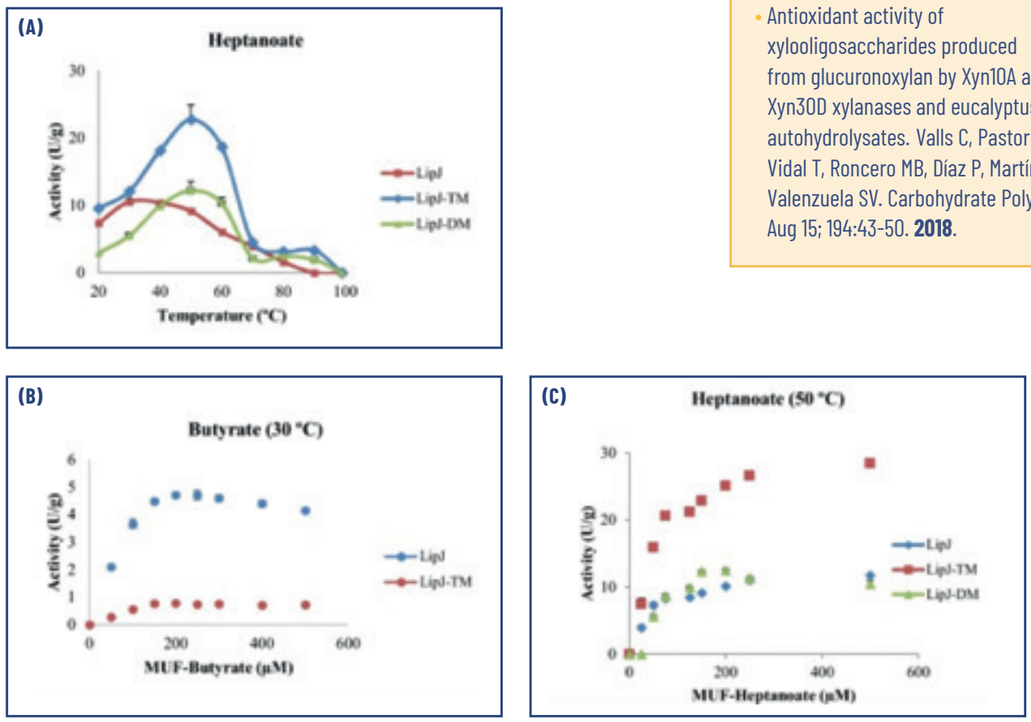


Figure 2. Generation of bio-nanoparticles produced in cellulosic sources: Field Emission Scanning Electron Microscopy image of Bacterial cellulose/ Ag nanoparticles composite

The group is currently working on the biochemical characterization and genetic manipulation of Carbohydrate Active Enzymes and Lipases from the early stages of sampling, cloning, purification up to studies of structure-function relationship, enzyme engineering, application and the combination of the new enzymes on promising substrates developed by the group, like Bacterial Cellulose or Nanofibrillated Cellulose.

Figure 3. Design of enzymes for biotechnological application: Shift in Bacillus sp. JR3 esterase LipJ activity profile after addition of essential residues from family I.5 thermophilic lipases: Temperature (A) and kinetics (B,C) profile of lipase wild type LipJ and variants LipJ-DM and LipJ-TM



SELECTED PAPERS

- Alternative Oils Tested as Feedstocks for Enzymatic FAMEs Synthesis: Toward a More Sustainable Process. Infanzón B., Cesarini S., Martínez J., Pastor F.I.J., Diaz P. Biotechnology Progress. 33; 5. **2017**.
- A bacterial GH6 cellobiohydrolase with a novel modular structure. Cerda-Mejía L., Valenzuela S.V., Frías C., Diaz P., Pastor F.I.J. Applied Microbiology and Biotechnology. 101; 7. **2017**.
- Fast purification method of functional LPMOs from Streptomyces ambofaciens by affinity adsorption. Valenzuela S.V., Ferreres G., Margalef G., Pastor F.I.J. Carbohydrate Research. 448. **2017**.
- Bacterial cellulose for increasing barrier properties of paper products. Fillat A, Martínez J, Valls C, Cusola O, Roncero MB, Vidal T, Valenzuela SV, Diaz P, Pastor FIJ. Cellulose. 25; 10:6093-610. **2018**.
- Antioxidant activity of xylooligosaccharides produced from glucuronoxylan by Xyn10A and Xyn30D xylanases and eucalyptus autohydrolysates. Valls C, Pastor FIJ, Vidal T, Roncero MB, Díaz P, Martínez J, Valenzuela SV. Carbohydrate Polymers. Aug 15; 194:43-50. **2018**.

Selected Projects

This work is funded by the Spanish MINECO BIOFABCEL CTQ2017-84966-C2-2-R and ART2017 projects.

Singular Scientific Equipment

- Nanofibrillated cellulose preparation: Panda Plus 2000, for high-pressure homogenization
- Protein purification: ÄKTA protein purification system, for chromatographic separation of proteins
- Screening for activity: ASYS UVM340 Microplate reader / Agilent, Varian Cary Eclipse Fluorescence Spectrophotometer, for microplate

International Collaborations

- Peter Biely's Lab: Institute of Chemistry, Slovak Academy of Sciences, Bratislava, Slovakia.
- Sonia Rodriguez Giordano's Lab: Bioscience Department, Universidad de la República. Montevideo, Uruguay.
- Diana Ciolacu: "Petru Poni" Institute of Macromolecular Chemistry, Department of Physical Chemistry of Polymers. Iasi, Romania.
- Mirjam Kabel: Department of Agrotechnology and Food Sciences, Wageningen University & Research. Wageningen, Netherlands.
- Nawel Boucherba: Head of Team Microbial enzymes, president of the scientific council of the FNSL. University A/Mira of Bejaia.

2.2.27. Micro and Nanotechnology and nanoscopies for Electronic and Electrophotonic Devices (MIND) (NanoPhotoElectro)

Department of Electronics and Biomedical Engineering, Faculty of Physics

Team

- **Albert Cornet Calveras (Full Professor)**
- **Blas Garrido Fernández (Full Professor)**
- **Albert Cirera Hernández (Full Professor)**
- **Juan Daniel Prades Garcia (Full Professor and ERC Starting Grant)**
- **Albert Romano Rodríguez (Associate Professor)**
- **Paolo Pellegrino (Associate Professor)**
- **Daniel Navarro Urrios (Postdoctoral Researcher Ramón y Cajal)**
- **Sergio Hernández Márquez (Associate Professor)**
- **Cristian Fàbrega Gallego (Tenure-Track Lecturer)**
- **Francisco de P. Hernandez Ramirez (Adjunct Lecturer)**
- **Aïda Varea Espelt (Adjunct Lecturer)**
- **Olga Casals Guillén (Postdoctoral Researcher)**
- **Julià López Vidrier (Postdoctoral Researcher Juan de la Cierva)**
- **Josep Oriol Blazquez Gomez (PhD Student)**

SELECTED PAPERS

- *A review on efficient self-heating in nanowire sensors: Prospects for very-low power devices. Fàbrega, C.; Casals, O.; Hernández-Ramírez, F.; Prades, J.D. Sensors and Actuators B-Chemical, 256, 797 - 811.* **2017**.
- *Highly Specific and Wide Range NO2 Sensor With Color Readout. Fabrega, C.; Fernández, L.; Monereo, O.; Pons-Balagué, A.; Xuriguera, E.; Casals, O.; Waag, A.; Prades, J. D.ACS Sensors 2, 1612 - 1618.* **2017**.
- *Selectively arranged single-wire based nanosensor array systems for gas monitoring. Chmela, O.; Sadílek, J.; Domènech-Gil, G.; Samà, J.; Somer, J.; Mohan, R.; Romano-Rodríguez, A.; Hubálek, J.; Vallejos, S. Nanoscale 10, 9087-9096.* **2018**.

- **Adrià Huguet Ferran (PhD Student)**
- **Alexander Cabal Tato (PhD Student)**
- **Ismael Gabaldon Saucedo (PhD Student)**
- **Juan Luis Frieiro Castro (PhD Student)**
- **Guillem Domènech Gil (PhD Student)**
- **Elena López Aymerich (PhD Student)**

Research

The activities developed in this biennium 2017-2018 can be named Development of Advanced Micro and Nanosystems. They cover from basic science (physics, chemistry, materials and nanoscience) to applied and technological topics (applied physics, engineering, micro and nanofabrication), always focusing on addressing specific societal problems. The three main topics are described briefly in the following:

1. Fabrication of advanced nanomaterials, their integration into nanodevices and the development of nanosystems for gas sensing applications. This is supported by a project financed by MINECO (TEC2016-76898-C6-2-R). This activity has a focus on the fabrication of crystalline metal oxide nanowires (NWs) for their use in gas sensing. A second aspect and to avoid the transfer of the NWs to the microhotplates (MHP) of the final chip, a new route has been set-up that allows the site-selective growth of the NWs directly on top of the MHP. It consists in modifying the classical vapor-liquid-solid growth method. Furthermore, this methodology has allowed growing different NWs onto different MHPs of the same chip. The different gas sensing pattern has allowed this chip to constitute a nano-electronic-nose, which provides gas discrimination and quantification.

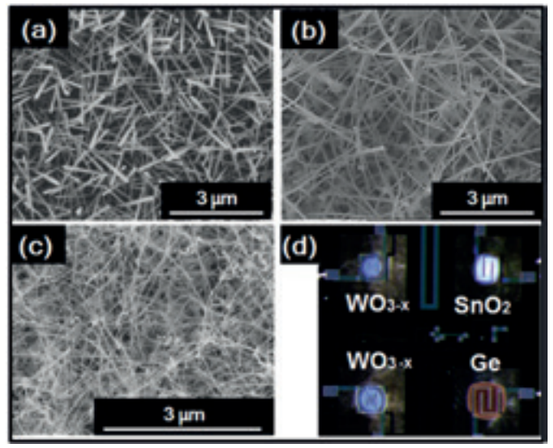


Figure 1: Localised growth of Nanowires on top of micromembranes and their gas response as an electronic nose.

2. Development of a nanosystem for the assessment of mechanical stresses in living tissues, started in an Explora project (TEC2014-62144-EXP). This is a truly interdisciplinary work, developed together with scientists from the Department of Genetics of UB and nanobiotechnologists from the Technical University of Denmark, aiming at developing a system that allows continuous monitoring the stresses of the tissues under disease conditions.
3. Development of ultra low power gas sensors, targeting improvements 3 orders of magnitude better than the state-of-the-art (i.e. a reduction from ~10mW down to ~10µW). This has been achieved by means of miniaturization and integration of the sensor materials with microLED devices, that supply the energy needed to activate the gas-surface interactions needed to trigger a response to gases in a much more energy efficient way, compared to the standard heat-based devices and compared to previous much bulkier implementations based on large LEDs. This activity has been carried out in

- *Site-specific growth and in situ integration of different nanowire material networks on a single chip: towards a nanowire-based electronic nose for gas detection.* Hrachowina, L.; Domènech-Gil, G.; Pardo, A.; Seifner, M. S.; Gràcia, I.; Cané, C.; Romano-Rodríguez, A.; Barth, S. *ACS Sensors 3, 727-734.* **2018**.
- *Sensitivity-Selectivity Trade-Offs in Surface Ionization Gas Detection. Müller, G.; Prades, J.D.; Hackner, A.; Ponzoni, A.; Comini, E.; Sberveglieri, G. Nanomaterials 8, 1 - 22.* **2018**.

close cooperation with the Technical University of Braunschweig and the Institut de Microelectrònica de Barcelona (IMB-CNM-CSIC), that provide GaN foundry services within the ERC Starting Grant "BetterSense" project.

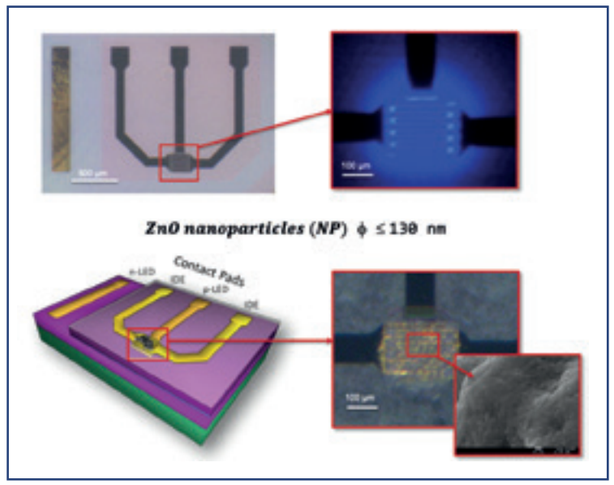


Figure 2: Micro Light-plate sensor based on ZnO nanoparticles

Selected Projects

- *Innovación tecnológica en micro y nanosensores para monitorización de calidad de aire y control medioambiental*
  Program: RETOS de la Sociedad
  Funding Agency: Ministerio de Economia y Competitividad
  Reference: TEC2016-76898-C6-2-R. 2017-2020
  IP: Albert Romano Rodriguez / Mauricio Moreno Sereno
- *Monitorización bidimensional de tensiones mecánicas en tejidos biológicos*
  Program: Proyectos "Explora Ciencia" y "Explora Tecnología" 2014
  Funding Agency: Ministerio de Economia y Competitividad
  Reference: TEC2014-62144-EXP. 2015-2018
  IP: Albert Romano Rodriguez
- *Nanodevice Engineering for a Better Chemical Gas Sensing Technology (BetterSense)*
  Program: ERC Starting Grant, 7th Framework Program, IDEAS
  Funding Agencia: European Union
  Reference: 336917. 2014-2019
  IP: Juan Daniel Prades Garcia

International Collaborations

- Research Center: Technical University of Denmark (DTU)
  Group leader: Winnie E. Svendsen. City: Lyngby (Denmark)
- Research Center: Goethe University of Frankfurt
  Group leader: Sven Barth. City: Frankfurt (Germany)
- Research Center: Albrechts-Ludwig Universität Freiburg
  Group leader: Jürgen Wöllenstein. City: Freiburg im Breisgau (Germany)
- Research Center: TU Braunschweig
  Group leader: Andreas Waag. City: Braunschweig (Germany)

2.2.28. Mineral Resources Research Group (NanoBio)

Department of Mineralogy, Petrology and Applied Geology, Faculty of Earth Sciences

Team

- **Josep Roqué Rosell (Tenure-Track Lecturer)**
- **Joaquín Antonio Proenza (Associate Professor)**
- **Joan Carles Melgarejo Draper (Associate Professor)**
- **Maria Abigaíl Jiménez Franco (Invited Postdoctoral Researcher)**

Research

We are group of scientists developing research in mineralogy at nanoscale by using cutting edge research techniques such as Transmission Electron Microscopy (TEM) and Synchrotron Radiation Sources (SRS) to explore and understand the geological and biological interactions taking place in minerals. The task that we develop consists of the study at nanoscale of the metals partitioning in geological systems, the study of natural nanoparticles aggregation, the study of nanoporosity in rocks and soils, the study of the stability of nanominerals and the *ab-initio* structure determination of nanominerals. Our research has a direct impact on the integral study of mineral resources (from exploration to the metallogenetic studies), on the possible applications of their minerals, on the environmental impact and the sustainability of these resources. In these fields we have an ample credited experience, both in the research and teaching levels. At the moment we are developing these research and educational lines in Europe (Catalonia, Spain, Bosnia-Herzegovina, Croatia, Bulgaria and Italy), America (Canada, Cuba, Mexico, Dominican Republic, Colombia, Argentina, Nicaragua and Brazil) and Africa (Angola and Egypt).

1. Research highlights

1.1. Nanoscale partitioning of Ru, Ir, and Pt in base-metal sulfides from the Caridad chromite deposit, Cuba.

We report new results of a combined focused ion beam and high-resolution transmission electron microscopy (FIB/HRTEM) investigation of platinum-group elements (PGE)-rich base-metal sulfides. The Ni-Fe-Cu base-metal sulfides (BMS) studied are millerite (NiS), pentlandite [(Ni,Fe)9S8], pyrite (FeS2), and chalcopyrite (CuFeS2). These BMS were found forming composite inclusions (<60 mm across) within larger unaltered chromite from the Caridad chromite deposit, which is hosted in the mantle section of the Mayarí-Baracoa Ophiolite in eastern Cuba. Electron probe microanalysis of BMS revealed PGE values of up to 1.3 wt%, except for pentlandite grains where PGE concentrations can reach up to 12.8 wt%. Based on the amount of Ru, two types of pentlandite are defined: (1) Ru-rich pentlandite with up to 8.7 wt% of Ru and <3.5 wt% of Os, and (2) Ru-poor pentlandite with Ru <0.4 wt% and Os <0.2 wt%. Ru-rich pentlandite contains Ir-Pt nanoparticles, whereas the other sulfides do not host nanometer-sized platinum-group minerals (PGM). The Ir-Pt inclusions are found as: (1) idiomorphic, needle-shape (acicular) nanoparticles up to 500 nm occurring along the grain boundar¬ies between Ru-rich pentlandite and millerite, and (2) nanospherical inclusions (<250 nm) dispersed through the matrix of Ru-rich pentlandite.

SELECTED PAPERS

- The accumulation of Ni in serpentines and garnierites from the Falcondo Ni-laterite deposit (Dominican Republic) elucidated by means of μXAS. Roqué-Rosell, J., Villanova-de-Benavent, C. & Proenza, J. A. Geochim. Cosmochim. Acta. 198, 48-69. **2017**.
- Nanoscale partitioning of Ru, Ir, and Pt in base-metal sulfides from the Caridad chromite deposit, Cuba. González-Jiménez, J. M., Deditius, A., Gervilla, F., Reich, M., Suvorova, A., Roberts, M. P., Roqué, J. & Proenza, J. A. Am. Mineral. 103, 1208–1220. **2018**.
- Au crystal growth on natural occurring Au—Ag aggregate elucidated by means of precession electron diffraction (PED). Roqué Rosell, J., Portillo Serra, J., Aiglsperger, T., Plana-Ruiz, S., Trifonov, T. & Proenza, J. A. J. Cryst. Growth. 483, 228-235. **2018**.

HRTEM observations and analysis of the selected-area electron diffraction patterns revealed that nanoparticles of Ir-Pt form domains within Ru-rich pent¬landite. Fast Fourier transform analyses of the HRTEM images showed epitaxy between Ir-Pt domain and PGE-poor millerite, which argues for oriented growth of the latter phase. These observations point to sub-solidus exsolution of the Ir-Pt alloy, although the presence of nanospherical Ir-Pt inclu¬sions in some other grains suggest the possibility that Ir-Pt nanoparticles formed in the silicate melt before sulfide liquid immiscibility. These Ir-Pt nanocrystals were later collected by the sulfide melt, preceding the formation of Ru-rich pentlandite. Early crystallization of the Ru-rich pentlandite and Ir-Pt nanoparticles led to the efficient scavenging of PGE from the melt, leaving a PGE-poor sulfide residue composed of millerite, pyrite, chalcopyrite, and a second generation of PGE-poor pentlandite [1].

1.2. Au crystal growth on natural occurring Au—Ag aggregate elucidated by means of precession electron diffraction (PED).

In the present work, a lamella from an Au—Ag aggregate found in Ni-laterites has been examined using Transmission Electron Microscope to produce a series of Precision Electron Diffraction (PED) patterns. The analysis of the structural data obtained, coupled with Energy Dispersive X-ray microanalysis, made it possible to determine the orientation of twinned native gold growing on the Au—Ag aggregate. The native Au crystal domains are found to have grown at the outermost part of the aggregate whereas the inner core of the aggregate is an Au—Ag alloy (4 wt% Ag). The submicron structural study of the natural occurring Au aggregate points to the mobilization and precipitation of gold in laterites and provides insights on Au aggregates development at supergene conditions. This manuscript demonstrates the great potential of electron crystallographic analysis, and in particular, PED to study submicron structural features of micron sized mineral aggregates by using the example of a gold grain found in a Ni-laterite deposits [2].

1.3. The accumulation of Ni in serpentines and garnierites from the Falcondo Ni-laterite deposit (Dominican Republic) elucidated by means of μXAS.

Ni-bearing serpentines and garnierites (Ni-bearing Mg-phyllosilicates) are the main Ni ores in the Falcondo Ni-laterite deposit (Dominican Republic). In the present paper a set of garnierite samples and the associated Ni-bearing serpentines with characteristic mineral compositions and textures, from the saprolite horizon, were studied by EMPA, μXRF and μXAS. The ultimate goal is to elucidate, for the first time, the Fe speciation and the Ni local environment of saprolite ores from Ni-laterites of the Dominican Republic. The chemical composition of the minerals has been obtained by means of EMPA and the Ni, Fe and Cr elemental maps obtained by μXRF allowed distinguishing the saprolite fragments containing Ni-bearing serpentines and Fe oxyhydroxides from the garnierite veins. The Fe K-edge μXANES demonstrated that Fe in the Ni-poor primary serpentine is mostly in the Fe^{2+} form, whereas in the Ni-bearing serpentine constituting the bulk of the saprolite and in the Fe-bearing garnierite Type I Fe was in the form of Fe^{3+}. In parallel, the local environment of Ni determined by means of Ni K-edge μEXAFS confirmed that in Ni-poor primary serpentines Ni formed a homogeneous Ni–Mg solid solution, in garnierites formed Ni–Ni clusters, and in Ni-bearing secondary serpentines Ni was found in Ni–Mg and Ni–Ni mixed sites. This paper explains the accumulation of Ni, the speciation of Fe in garnierites with various mineral compositions and in Ni-bearing serpentines from the saprolite horizon in Ni-laterite deposits [3].

1.4. Fibrous Platinum-Group Minerals in "Floating Chromitites" from the Loma Larga Ni-Laterite Deposit, Dominican Republic

This contribution reports on the observation of enigmatic fibrous platinum-group minerals (PGM) found within a chromitite body included in limonite ("floating chromitite") from Ni-laterites in the Dominican Republic. Fibrous PGM have a Ru-Os-Ir-Fe dominated composition and are characterized by fibrous textures explained by grain-forming fibers which are significantly longer (1–5 μm) than they are wide (~100 nm). Back-scattered electron (BSE) images suggest that these nanofibers are platinum-group elements (PGE)-bearing and form <5 μm thick layers of bundles which are oriented orthogonal to grains' surfaces. Trace amounts of Si are most likely associated with PGE-bearing nanofibers. One characteristic fibrous PGM was studied in detail: XRD analyses point to ruthenian hexaferrum. However, the unpolished fibrous PGM shows numerous complex textures on its surface which are suggestive for neoformation processes: (i) features suggesting growth of PGE-bearing nanofibers; (ii) occurrence of PGM nanoparticles within film material (biofilm?) associated with PGE-bearing nanofibers; (iii) a Si-rich and crater-like texture hosting PGM nanoparticles and an Ir-rich accumulation of irregular shape; (iv) complex PGM nanoparticles with ragged morphologies, resembling sponge spicules and (v) oval forms (<1 μm in diameter) with included PGM nanoparticles, similar to those observed in experiments with PGE-reducing bacteria. Fibrous PGM found in the limonite may have formed due to supergene (bio-) weathering of fibrous Mg-silicates which were incorporated into desulphurized laurite during stages of serpentinization [4].

Selected Projects

- *Mineralogía y geoquímica de Ni, Co y de los elementos del grupo del plantino (EGP) en lateritas niquelíferas.*
  IP: Joaquin Antonio Proenza Fernandez (Departament de Mineralogia, Petrologia i Geologia Aplicada). Official Code: CGL2006-07384/. Institution: UB
- *Procesos metalogenéticos de enriquecimiento supergénico de Co y elementos del grupo del platino (EGP) en lateritas niquelíferas.*
  IP: Joaquin Antonio Proenza Fernandez (Departament de Mineralogia, Petrologia i Geologia Aplicada). Oficial Code: CGL2009-10924. Institution: UB.
- *Complejos ultramáficos oceánicos en márgenes de placa convergentes: un registro petrológico, geoquímico y metalogenético de la tectónica global (región del Caribe).*
  IP: Joaquin Antonio Proenza Fernandez (Departament de Mineralogia, Petrologia i Geologia Aplicada). Oficial Code: CGL2012-36263. Institution: UB.
- *Diamante, circón y otros minerales 'exóticos' en cromititas ofiolíticas y rocas asociadas. Implicaciones para la geodinámica mantélica.*
  IP: Joaquin Antonio Proenza Fernandez (Departament de Mineralogia, Petrologia i Geologia Aplicada). Oficial Code: CGL2015-65824-P. Institution: UB

2.2.29. Nanobioengineering and Biomaterials Unit (NanoBio)

Department of Electronics and Biomedical Engineering, Faculty of Physics

Team

- **Josep Samitier Martí (Full Professor)**
- **Oscar Castaño Linares (Associate Professor)**
- **Romén Rodríguez Trujillo (Tenure-Track Lecturer)**
- **Mònica Mir Llorente (Adjunct Lecturer)**

Research

The group is devoted to the application of nanotechnology and biomaterials for the development of new systems, protocols and biomedical devices with the aim of creating new diagnostic platforms, models and biological microenvironments, and regenerative therapies. The main research activities of the group include the biochemical engineering, soft lithography en microfabrication techniques, functionalization of biomaterials integrated with microfluidic systems and the three-dimensional scaffolding of biodegradable and bioactive biomaterials.

Bioengineering microdevices are used to study cellular responses to biomolecular compounds applied to Organ-on-Chip devices, or for the development of new laboratory-based biosensors on a chip. The objective is to manufacture microsystems that contain living cells that recapitulate the functions at the level of tissues and organs in vitro and new portable diagnostic devices that can be used as point of care systems.

We design, manufacture and characterize bioactive and biodegradable materials and investigate their interactions with biological entities, both in terms of their fundamental aspects and with specific applications for tissue engineering purposes in mind. The objective is the repair and functional restoration of tissues or organs through 3D scaffolding, cells and signals.

We are a truly multidisciplinary team composed of researchers and students from very diverse backgrounds. The projects carried out by the group focus on clinical and industrial needs.

Selected Projects

- *NanoVax Engineered nanovaccines for anti-tumour immuno-therapy* (2016-2019) EURONANOMED 2. Josep Samitier / Lorenzo Albertazzi
- *MASCTN-Training Training on Advanced Stem Cell Technologies in Neurology*. PI: Josep Samitier. European Commission MARIE CURIE - ITN/813851

SELECTED PAPERS

- *DNA-origami-driven lithography for patterning on gold surfaces with sub-10 nm resolution.* Gállego, Isaac, Manning, Brendan, Prades, Joan Daniel, Mir, Mònica, Samitier, Josep, Eritja, Ramon *Advanced Materials*, 29, 1603233. **2017**.

- *Instructive microenvironments in skin wound healing: Biomaterials as signal releasing platforms.* Castaño, O., Pérez-Amodio, S., Navarro, C., Mateos-Timoneda, M.A., Engel, E. *Advanced Drug Delivery Reviews* 129, 95-117. **2018**.

- *Directed flow of micromotors through alignment interactions with micropatterned ratchets.* Katuri, Jaideep, Caballero, David, Voituriez, R., Samitier, Josep, Sanchez, Samuel. *ACS Nano* 12, (7), 7282-7291. **2018**.

- *Long distance electron transfer through the aqueous solution between redox partner proteins.* Lagunas, A., Guerra-Castellano, A., Nin-Hill, A., Díaz-Moreno, I., De la Rosa, M. A., Samitier, J., Rovira, C., Gorostiza, P., *Nature Communications* 9, (1), 5157. **2018**.

- *Bacteria Detection and Differentiation Using Impedance Flow Cytometry.* Casper Hyttel Clausen, Maria Dimaki, Christian Vinther Bertelsen, Gustav Erik Skands , Romen Rodriguez-Trujillo, Joachim Dahl Thomsen and Winnie E. Svendsen. *Sensors*, 18(10), 3496. **2018**.

Singular Scientific Equipment

- Nanofabrication and nanomanipulation
  - 3D Printing system for microfluidic devices
  - Soft lithography en microfabrication techniques
  - Graphtech
  - Electrospinning device
  - Spin-coater
  - Combustion furnace
  - High temperature furnace
  - Ball mill
  - Inert atmosphere facilities
  - Sol-gel facilities
- Characterization
  - Potentiostates
  - Optical Waveguide Lightmode Spectroscope (OWLS)
  - Atomic Force Microscope (AFM)
  - Optical Microscopes (white light/epifluorescence)
  - Electrical Impedance spectroscopy (EIS)
  - Multi-frequency Lock-in Amplifier
  - Sub-femtoamp Remote SourceMeter Instrument
  - Surface characterization equipment (contact angle, Z potential)
  - Differential Scanning Calorimetry (DSC)
  - Soft tissue mechanical testing machine
  - Peptide synthesizer
  - Vibrational viscosimeter
- Molecular/cell biology
  - Cell culture facilities
  - Molecular Biology equipment: protein and DNA electrophoresis
  - Thermocycler (PCR)
  - Biological safety cabinet (class II)
  - Microwell plate readers
  - Protein and DNA electrophoresis systems
  - Microincubator Okolab
  - Nanodrop spectrophotometer
  - CO_2 incubator for cells
  - Cell culture cabin

- Microfluidics
  - › High precision syringe pumps
  - › Peristaltic pumps

International Collaborations

- Dr. Adrian Carretero, Institut d'Electronique et des Systèmes, Montpellier, France
- Dr. Graham Johnson, Uniscan Instruments Ltd, Buxton, UK
- Dr. Izabella Rajzer Institute of Textile Engineering and Polymer Materials, University of Bielsko-Biala, Poland
- Dr. Nicole Jaffrezic, Université Claude Bernard Lyon 1, France
- Prof. Albert Folch, Dpt. of Bioengineering, University of Washington, USA
- Prof. Albert van den Berg, University of Twente, The Netherlands
- Prof. Andre Bernard, Institut für Mikro- und Nanotechnologie (MNT-NTB), Buchs, Switzerland
- Prof. E. Faszewski, Wheelock College, Boston, USA
- Prof. G. Fuhr, FhG Biomedicine, St. Ingbert, Germany
- Prof. H. Börner Max, Planck Institute of Colloids and Interfaces, Golm, Germany
- Prof. Jean-Louis Marty, U. de Perpignan Via Domitia, France
- Prof. Juan C. Izpisúa, Salk Institute for Biological Studies, La Jolla, California
- Prof. Kevin Healy Biomaterials & Tissue Engineering Laboratory, University of California at Berkeley, USA
- Prof. Matthew Dalby, University of Glasgow, UK
- Prof. Paolo Dario, Scuola Superiore Sant'Anna (SSSA), Pontedera, Italy
- Prof. Roger D. Kamm, Biological Engineering, Massachusetts Institute of Technology (MIT), Cambridge, USA

2.2.30. NanoBioPharma (NanoPharmaMed)

Department of Pharmacy and Pharmaceutical Technology and Physical-Chemical, Faculty of Pharmacy and Food Sciences

Team

- **Ana Calpena Campmany (Associate Professor)**
- **Mireia Oliva (Associate Professor)**
- **Lyda Halbaut Bellowa (Associate Professor)**
- **Helen Lissette Alvarado Bonilla (Adjunct Lecturer)**
- **Mireia Mallandrich (Adjunct Lecturer)**
- **Joaquim Suñer Carbó (Adjunt Lecturer)**
- **Marcelle Silva de Abreu (External Collaborator)**
- **Guadalupe Del Carmen Abrego Escobar (External Collaborator)**
- **Beatriz Clares Maveros (External Collaborator)**

SELECTED PAPERS

- *Developing Transdermal Applications of Ketorolac Tromethamine Entrapped in Stimuli Sensitive Block Copolymer Hydrogels.* Mallandrich M., Fernández-Campos F., Clares B., Halbaut L., Alonso C., Coderch L., Garduño-Ramírez M.L., Andrade B., del Pozo A., Lane M.E., Calpena A.C. *Pharmaceutical Research.* Vol: 34 . **2017**.

Research

The NanoBioPharma Group is interested on the study and development of control released nanostructured components for transdermal application for the treatment of inflammatory processes.

2.2.31. Nanoenergy and Electronic Materials (M2E) Group (NanoEnergy)

Department of Electronics and Biomedical Engineering, Faculty of Physics

Team

- **Joan Ramon Morante Lleonart (Full Professor)**

Research activity description

M2E investigates the mechanisms and processes of exchange or transformation of energy at the nano-scale, mainly between photons, phonons, charge carriers and molecules such as CO_2, H_2O or H_2. These aspects focus our activity and interest in implementing the methodologies and processes of energy storage with real systems applicable in the different parts of the energy system such as generation, transport, distribution as well as at the final user level considering the use of intelligent gas and electricity networks as well as its interconnectivity in an increasingly electrified society.

In this context, it is highly relevant to consider as a renewable and sustainable energy source that one coming from the sun either as direct solar irradiation (photons), such as photovoltaic (load carriers) or as thermal energy (phonons) or its combination to be able to capture and store solar energy. In addition, these methodologies are also valid or adaptable for other renewable sources that produce electrical or thermal energy that allow the thermoconversion, the electroconversion and the bioconversion a part from the photoelectronconversion. Moreover, these procedures become key to establishing the requirements for a descarbonized society with a carbon based circular economy loop (CO_2, reduction, fuel, oxidation, CO_2) or even hydrogen (H_2O, reduction, hydrogen, oxidation) - H_2O) or other substances where chemical energy is produced by transformation directly from the sun by the action of photons or indirectly via renewable electricity and / or thermal energy. Thus, the research activity lines are concreted in:

Chemically based energy storage: 1. Solar Fuels; 2. Synthetic Fuels; 3. Materials, components and scalability of reactors for production.

Electrochemically based energy storage: 1. Flow batteries for high demand energy capacity; 2. Photo batteries; 3. Supercapacities for high demand of power capacity.

Fully autonomous systems for IoT applications: 1. Mechanisms and Processes of transfer of energy to nano scale; 2. Thermoelectricity, thermoelectric systems and applications; 3. Systems of capture of energy and storage at nano and micro scale.

- *Cytotoxic evaluation of (2s)-5,7-dihydroxy-6-prenylflavanone derivatives loaded PLGA nanoparticles against MiaPaCa-2 cells.* Andrade-Carrera B., Clares B., Noé V., Mallandrich M., Calpena A.C., García M.L., Garduño-Ramírez M.L. Molecules. Vol: 22. **2017**.
- *Development of Clotrimazole Multiple W/O/W Emulsions as Vehicles for Drug Delivery: Effects of Additives on Emulsion Stability.* Suñer J., Calpena A.C., Clares B., Cañadas C., Halbaut L. *AAPS PharmSciTech.* Vol: 18. **2017**.
- *Design, Characterization, and Biopharmaceutical Behavior of Nanoparticles Loaded with an HIV-1 Fusion Inhibitor Peptide.* Ariza-Sáenz M., Espina M., Calpena A., Gómara M.J., Pérez-Pomeda I., Haro I., García M.L. *Molecular Pharmaceutics.* Vol: 15. **2018**.
- *Development of a mucoadhesive delivery system for control release of doxepin with application in vaginal pain relief associated with gynecological surgery.* Sanz R., Clares B., Mallandrich M., Suñer-Carbó J., Montes M.J., Calpena A.C. *International Journal of Pharmaceutics.* Vol: 535. **2018**.

Main research lines active in the group are:

A. Chemically based energy storage:

A. 1. Solar Fuels:

Mechanisms, Materials, Components and Devices for a Solar Refinery ("Artificial Photosynthesis"): Global aim: to store solar energy by producing solar fuels such as hydrogen, formic acid, "syngas" and methanol. Specific aims: i) hydrogen: development of knowledge and technology to achieve systems (free bias & non free bias) with solar conversion factors with hydrogen STH> 14% and costs lower than € 3 / kg. ii) CO_2 reduction: development of knowledge and technology to achieve, under similar conditions, systems with solar conversion factors for STF fuels> 10%. iii) Physico-chemical improvement of the separation systems of the products derived from the CO_2 photo reduction to achieve better efficiencies and yields in the final product. iv) mechanisms and processes for the self regeneration of catalysts, nano influence. v) systems for photo-catalysis.

A. 2. Synthetic Fuels:

Mechanisms, Materials, Components and Devices for the production of synthetic fuels, especially Biomethane or "Syngas", from biogenic sources of carbon such as mud from water treatment plants or waste treatment. Development of PEM systems for electrolysis and co-electrolysis of CO_2 and H_2O to produce H_2 and / or syngas for the synthesis of fuel. Main aim: production of synthetic fuels of biogenic origin (exempt from positive CO_2 emissions). Specific aims: i) Cold plasma technology for the production of biomethane at low temperatures, adiabatic process, with high selectivity (> 98) and high conversion (> 90%). ii) Production and use of syngas for the production of methanol from the catalyst improvements, study and improvement of efficiency and productivity of the process. iii) Purification and effects of the impurities on the process itself and the catalysts used. Regeneration and life of catalysts, plasma mechanisms.

A.3. Materials, components and scalability of reactors for production:

Physical and chemical analysis and engineering design to achieve a modular reactor technology to optimize parameters and analysis of their scalability. Specific aims: unit cells and modules based on photo-electro-chemical and photocatalysis processes for solar fuels: i) hydrogen, ii) CO_2 reduction producers and iii) modular reactors based on cold plasma units for synthetic fuels.

SELECTED PAPERS

- *Compound Copper Chalcogenide Nanocrystals.* Claudia Coughlan, Maria Ibáñez,Oleksandr Dobrozhan, Ajay Singh, Andreu Cabot* and Kevin M. Ryan*. *Chem. Rev.*, 117, 5865–6109. **2017**.

- *Recent developments in organic redox flow batteries: A critical review.* P.Leunga; A.A.Shah; L.Sanz; C.Flox; J.R.Morante; Q.Xu; M.R.Mohamed; C.Ponce de León; F.C.Walsh. *Journal of Power Sources.* Vol 360, Pages 243-283. **2017**.

- *Enhanced photoelectrochemical water splitting of hematite multilayer nanowire photoanodes by tuning the surface state via bottom-up interfacial engineering.* PengYi Tang, HaiBing Xie, Carles Ros, LiJuan Han, Martí Biset-Peiró, YongMin He, Wesley Kramer, Alejandro Pérez Rodríguez, Edgardo Saucedo, José Ramón Galán-Mascarós, Teresa Andreu, Joan Ramon Morante* and Jordi Arbiol*. *Energy Environ. Sci.*, Vol 10, 2047. **2017**. + journal cover.

- *Bottom-up engineering of thermoelectric nanomaterials and devices from solutionprocessed nanoparticle building blocks.* Silvia Ortega, Maria Ibáñez, Yu Liu, Yu Zhang, Maksym V. Kovalenko, Doris Cadavid* and Andreu Cabot*. *Chem. Soc. Rev.*, 46, 3510. **2017**.

- *A prototype reactor for highly selective solar-driven CO_2 reduction to synthesis gas using nanosized earth-abundant catalysts and silicon photovoltaics.* Félix Urbain, Pengyi Tang, Nina M. Carretero,Teresa Andreu,Luis G. Gerling, Cristobal Voz, Jordi Arbiol and Joan Ramon Morante. *Energy Environ. Sci.* 10, 2256. **2017**.

B. Electrochemically based energy storage:

B.1. Flow batteries for high demand energy capacity:

Beyond the current forms of lithium technologies where energy density and power density are correlated, there are storage technologies where energy and power capacities are decoupled and allow the use of different types of materials for electrodes, electrolytes, active species and membranes, which allows to respond to many needs beyond transport where a very high energy density is a key point. Main goal: electrochemical energy storage beyond the lithium. Specific goals: i) High power density flow batteries> 1.5W / cm2 in stacks using electrolyte with high molarity with additives, wide range of temperatures, high current densities> 250mA / cm^2 based on new electrode materials and improved membranes. ii) Alternative flow-based batteries based on organic, ionic and semisolid liquids. iii) air metal batteries and circular economy of its constituents and products.

B.2. Photo batteries:

Mechanisms, Materials, Components and Devices to develop a battery with direct recharge from the solar illumination. Main objective: development of concepts, materials and systems to implement a photobattery aimed at self-consumption and / or autonomous systems. Specific objectives: i) mechanisms, materials, structure and configuration of photoelectrodes. ii) definition of a loading / unloading strategy based on different redox and electrolyte pairs. Reference will be encrypted in Vanadi. iii) modeling and engineering of prototypes.

B.3. Supercapacities for high demand power capacity:

These types of devices become an essential tool to respond to the demand for power peaks of the current / future electric grids. General objectives: application of new Nanomaterials with very high porosity for supercapacity of very high capacity> 100F / g and many fast response times> 10V / s. Specific objectives: i) processes and characterization of nano carbon fibers and use of additives and graphene ii) implementation of prototype type cells button and punch. iii) development of flow-based supercapacities

C. Fully autonomous systems for IoT:

C.1. Mechanisms and Processes of transfer of energy to nano scale:

Studies in nanomaterials and nanosciences. General objectives: study of basic phenomena. Specific objectives: i) control of parameters in the synthesis of materials ii) design of nano-structures iii) implementation of bimetallic catalytic materials and based on oxidized transition metal or as calcogenous (2D).

C.2. Thermoelectricity, thermoelectric systems and applications:

General objectives: implementation of thermoelectric materials with parameters zT> 1. Particular objectives: new thermoelectric materials ii) implementation of modules iii) high temperature gradient development.

C.3. Systems of capture of energy and storage at nano and micro scale:

General objective: materials and concepts for micro-batteries and / or microsupercapacities for autonomous systems. Particular objectives: i) materials and deposition of layers by microbanks. ii) materials and processes for microsupercap iii) implementation of autonomous systems including capture of energy, storage, sensors and communications module (the latter commercial).

Selected Projects

- CEOPS: CO²-Loop for Energy storage and conversion to Organic chemistry. FP7-NMP-309984. Processes through advanced catalytic Systems. IP: Joan R. Morante. Horizon 2020. 2016-2019
- HELIS: High energy lithium sulphur cells and batteries H2020-NMP-666221. IP: Joan Ramon Morante. Horizon 2020. 2015-2019

Singular Scientific Equipment

- Functional nano materials laboratory
- Electrochemical batteries laboratory
- Photoelectroconversion and CO2 laboratory
- Thermoconversion and catalysis laboratory
- Environmental energy collectors and 2D storage laboratory

International Collaborations

- The research group coordinates and/or participates in some networks; xarxa d'excel·lència MINECO BAT-FLU (Bateries de Flux Redox); FOTO-FUEL (Red de excelencia en producción de combustibles solares), Materials Avançats per a l'Energia (XARMAE) de la direcció General de Recerca de la Generalitat i RIS3CAT energia de la Generalitat de Catalunya. It also has the recognition of TECNIO, by ACCIO Generalitat de Catalunya.
- Due to the intense activity of the group in European projects, the group collaborates with various institutions and companies at European and international level, such as: Commissariat à l'énergie atomique et aux énergies alternatives (CEA), C.T.G. SPA – Italcementi, Instituto Superior Técnico (IST), OMNIDEA, Ecole Nationale Supérieure de Chimie Paris (ENSCP), Faculdade de Ciências e Tecnologia da Universidade Nova de Lisboa (NOVA), GDF-Suez Energy Romania, European Materials Research Society, Chemie-Cluster Bayern, University of Cologne UNICO, Fraunhofer Institute for Mechanics of Materials IWM, Swiss Federal Institute of Technology Zurich (ETH), University of Warsaw (UW), Tampere University of technology (TUT), Consorzio Interuniversitario Nazionale per la Scienza e Tecnologia dei Materiali (INSTM), Siemens AG SAG, Sachtleben Pigment GmbH SC, Repsol i Gas Natural.
- M2E has scientific collaboration international recognized research groups. One of the fields in which the group has established partnerships with national and international groups is that of nano-energy research. Therefore, there is a special emphasis on the transfer of energy to the nano-scale using low-dimensional materials (nano tubes of carbon, graphene, quantum graphene points, 2D materials etc.). Specifically, part of these collaborations focuses on the study of the functionalization of these materials, their surface treatment and on the processes and mechanisms that can take place.
- In the field of 1D structures such as semiconductor nanowires for applications in new energies, the team have collaborations with other groups: Prof. Anna Fontcuberta i Morral, EPFL (Lausanne, Switzerland), el Prof. Martin Eickhoff, Bremen Universität, Bremen (Germany), professor Rossi CNRS Montréal (Canada) and Prof. A. Vomiero (Lula Sweden).
- In the field of the application of nanostructures for new energies and catalysis the researchers have collaborations with Prof. Brian Korgel from University of Texas at Austin (USA), Prof. Wolfgang Schumann from Ruhr Universität Bochum, (Bochum, Germany), Prof. Maksym V. Kovalenko, Swiss Federal Institute of Technology, ETH (Zurich, Switzerland), Dr. Mauro Epifani, CNR-Istituto per Microelettronica Microsistemi, CNR-IMM (Lecce, Italy), Prof. Jose Ramon Galan-Mascaros, Institut Català d'Investigació Química (ICIQ), and Prof. Jordi Arbiol ICN2

- In the analysis of the mechanisms of growth and application of 2D structures (graphene, MoS2, MoTe2, etc.) in energy and photonics, we have collaborations among others with the groups of the Dra. Esther Alarcón-Lladó, FOM Institute AMOLF, (Amsterdam, Netherlands), Prof. Anna Fontcuberta i Morral, EPFL (Lausanne, Switzerland), Prof, Davide Barreca (Universitat de Padova), Prof. Lars Osterlund d'Uppsala. En temes de bateries i supercaps es te entre altres col·laboracions amb el professor Y Gogotsi de la universitat de Drexel USA , amb el professor Walsh de la universitat de Southampton , la professora C. Engstrom de la U. Uppsala, la professora F. Montmajor de la Universitat tècnica de Lisboa.
- Professor J.R.Morante is member and vice-president of the executive committee from European Materials Research Society and member of some congresses organizing committee (TCM transparent conductive materials, Eurosensors,.....). He is also editor in chief of the Journal of Physics D: Applied Physics from the English Institute of Physics (IOP).
- Finally it is also to note the collaboration of the research team with private companies: REPSOL, Gas Natural Fenosa, FAE, IDIADA, RDflow, EDP (Hidrocantabrico energía), Zigor, Cidete, Albufera, ...

2.2.32. Nanomalaria Group (NanoBio)

Team

- **Santiago Imperial Ródenas (Professor. Department of Biochemistry and Molecular Biology, Faculty of Biology)**
- **Xavier Fernández Busquets (External collaborator- IBEC-CRESIB)**
- **Carlota Roca Martínez (PhD Student)**

Research

Malaria is arguably one of the main medical concerns worldwide because of the numbers of people affected, the severity of the disease and the complexity of the life cycle of its causative agent, the protist Plasmodium spp. The clinical, social and economic burden of malaria has led for the last 100 years to several waves of serious efforts to reach its control and eventual eradication, without success to this day. With the advent of nanoscience, renewed hopes have appeared of finally obtaining the long sought-after magic bullet against malaria in the form of a nanovector for the targeted delivery of antimalarial drugs exclusively to Plasmodium-infected cells. Nanotechnology can also be applied to the discovery of new antimalarials through single-molecule manipulation approaches for the identification of novel drugs targeting essential molecular components of the parasite. Finally, methods for the diagnosis of malaria can benefit from nanotools applied to the design of microfluidic-based devices for the accurate identification of the parasite's strain, its precise infective load, and the relative content of the different stages of its life cycle, whose knowledge is essential for the administration of adequate therapies. The benefits and drawbacks of these nanosystems have to be considered in different possible scenarios, including economy-related issues that are hampering

SELECTED PAPERS

- *Biophysical characterization of the association of histones with single-stranded DNA.* Wang, Y., van Merwyk, L., Tönsing, K., Walhorn, V., Anselmetti, D., and Fernàndez-Busquets, X. Biochim. Biophys. *Acta* 1861, 2739-2749. **2017**.
- *Heparin: new life for an old drug.* Aláez-Versón, C.R., Lantero, E. and Fernàndez-Busquets, X. *Nanomedicine* 12, 1727-1744. **2017**.
- *Adaptation of targeted nanocarriers to changing requirements in antimalarial drug delivery.* Marques, J., Valle-Delgado, J.J., Urbán, P., Baró, E., Prohens, R., Mayor, A., Cisteró, P., Delves, M., Sinden, R.E., Grandfils, C., de Paz, J.L., García-Salcedo, J.A., and Fernàndez-Busquets, X. *Nanomedicine: NBM* 13, 515-525. **2017**.

the progress of nanotechnology-based medicines against malaria with the dubious argument that they are too expensive to be used in developing areas. Unfortunately, it is true that the application of nanoscience to infectious disease has been traditionally neglected. Thus, extra ingenuity is demanded from us: malaria-oriented nanomedicines not only need to work spotless; they have to do so in a cost-efficient way because they will be deployed in low-income regions.

The driving force of the Nanomalaria group is our personal commitment to applying nanomedicine to infectious diseases of poverty through several research lines: (i) Exploration of different types of encapsulating structure (liposomes, synthetic and natural polymers), targeting molecule (protein, polysaccharide, nucleic acid aptamers), and antimalarial compound (e.g. new structures derived from marine organisms and antimicrobial peptides) for the assembly of nanovectors capable of delivering their drug cargo with complete specificity to diseased cells. (ii) Study of metabolic pathways present in Plasmodium but absent in humans, with the aim of identifying specific enzymes as therapeutic targets. (iii) Use of glycosaminoglycans for innovative antimalarial strategies. (iv) Design of new methods for the targeted drug delivery to Plasmodium stages in the mosquito vector. (v) Investigation of novel drugs against insect-borne diseases working through radically new mechanisms. (vi) Extension of our activities to new pathologies (leishmaniasis).

- *2-picolylamine derivatization for high sensitivity detection of abscisic acid in apicomplexan blood-infecting parasites.* Moles, E., Marcos, J., Imperial, S., Pozo, O.J., and Fernàndez-Busquets, X. *Talanta* 168, 130-135. **2017**.
- *ImmunoPEGliposomes for the targeted delivery of novel lipophilic drugs to red blood cells in a falciparum malaria murine model.* Moles, E., Galiano, S., Gomes, A., Quiliano, M., Teixeira, C., Aldana, I., Gomes, P. and Fernàndez-Busquets, X. *Biomaterials* 145, 178-191. **2017**.

Selected Projects

- 2018-2021: Research grant, ERA-NET Cofund EURONANOMED III. European innovative research & technological development projects in nanomedicine.
  Project title: *NANOpheles. Development of nanovectors for the targeted delivery in Anopheles mosquitoes of agents blocking transmission of Plasmodium parasites*. (EURONANOMED2017-178).
- 2014-2017: Research grant, Fondazione CARIPLO call Science and Technology Research on Advanced Materials.
  Project title: *Amphoteric polyamidoamines as innovative tools to selectively direct antimalarial drugs towards Plasmodium-infected red blood cells*. (Ref. 2013-0584).
- 2015-2018: Research grant, Biotechnology Programme, Ministry of Economy and Competitivity, Spain.
  Project title: *Engineering of nanovectors for the delivery of antimalarial drugs to Plasmodium transmission forms*. (BIO2014-52872-R).

International Collaborations

- Dario Anselmetti, Universität Bielefeld, Germany. Single molecule force spectroscopy.
- Elisabetta Ranucci, Università degli Studi di Milano, Italy. Polyamidoamine nanoparticle synthesis.
- Inga Siden-Kiamos, Foundation for Research and Technology – Hellas, Heraklion, Greece. Development of the malaria parasite within the mosquito.
- Paula Gomes, Universidade do Porto, Portugal. Development of new antimalarial drugs.
- Fatima Nogueira, Universidade Nova de Lisboa, Portugal. Antimalarial drug assays in Plasmodium-infected mosquitoes and mice.
- Christian Grandfils, University of Liège, Belgium. Biomaterials research.

- Eduardo Prata Vilanova, Universidade Federal do Rio de Janeiro, Brazil. Exploration of sulfated polysaccharides of marine origin as antimalarials.
- Maria Manconi, Università di Cagliari, Italy. Liposome technology.
- Krijn Paaijmans, Arizona State University, Tempe, USA. Administration of drug nanocarriers to Anopheles mosquitoes.
- Kim Williamson, Uniformed Services University of the Health Sciences, Bethesda, USA. Basic biology of bacterial, viral, and parasite diseases.
- Juan José Valle-Delgado, Aalto University, Helsinki, Finland. Atomic force microscopy.
- Ellen Faszewski, Boston University, USA. Marine sponge cell adhesion.
- Jos Paulusse, University of Twente, The Netherlands. Encapsulation of peptides in tailor-made multifunctionalized nanocarriers and polyamidoamine-derived nanogels.

2.2.33. Nanostructure of Biomembranes Group (NanoBio)

Department of Pharmacy and Pharmaceutical Technology and Physical-Chemical, Faculty of Pharmacy and Food Sciences

Team

- **Jordi Borrell Hernández (Full Professor)**
- **Maria Teresa Montero Barrientos (Associate Professor)**
- **Òscar Domènech Cabrera (Associate Professor)**
- **Martha Leticia Vázquez González (Adjunct Lecturer)**
- **Adrià Botet Carreras (PhD Student)**

Research

The Nanostructures of Biomembranes Group has traditionally worked with spectroscopic techniques, particularly spectrofluorimetry, NMR, DSC, Langmuir monolayers and Langmuir Blodgett films and more recently, with the Atomic Force Microscope (AFM).

What characterizes the group is the fact that we combine the application of these techniques with molecular biology methods for which we are self-sufficient. Specifically, we obtain the proteins under investigation, lactose permease, NorA or KcsA, from Escherichia coli cultures. These proteins are models of efflux pump proteins related with the drug resistance in bacteria. We can extract the proteins from the cell membrane and after purification, we finally reconstitute them into membrane models of desired compositions. Spectrofluorometric studies of surface potential or FRET tell us about the interactions between proteins and the lipids that surround it. The characterization of the membrane models with the AFM allows the visualization and interaction (Force Spectroscopy) with an individual molecule of protein giving us the idea of the necessary force to take it out of

SELECTED PAPERS

- *Amphotericin B releasing topical nanoemulsion for the treatment of candidiasis and aspergillosis.* Sosa, L., Clares, B., Alvarado, H.L., Bozal, N., Domènech, Ò., Calpena, A.C. Nanomedicine: Nanotechnology, *Biology, and Medicine* 13(7), 2303-2312. **2017**.
- *A biophysical study of gene nanocarriers formed by anionic/zwitterionic mixed lipids and pillar[5]arene polycationic macrocycles.* Barrán-Berdón, A.L., Martínez-Negro, M., García-Río, L., Domènech, Ò., Tros De Ilarduya, C., Aicart, E., Junquera, E. *Journal of Materials Chemistry* B 5(17), 3122-3131. **2017**.
- *Critical Temperature of 1-Palmitoyl-2-oleoyl-sn-glycero-3-phosphoethanolamine Monolayers and Its Possible Biological Relevance.* Borrell, J.H., Domènech, Ò. Journal of Physical Chemistry B 121(28), 6882-6889. **2017**.

the membrane. This information is important to understand how proteins are inserted in cell membranes and how they perform their function. Altering the membrane lipid composition modifies these force profiles suggesting a possible approach to inhibit the functionality of the protein when inserted in the membrane.

Selected Projects

- *Nanobioenginyeria i Nanobioelectrònica*, SIC-BIO.SGRC- Ajuts de Suport als Grups de Recerca de Catalunya (SGR) 2017SGR1079 2018-2021. IP. Josep Samitier Martí
- *Microscopio de barrido de fuerzas eléctricas para medidas electrofisiológicas a la nanoescala.* IP. Gabriel Gomila. TEC2016-79156-P. Ministerio de Economía y Competitividad (MCOC). 2016-2019
- *Breaking the Borders of Antimicrobial Resistance. Searching New Antimicrobial Compounds against Multi-Drug Resistant Bacteria: A Study of Policationic AMPS and Lipid Nanoparticles.* Fundació La Marató (TV3) (FMTV). 2018-2021. IP: Miquel Viñas Ciordia

Singular Scientific Equipment

- Multimode IV Atomic Force Microscope from Bruker controlled by Nanoscope V electronics equipped with a 15 µm scanner.
- Two KSV Nima Langmuir troughs equipped with surface pressure balance, surface potential and Brewster Angle Microscope (BAM).
- SLM Aminco 8100 Spectrofluorometer equipped with Xenon Lamp and thermostatted cuvette holder.

International Collaborations

- Ronald H. Kaback. Department of Physiology. University of California, Los Angeles, USA. Physicochemical studies of Lactose permease (Lac Y) protein in model membranes
- Pierre Emmanuel Milhiet. Structural Biochemistry Centre CNRS UMR 5048 - UM - INSERM U 1054, Montpellier, France. Physicochemical studies of Macromolecules - model membrane interactions by AFM.
- Marie-Paule Mingeot Leclercq. Department of Cellular and Molecular Pharmacology, Catholic University of Louvain, Brussels, Belgium. Macromolecules - model membrane interactions
- Manuel Prieto. Molecular Physical Chemistry Centre, Technical University of Lisbon, Portugal. FRET fluorescence studies between membrane proteins and lipids in the annular region.

SELECTED PAPERS

- *Mapping phase diagrams of supported lipid bilayers by atomic force microscopy.* Borrell, J.H., Montero, M.T., Domènech, Ò. *Microscopy Research and Technique* 80(1), 4-10. **2017**.
- *Characterization and lipid phase effect on the interaction of GBV-C E2-derived peptide, P6-2VIR576, with lipid membranes relating it with the HIV-1 FP inhibition.* Girona, V., Domènech, Ò., Prat, J., Ortiz, A., Muñoz-Juncosa, M.M., Pujol, M. Colloids and Surfaces A: *Physicochemical and Engineering Aspects.* 554, 187-196. **2018**.

2.2.34. Nanostructured systems for controlled drug delivery (NanoPharmaMed)

Department of Pharmacy and Pharmaceutical Technology and Physical-Chemical, Faculty of Pharmacy and Food Sciences

Team

- **M. Luisa García López (Full Professor)**
- **Espina García Marta (Associate Professor)**
- **Fidencia Gamisans Linares (Adjunct Lecturer)**
- **Elena Sanchez Lopez (Adjunct Lecturer)**
- **Amanda Cano Fernández (Adjunct Lecturer)**

Research

The research group develops and assesses nanostructured systems of controlled released in order to treat neurodegenerative diseases or ocular inflammation.

Selected Projects

- *Aplicación de criterios de calidad basada en el diseño al proceso de liofilización de sistemas nanoestructurados para el tratamiento de enfermedades neurodegenerativas*. MAT2014-59134-R. IP: Garcia Lopez, M. Luisa. Ministerio de Economia y Competitividad. 2015-2017.

Singular Scientific Equipment

- Particle size analyzers (Nanozeta sizer y difracción lasser)
- Homogenizers (ultrasound and high pression piston-gap)
- Thermal Analysis Systems (DSC, TG, thermomicroscopy)
- Otical Analyzer (Turbiscan Lab)
- Liofilizers (Lyo Quest y Lyo Beta), SPRAY DRIED, ROTAVAPORES
- Corneal camera, Franz cells
- HPLC

International Collaborations

- Group of Pharmaceutical Technology, Faculty of Pharmacy, University of Coimbra, Coimbra, Portugal

SELECTED PAPERS

- *New potential strategies for Alzheimer's disease prevention: pegylated biodegradable dexibuprofen nanospheres administration to APPswe/PS1dE9.* Sánchez-López E., Ettcheto M., Egea M.A., Espina M., Calpena A.C., Folch J., Camins A., García M.L. *Nanomedicine: Nanotechnology, Biology, and Medicine. Vol 13.* **2017**.
- *Dexibuprofen prevents neurodegeneration and cognitive decline in APPswe/PS1dE9 through multiple signaling pathways. Ettcheto M., Sánchez-López E., Pons L., Busquets O., Olloquequi J., Beas-Zarate C., Pallas M., García M.L., Auladell C., Folch J., Camins A. Redox Biology. Vol 13.* **2017**.
- *Epigallocatechin-3-gallate loaded PEGylated-PLGA nanoparticles: A new anti-seizure strategy for temporal lobe epilepsy.* Cano A., Ettcheto M., Espina M., Auladell C., Calpena A.C., Folch J., Barenys M., Sánchez-López E., Camins A., García M.L. *Nanomedicine: Nanotechnology, Biology, and Medicine.* **2018**.
- *Development of fluorometholone-loaded PLGA nanoparticles for treatment of inflammatory disorders of anterior and posterior segments of the eye.* Gonzalez-Pizarro R., Silva-Abreu M., Calpena A.C., Egea M.A., Espina M., García M.L. *International Journal of Pharmaceutics.* **2018**.
- *Memantine loaded PLGA PEGylated nanoparticles for Alzheimer's disease: In vitro and in vivo characterization.* Sánchez-López E., Ettcheto M., Egea M.A., Espina M., Cano A., Calpena A.C., Camins A., Carmona N., Silva A.M., Souto E.B., García M.L. *Journal of Nanobiotechnology.* **2018**.

2.2.35. Nanosystems Statistical Physics (NanoMet)

Department of Condensed Matter Physics, Faculty of Physics

Team

- **Miguel Rubí Capaceti (Full Professor)**
- **Andrés Arango Restrepo (PhD Student)**

Research

The research in the group is focused Non-equilibrium statistical physics, Non-equilibrium nanoscale phenomena, Mesoscopic non-equilibrium thermodynamics, Transport in confined Systems, Biophysics, Magnetization dynamics.

Selected Projects

- *Procesos de no equilibrio y transformaciones energéticas en pequeñas escalas: sistemas autoensamblados, confinados y activos*. FIS2015-67837-P. IP: Rubi Capaceti, Jose Miguel. Ministerio de Economia y Competitividad. 2016-2018
- *Física Estadística*. SGR. 2017SGR884. IP: Rubi Capaceti, Jose Miguel. Agència de Gestió d'Ajuts Universitaris i de Recerca (AGAUR). 2017-2020

SELECTED PAPERS 2.2.35.

- *Lateral-drag propulsion forces induced by anisotropy.* Nefedov I.S., Rubi J.M. *Scientific Reports*, 7. **2017**.
- *Radiative Heat Shuttling. Latella I., Messina* R., Rubi J.M., Ben-Abdallah P. Phys. Rev. Lett. 121. **2018**.
- *Prediction of Protein Configurational Entropy (Popcoen).* Goethe M., Gleixner J., Fita I., Rubi J.M. *Journal of Chemical Theory and Computation*, 14, 3. **2018**.
- *Determinants of population responses to environmental fluctuations.* Vilar J.M.G., Rubi J.M. *Scientific Reports*, 887. **2018**.
- *Nonequilibrium self-assembly induced Liesegang rings in a non-isothermal system.* Arango-Restrepo A., Barragán D., Rubi J.M. *Physical Chemistry Chemical Physics*, 7. **2018**.

2.2.36. Organic Materials Unit (NanosMat)

Department of Inorganic and Organic Chemistry, Faculty of Chemisty

Team

- **Maria Dolors Velasco Castrillo (Associate Professor)**
- **Jaume García Amorós (Associate Professor)**
- **Alba Cuadrado Santolaria (PhD Student)**
- **Roger Bujaldón Carbó (PhD Student)**

Research

One of the major challenges of the research in the Organic Materials group will be the programming of different properties (optical, electronic, luminescent or magnetic) into liquid single crystal elastomers (LSCE), i.e. weakly cross-linked polymer networks that combine the elasticity of conventional rubbers with the long-range molecular order of liquid crystals, which reaches the macroscopic level. Unraveling the different structural and environmental factors that might influence the behavior of the active components in this medium is crucial to obtain actuators with the expected abilities, for example, efficient optical mechanotransducers (mechanical-optical field) with either inverse (fluorescence increases upon stretching of the LSCE) or multiple responses (emission intensity changes at two different wavelengths upon the application of a single mechanical force); effective artificial muscle-like actuators capable of experiencing sophisticated deformations upon suitable activation (optical-magnetic-mechanical field) or flexible electronic devices (electric-mechanical field).

Our research group has garnered a solid background in organic synthesis, macromolecular chemistry and materials chemistry and physics over the years. Specifically, and as a result of the research performed during the last projects, we have got experience in the design and synthesis of highly conjugated organic heterocycles with luminescent and semiconductor properties, and potential magnetic behaviour. The Organic Materials group investigates in the design and comprehension of the different factors that influence the semiconductor behaviour of organic materials and in the Interface engineering and solid-state organization for organic thin-film transistors. We are also engaged in the development of molecular and macromolecular liquid-crystalline systems for different applications. We have defined for the first time distinct mesogenic systems, based on the carbazole and porphyrin cores, with potential technological interest. Furthermore, light-sensitive azo derivatives have been introduced into liquid-crystalline elastomeric networks in order to produce efficient and rapid optically-controlled artificial muscle-like actuators. The latter research was funded by the European project "FUnctional Liquid-Crystalline Elastomers" (FULCE) of which Prof. Dr. h.c. H. Finkelmann, a worldwide leader in the field of macromolecular chemistry and physics, was its coordinator. On the other hand, the decoration of the azobenzene core with appropriate electron donating and electron withdrawing organic functions has led to the development of a wide palette of azo dyes endowed with switching speeds down to the nanosecond time window.

SELECTED PAPERS 2.2.36.

- *Easy accessible blue luminescent carbazole-based materials for Organic Light-Emitting Diodes.* Reig, M.; Gozálvez, C.; Bujaldón, R.; Bagdziunas,G.; Ivaniuk, K.; Kostiv, N.; Volyniuk,D.; Grazulevicius, J. V.; Velasco, D. Dyes and Pigments. **2017**. 137, 24-35.
- Tuning the ambipolar charge transport properties of tricyanovinyl-substituted carbazole-based materials Reig, M.; R.; Bagdziunas, G.; D. Volyniuk, D.; Grazulevicius, J. V.; Velasco, D. Physical Chemistry Chemical Physics. **2017**. 19, 6721-6730.
- *Smectic-B liquid single crystal elastomers as efficient optical mechanotransducers* Escalera-López, D.; Garcia-Amorós, J.; Velasco, D. *Macromolecular Chemistry and Physics*. **2018**. 219, 1700550. Front cover.

Selected Projects

- Nuevos materiales orgánicos y su uso para la modulación y transformación de la energía. Programa Nacional de ciencias y tecnologías químicas CTQ2015-65770-P. IP: M. Dolores Velasco Castrillo. Ministerio de Economía y Competitividad. 2016-2018.

Singular Scientific Equipment

- Polarised Optical Microscopy
- Photoisomerization set-up
- Heating centrifuge

International Collaborations

- Dr. O. Poizat (Laboratoire de Spectrochimie Infrarouge et Raman CNRS, Université de Lille1 Sciences et Technologies, Université Lille Nord de France, Villeneuve d'Ascq Cedex, France).
- Dra. M. M. M. Raposo (Centro de Química, Universidade do Minho, Braga,Portugal).
- Dr. J. V. Grazulevicius (Department of Polymer Chemistry and Technology, Kaunas University of Technology, Lithuania).
- Dr. V. Jankauskas (Department of Solid State Electronics, Vilnius University, Vilnius, Lithuania).

- *Solid-state organization of n-type carbazole-based semiconductors for organic thin-film transistors.* Reig, M.; Puigdollers, J; Velasco, D. *Physical Chemistry Chemical Physics*. **2018**. 20, 1142-1149.
- *Interface engineering and solid-state organization for triindole-based p-type organic thin-film transistors.* Reig, M.; Bagdziunas, G.; Ramanavicius, A.; Puigdollers, J.; Velasco, D. *Physical Chemistry Chemical Physics*. **2018**. 20, 17889 -17898.

2.2.37. Peptides and Proteins: Physicochemical Studies (NanoBio)

Department of Pharmacy and Pharmaceutical Technology and Physical-Chemical, Faculty of Pharmacy and Food Sciences

Team

- **Victòria Girona Brumós (Full Professor)**
- **Yolanda Cajal Visa (Associate Professor)**
- **Josefina Prat Aixelà (Associate Professor)**
- **Montserrat Pujol Cubells (Associate Professor)**
- **Montserrat Muñoz Juncosa (Associate Professor)**

Research

Peptides and Proteins: Physicochemical Studies Group during 2017 and 2018 has been developing its activity in two research lines a) Biophysical studies of surface-active GBV-C peptides as potential inhibitors of HIV-1 FP peptide and b) The performance of biophysical and microbiological studies of multifunctional polycationic peptide constructions with membrane activity. Concerning HIV-1 FP inhibition, its research focused specifically on the effect of lipid phase in the process that takes place. Findings corroborate that 1) GBV-C peptides interact with HIV-1 FP providing a kind of peptide-peptide complex that produces a change of LE / LC phase extension and avoid the HIV-1 FP action at membrane level; 2) the interaction occurs at the LE / LC border.

The line of research on new antibiotic lipopeptides has developed new candidate molecules with MICs in the micromolar range for both Gram positive and Gram negative bacteria (patents WO2010/029196, WO2011/110716, PCT/ES2014/070286). Biophysical studies with model membranes in combination with flow cytometry and TEM observation in susceptible bacteria are indicative of a membrane-based mechanism of action. The project is part of the European consortium ENABLE (European Network for AntiBiotic Lead Engine). This is the one only project in Europe to develop new antibiotics against Gram negative bacteria funded by the Innovative Medicines Inititiave (IMI) (7th framework program and EFPIA, the European Federation of Pharmaceutical Industries and Associates; see http://www.imi.europa.eu/content/enable).

Selected Projects

- *European Gram-negative Antibacterial Engine* (ENABLE).
  IP: Francesc Rabanal Anglada. Tipus de contracte/programa: COOPERATION. HEALTH. Seventh Framework Programme (FP7). Health. 2014-2020.
- *Design of an age-dependent corneal membrane model for in vitro interaction studies of biodegradable polymeric nanoparticles. In vitro/ex vivo/in vivo correlation.*
  IP: Elena Sánchez López. Ajuts a la Recerca Institut de Nanociència i Nanotecnologia de la UB. IN²UB. (ART 2018) 2018 -2019
- *Determinació de la possible desnaturalització de la lactoferrina microencapsulada.*
  IP: Yolanda Cajal Visa. Fundació Bosch i Gimpera. 2017

Singular Scientific Equipment

- Langmuir Balance KSV 5000 with Dipper and surface potential
- KSV – Nima Micro BAM

SELECTED PAPERS

- *Interaction of the GBV-C E2 derived peptide, P6-2VIR576, with anionic phospholipid membranes.* Ortiz,A.; Girona,V.; Prat,J.; Muñoz-Juncosa,M.; Alsina,M.M.; Pujol,M. *Colloids and Surfaces A* 532: 483-492. **2017**.
- *Recent advances and perspectives in the design and development of polymyxins.* Rabanal Anglada, Francesc; Cajal Visa, Yolanda Carlota. *Natural Product Reports*, 34: 886-908. **2017**.
- *Characterization and lipid phase effect on the interaction of GBV-C E2-derived peptide, P6-2VIR576, with lípid membranes relating it with the HIV-1 FP inhibition.* Girona,V.; Domènech,O.; Prat,J.; Ortiz,A.; Muñoz-Juncosa,M.; Pujol,M. *Colloids and Surfaces A*, 554: 187-196. **2018**.

2.2.38. Pharmaceutical Nanotechnology (NanoPharmaMed)

Department of Pharmacy and Pharmaceutical Technology and Physical-Chemical, Faculty of Pharmacy and Food Sciences

Team

- **M. José García Celma (Full Professor)**
- **Immaculada Dinarès Milà (Professor)**
- **M. Àngels Salvadó Lladós (Professor)**
- **Marta Monge Azemar (Adjunct Lecturer)**
- **Esteban Figueroa Becerra (PhD Student)**

Research

The research group Pharmaceutical Nanotechnology belongs to the University of Barcelona (UB) and it is ascribed to the Faculty of Pharmacy and Food Sciences. The members of the research team belong to the Department of Pharmacy and Pharmaceutical Technology and Physicochemistry and to the Department of Pharmacology, Toxicology and Chemical Therapeutics. The research group is leaded by María José García Celma. The team is a part of the Consolidated Group on Surfactants (CSIC-UB) (2017SGR1778), recognised by the Government of Catalonia (Generalitat de Catalunya), since 1994. The UB team is a R+D Associated Unit to the Spanish Research Council (CSIC), entitled "Pharmaceutical Nanotechnology" leaded by María José García Celma. Members of the team belong to the QCI group in the Networking Research Center on Bioengineering, Biomaterials and Nanomedicine (CIBER-BBN), since January 2008 and to the QCI centre, in the TECNIO network of research centres, that provide technological support to industries. All the members of the research team belong to the Nanoscience and Nanotechnology Institute (IN²UB) and Dr. García Celma is a member of the managing board.

The research interests of the group have focused to the development of novel controlled drug delivery dosage forms based on nanostructured surfactant and polymeric systems. Important contributions are the studies on formation and characterization of hydrogels, microemulsions, nano-emulsions, highly concentrated emulsions as drug carriers and the use of some of these colloidal systems as templates for the preparation of nanoparticles and solid foams. Incorporation and release of drugs and biomolecules have been investigated in these nanostructured formulations. The effective incorporation of drugs and biomolecules can facilitate the therapy of various diseases or physiological disorders of high incidence in the population and/or difficult to treat. Ionic liquids have been developed to improve the water solubility of some drugs without affecting the pharmacological activity, and allowing the encapsulation of these drugs in the

SELECTED PAPERS

- *Microemulsions and nano-emulsions for cosmetic applications.* C. Solans, M.J. García-Celma. *Cosmetic Science and Technology: Theoretical Principles and Applications*, 1st edition. (K. Sakamoto, R. Lochhead, H. Maibach, Y. Yamashita, eds.) Elsevier, Cambridge. Pag. 507-518. **2017**.
- *Versatile methodology to encapsulate gold nanoparticles in PLGA nanoparticles obtained by nano-emulsion templating.* C. Fornaguera; N. Feiner-Gracia; A. Dols-Pérez; M.J. García-Celma; C. Solans. *Pharmaceutical Research.* Vol: 34. Num: 5. Pag: 1093-1103. **2017**.
- *DHA and L- Carnitine loaded chitosan hydrogels as delivery systems for topical application.* I. Solé, S. Vilchez, J. Miras, N. Montanyà, M.J. García-Celma, J. Esquena. *Colloids and Surfaces A. Physicochemical and Engineering Aspects.* Vol: 525. Pag: 85-92. **2017**.
- *Hyaluronan based materials with catanionic sugar-derived surfactants as drug delivery systems.* F. Roig; M. Blanzat; C. Solans; J. Esquena; M.J. García-Celma. *Colloids and Surfaces B: Biointerfaces.* Vol: 164. Pag: 218- 223. **2018**.
- *Cell penetrating peptide grafting of PLGA nanoparticles to enhance cell uptake.* N. Feiner-Gracia, A. Dols-Pérez, M. Royo, C. Solans, M.J. García-Celma, C.Fornaguera. *European Polymer Journal.* Vol: 108. Pag: 429 -438. **2018**.

nanocarriers. The group maintains collaboration with important universities and research centers, which currently include the University of Lorraine and the University Paul Sabatier in Toulouse (France), Krakow University of Technology (Poland), Universidad de Guadalajara (México) and the University of Chile.

Researchers (CSIC staff) in the consolidated research group, QCI group (CIBER-BBN) and QCI center (TECNIO) that collaborate with the group:

- Dr. Conxita Solans (Professor)
- Dr. Jordi Esquena (Tenured scientist)
- Dr. Carlos Rodríguez (Tenured scientist)
- Dr. Gabriela Calderó (postdoctoral Researcher)

Selected Projects

- *Estrategias de formacion y estabilizacion de emulsiones agua-en-agua para aplicaciones farmacéuticas y alimentarias innovadoras*. CTQ2016-80645-R.
  IP: C. González Azón y M.J. García-Celma. Programa estatal de investigación, desarrollo e innovación orientada a los Retos de la Sociedad.2017-2019 (extedend: 2020)
- *Development of innovative formulations for the delivery of actives into the skin* (Ref. FBG-308810). Almirall, S.A. (Doctorado industrial). IP: M.J. García-Celma. 2016-2019
- *Nanoencapsulated active ingredients for the conditioning of the hair, the repair-reconstruction, the sheen and the maintenance of the color* (Ref. FBG-309702). IP: M.J. García. Beautyge, S.L. 2017-2018

Singular Scientific Equipment

- Vision® G2 Elite 8™ (Hanson Research): Dissolution tester with automated sampling.
- Microette™ Automated Test System (Hanson Research), with 6 Franz diffusion cells.
- VASCO nanoparticle size analyzer (Cordouan): DLS.
- Zetasizer Nano ZS (Malvern Instruments): DLS, zeta potential.
- Heracell CO_2 incubator (Thermo Scientific).
- Biosafety cabinet.
- Plasma reactor.

2.2.39. Physics in Nanobiophysics (NanoBio)

Department of Condensed Matter Physics, Faculty of Physics

Team

- **Aurora Hernandez Machado (Full Professor)**

Research

The research group is focused on dynamics of interfaces in nanotechnology, fluidics and biophysics, including the measure of the viscosity of Newtonian and nonNewtonian, being particularly interested on the rheology of blood, the stability and dynamics of biological membranes, vesicles, fuids and angiogenesis by both at the mathematical modeling level and experimentally.

Selected Projects

Biomecánica de biofluidos a la micro y nanoescala. FIS2016-78883-C2-1-P. IP: Hernandez Machado, Aurora. 2016-2019

SELECTED PAPERS

- *Elastic and dynamic properties of membrane phase-field models.* Lázaro G.R., Pagonabarraga I., Hernández-Machado A. *European Physical Journal* E. 40:77. **2017**.
- *Front microrheology of the non-Newtonian behaviour of blood: Scaling theory of erythrocyte aggregation by aging.* Trejo-Soto C., Costa-Miracle E., Rodriguez-Villarreal I., Cid J., Castro M., Alarcon T., Hernandez-Machado A. *Soft Matter*, 16. **2017**.
- *Front Microrheology of Biological Fluids.* Trejo-Soto C.A., Costa-Miracle E., Rodriguez-Villarreal A.I., Cid J., Castro M., Alarcón T., Hernández-Machado A. *Journal of Physics: Conference Series.* **2018**.

2.2.40. Self-organized complexity and self-assembling materials (SOC&SAM) (NanoBio, NanosMat)

Department of Materials Science and Physical Chemistry, Faculty of Chemistry)

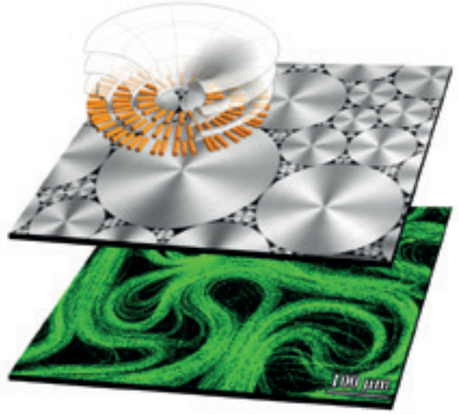
Team

- **Francesc Sagués Mestre (Full Professor)**
- **Jordi Ignés Mullol (Associate Professor)**
- **Joan-Anton Farrera Piñol (Associate Professor)**
- **Mohammad Tahghighi (PhD Student)**
- **Berta Martínez Prat (PhD Student)**
- **Josep Maria Pagès Casas (PhD Student)**

Research

The Self-organized Complexity and self-assembling Materials Group (SOC&SAM) performs basic research in the field of soft Nanotechnology. A significant part of our work is devoted to the study of composite systems in which anisotropic fluids (liquid crystals) are organized by contact with ordered surfactant monolayers or protein gels or by the presence of colloidal inclusions. We take advantage of the coupling of liquid crystals with external electric or magnetic fields to build responsive materials whose organization we can control.

A significant part of our current effort is in the context of active soft materials, where we have studied the aqueous gel that forms in-vitro when the molecular motor protein kinesin is combined with self-assembled microtubules of the cytoskeleton protein tubulin. In the presence of ATP, and when depleted on an interface with an immiscible liquid, the system self-assembles into dynamic bundles with two-dimensional long-range orientational order. We have taken advantage of the coupling of this material with an oil interface to demonstrate that the dynamics of the active material can be controlled by exerting an influence on an anisotropic interface, either with a magnetic field or with intrinsic viscosity contrasts. Using microfluidic techniques, we prepare ensemble of



The organization of active bundles of tubulin (fluorescence confocal image, bottom) is influenced by the soft patterning at the interface with a smectic-A liquid crystal (reflection confocal image, top). The organization of oil molecules in layers (sketch) determines an anisotropic interfacial viscosity.

microdroplets including the active gel to study the response of this material in confined geometries.

In the context of colloidal transport, we have developed a strategy to command the self-assembly and to drive ensembles of microscale solid or liquid inclusions in confined geometries. This is achieved by using non-linear electrophoresis mediated by a liquid crystal medium as driving force, and light-induced control of the local mesogen to steer the moving colloids. The developed strategy allows to study transitions between different forms of aggregation of colloidal ensembles, and to prepare a model system to explore the phenomena of clogging at the microscale.

From a more applied perspective, we have employed the Langmuir-Blodgett technique to control the assembly of gold nanoparticle monolayers for the detection of analytes by means of Surface-Enhanced Raman Scattering. This allows to tune the optimal lateral packing of plasmonic hot-spots for unprecedented versatility and reproducibility.

Selected Projects

- *Portable Low-cost Raman Probe for Chemical Contaminant IDentification* (RaPID). IP: Jordi Ignés. NATO SPS 985250. 2017-2019
- *Fenómenos de no-equilibrio en Materia Blanda: de fluidos complejos a tejidos celulares*, FIS2016-78507-C2-1-P. IP: Francesc sagué, Co-IP. Jordi Ignés. Ministerio de Economia y Competitividad. 2016-2019
- *Transport phenomena at the nanoscale (Nanotrans).* H2020 MSCA-ITN 2015

Singular Scientific Equipment

- Optical microscopes with temperature control. Polarizing, fluorescent, upright/inverted. Electric and magnetic control (1T permanent magnet).
- High sensitivity and high speed cameras.
- Langmuir-Blodgett setup with Brewster angle microscopes.
- Microfluidics equipment: plasma cleaner, FemtoJet, syringe pumps, Micro-forge.

International Collaborations

- ESPCI-ParisTech (T. López-León); University of Oxford (J. Yeomans); Ecole Normale Supérieure (P. Oswald); Univ. of Colorado (D. Schwartz, I. Smalyukh); U. Cal. Sta. Barbara (Z. Dogic, C. Marchetti); Brandeis University (S. Fraden); Kent State University (O. Lavrentovich); Max Planck MPIDS (R. Golestanian)

SELECTED PAPERS

- *Taming active turbulence with patterned soft interfaces.* P. Guillamat, J. Ignes-Mullol, F. Sagues. *Nat Commun* 8, 564. **2017**.
- *Active nematics.* A. Doostmohammadi, J. Ignes-Mullol, J. M. Yeomans, F. Sagues. *Nat Commun* 9, 3246. **2018**.
- *Active nematic emulsions.* P. Guillamat, Z. Kos, J. Hardouin, J. Ignes-Mullol, M. Ravnik, F. Sagues. *Sci Adv* 4, eaao1470. **2018**.
- *Inhomogeneous assembly of driven nematic colloids.* J. M. Pages, A. V. Straube, P. Tierno, J. Ignes-Mullol, F. Sagues. *Soft Matter*. **2018**.
- *Tailoring plasmonic response by Langmuir–Blodgett gold nanoparticle templating for the fabrication of SERS substrates.* M. Tahghighi, I. Mannelli, D. Janner, J. Ignés-Mullol. *Applied Surface Science* 447, 416. **2018**.

2.2.41. Solar and Photovoltaic Energy Group (NanoEnergy)

Team

- **Jordi Andreu Batallé (Associate Professor)**
- **Joan Bertomeu Balagueró (Associate Professor)**
- **José Miguel Asensi López (Associate Professor)**
- **Thomas Tom (PhD Student)**

Research

The Solar Energy Group of the University of Barcelona has been focused for long time in the development of new technologies for photovoltaic modules based on silicon thin films. These include modules based on p-i-n structures of amorphous and microcrystalline silicon and on heterojunction silicon solar cells. In addition to the development of the hot-wire chemical vapor deposition (HWCVD) for the silicon-based materials, activities in the field of transparent conducting oxides and light confinement strategies for using in thin film silicon solar cells are also being carried out.

The activity of the group has evolved to the research on new materials and structures for heterojunction solar cells based in crystalline silicon avoiding the use of doped layers. The aim is to substitute these layers by other materials that act as selective contacts (hole transport layers or electron transport layers) and can be deposited from simpler techniques and/or less dangerous precursor materials. In particular several transition metal oxides are being investigated.

Also the study of alternatives to ITO, which is the most currently used material as transparent electrode, is being carried out, with the aim of avoid the use of critical raw materials as indium. Structures dielectric-metal-dielectric with ultrathin metal layers are being investigated for such application.

Selected Projects

Células solares de heterounión de silicio de estructura no convencional. ENE2016-78933-C4-2-R. IP: Bertomeu Balagueró, Joan. Ministerio de Economia y Competitividad. 2016-2019.

SELECTED PAPERS

- *Investigation on the structural changes of ZnO:Er:Yb thin film during laser annealing to fabricate a transparent conducting upconverter.* Lluscà M., López-Vidrier J., Lauzurica S., Canteli D., Sánchez-Aniorte M.I., Molpeceres C., Antony A., Hernández S., Alcobé X., Garrido B., Bertomeu J. *Journal of Luminescence*. Vol: 185. **2017**.
- *Effect of the base pressure achieved prior deposition on the main properties of ZnO:Al films obtained by DC magnetron sputtering at room temperature for electrical contact use.* García-Valenzuela J.A., Andreu J., Bertomeu J. *Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films*. Vol: 35. **2017**.
- *Yttrium oxide passivation of porous silicon nanostructures for improved photoluminescence and optoelectronic properties.* Derbali L., El Whibi S., Zarroug A., Bertomeu J., Ezzaouia H. *Journal of Materials Science: Materials in Electronics*. Vol: 29. **2018**.
- *Modulation of argon pressure as an option to control transmittance and resistivity of ZnO:Al films deposited by DC magnetron sputtering: On the dark yellow films at 10 -7 Torr base pressures.* García-Valenzuela J.A., Cabrera-German D., Cota-Leal M., Suárez-Campos G., Martínez-Gil M., Romo-García F., Baez-Gaxiola M.R., Sotelo-Lermac M., Andreu J., Bertomeu J. *Revista Mexicana de Fisica*. Vol: 64. **2018**.

2.2.42. Solar Energy Materials and Systems (SEMS) Group (NanoEnergy)

Department of Electronics and Biomedical Engineering, Faculty of Physics

Team

- **Alejandro Pérez Rodríguez (Full Professor)**
- **Lorenzo Calvo Barrio (Adjunct Lecturer)**
- **Edgardo Saucedo Silva (External Collaborator-Senior Researcher at IREC)**
- **Victor Izquierdo Roca (External Collaborator-Senior Researcher at IREC)**
- **Marcel Placidi (External Collaborator-Senior Researcher at IREC)**

Research

The activities of the Solar Energy Materials and Systems Group (SEMS Group) are centred on the development of new materials and processes for advanced thin film PV technologies compatible with the requirements of sustainability, compatibility with industrial mass-production with very low environmental impact, high efficiency and low manufacturing cost. The SEMS Group is very active in the development of thin film technologies based on inorganic chalcogenide compounds, including technologies that are already at the industrial exploitations stage – as those related to Cu(In,Ga)(S,Se)2 (CIGS)- as well as emerging technologies based on new materials such as kesterite (Cu2ZnSn((S,Se)4 (CZTS)) compounds, and new low dimensional chalcogenides including Sb2Se3. This includes also an intense activity in the research and development of advanced characterization methodologies suitable for quality control and process monitoring applications.

The aim is the exploitation of the technological flexibility of chalcogenide based technologies for the development of device and process concepts suitable for next generation PV integrated components and systems, looking for an ubiquitous penetration of PV in all scenarios of human activity. This includes low weight flexible devices for light weight solar roofs, ceramic-based solar tiles for building integration, semi-transparent devices for glass based façades and solar windows, as well as solar harvesting devices for IoT applications.

Main research lines active in the group are:

- Development of new materials and device concepts for advanced cost-efficient PV: Kesterites, wide band-gap chalcogenides, alternative thin film PV semiconductors, bifacial cells, semi-transparent devices, multijunction concepts, alternative flexible / light weight / ceramic substrates;
- Low cost industrial compatible processes for sustainable high efficiency chalcogenide based technologies: Sequential process (sputtering), Electrodeposition, spray pyrolysis, chemical bath deposition, printing;

SELECTED PAPERS

- *Characterization of Cu2SnS3 polymorphism and its impact on optoelectronic properties.* Oliva, F., Arqués, L., Acebo, L., Guc, M., Sánchez, Y., Alcobé, X., Pérez-Rodríguez, A., Saucedo, E., Izquierdo-Roca, V. *Journal of Materials Chemistry* A 5, Vol: 5, 23863 – 23871. **2017**.
- *Structural polymorphism in "kesterite" Cu2ZnSnS4: Raman spectroscopy and first-principles calculations analysis.* Dimitrievska, M., Boero, F., Litvinchuk, A.P., Delsante, S., Borzone, G., Pérez-Rodríguez, A., Izquierdo-Roca. V. *Inorganic Chemistry* Vol: 56, 3467 - 3474. **2017**.
- *Double band gap gradients in sequentially processed photovoltaic absorbers from the Cu(In,Ga)Se2-ZnSe pseudobinary system.* Kondrotas, R., Oliva, F., Alcobe, X., Izquierdo-Roca, V., Perez-Rodriguez, A., Saucedo, E., Pistor, P. *Progress in Photovoltaics: Research and Applications* Vol: 26, 135 – 144. **2018**.
- *Understanding the cell-to-module efficiency gap in Cu(In,Ga)(S,Se)2 photovoltaics scale-up.* Bermudez V., Perez-Rodriguez A. *Nature Energy*. Vol: 3. **2018**.
- *How small amounts of Ge modify the formation pathways and crystallization of kesterites.* Giraldo, S.; Saucedo, E.; Neuschitzer, M.; Oliva, F.; Placidi, M.; Alcobé, X.; Izquierdo-Roca, V.; Kim, S.; Tampo, H.; Shibata, H.; Perez-Rodriguez, A.; Pistor, P. *Energy & Environmental Science* Vol:11 (3), 582 – 593. **2018**.

- Advanced characterization methodologies in thin film PV technologies: Development of techniques suitable for Quality Control & Process Monitoring (multi-wavelength resonant excitation Raman scattering, elastic light scattering, PL...).

Selected Projects

- *DURACIS: Advanced global encapsulation solutions for long term stability in industrial flexible PV technologies.* (PCIN-2017-041), 2017-2020. SOLAR-ERA.NET European Program. Acciones de Programación Conjunta Internacional, Agencia Estatal de Investigacion
- *INFINITE-CELL: International cooperation for the development of cost efficient kesterite/c-Si thin film next generation tandem solar cells.* (H2020-MSCA-RISE.2017-777968). H2020. 2017-2021
- *STARCELL: Advanced strategies for substitution of critical raw materials in photovoltaics* (H2020-NMBP-03-2016-720907). H2020. 2017-2019

Singular Scientific Equipment

- Thin Film Photovoltaics Laboratory of the SEMS group: The Laboratory constitutes a platform for the modelling, development and evaluation of new processes and materials in advanced PV thin film technologies before their industrial implementation. The Laboratory has developed its own PV baseline technologies including electrodeposition based CIGS processes and two-step PVD based CZTS processes scalable up to 10x10 cm2 substrates with efficiency values that are among the highest ones achieved at world level in these technologies (> 11.8% efficiency for new Indium- and Gallium-free CZTS based devices with processes avoiding the use of hazardous compounds). The infrastructure available at the Laboratory includes: Three sputtering systems for the deposition of front and back contacts in PV technologies, thermal evaporator, a complete electrochemical and chemical workshop, reactive thermal treatment equipment, rapid thermal processes equipment, spray pyrolysis system under inert atmosphere, X-ray fluorescence, advanced Raman and Photoluminescence spectrometers, AAA solar simulator and spectral response.

International Collaborations

- The SEMS group has well consolidated international collaborations with a broad network of R+D centers that are among the world leading research groups in chalcogenide PV technologies, as HZB (Berlin, Germany), EMPA (Zurich, Switzerland), TNO (Holland), University of Luxembourg, Free University Berlin (Germany), Uppsala University (Sweden), IPVF (CNRS, Paris, France), ZSW (Stuttgart, Germany), IMEC (Belgium), Imperial College (UK), Northumbria University (UK), Martin-Luther University (Halle, Germany), Aix-Marseille University (France), CEA-LITEN (Grenoble, France), AIST (Japan), as well as with relevant European companies from the PV Technologies and Energy sectors as Flisom AG (Switzerland), Sunplugged Solare Energiesysteme GmbH (Austria), Manz CIGS Technology (Germany), IMRA (Toyota group, France), Advanced Coatings and Constructions Solutions (AC&CS, Belgium), Electricité de France (France), IBM (Yorktown Heights, NY, USA), AST Sistemas SL (grupo AYESA, Spain), FAE SAE (Spain), Ecopol Tech S.L. (Spain), Lenz Instruments SL (Spain), Eliosys S.A. (Belgium), Midsummer AB (Sweden), Onyx Solar (Spain). These collaborations have been enhanced by the strong activity of the SEMS group in the launching and coordination of international collaborative projects in these fields, including projects from the FP7 and H2020 programmes of the European Commission and from the SOLAR-ERA.NET European cooperative action.

2.2.43. Statistical Physics of Bio-Nano Systems and Complex Matter (BioNanoComplex) (NanoMet)

Department of Condensed Matter Physics, Faculty of Physics

Team

- **Giancarlo Franzese (Associate Professor)**
- **Carlos Calero Borrallo (Adjunct Lecture)**
- **Oriol Vilanova Gabarrón (PhD Student)**
- **Sotiris Samatas (PhD Student)**
- **Luis Enrique Coronas Serna (PhD Student)**

Research

Our research activity focuses on Statistical Physics of Bio-Nano Systems and Complex Matter, including hydrated biological systems, proteins, membranes nanoparticles, colloids and glassy systems. We use computer simulations and analytic theories to understand the macroscopic properties of these complex systems.

Our recent studies focus on Water at Bio-Nano Interfaces. The interest is twofold:

1. For the fundamental understanding of basic science (Why water is so important for life? Which properties make water unique for biological processes? How water affects the dynamics of biomolecules? How can we model water-mediated Bio-Nano Interactions?).

2. For the applications (Can we design new proteins and drugs using our knowledge of the water anomalies? Can we control the water-mediated interactions responsible for protein-aggregation diseases, e.g., Alzheimer? How water regulates the interaction of nanoparticles with leaving cells? Can new materials, e.g., graphene, be used for nanomedicine? Can we engineer safe-by-design nanoparticle? Can we develop safe theranostic for hard-to-treat diseases, such as cancer?).

To give our contribution in answering these questions, we develop a multi-scale approach to simulate biological systems under realistic conditions (e.g., thousands of proteins hydrated by billions of water molecules). Our approach, based on a combination of atomistic models and in-house coarse-grain models, covers length-scales from 0.1 to 104 nm and time-scales from picoseconds to hours. We study by atomistic simulations how the dynamics and structure of water change at bio-interfaces (e.g., proteins or membranes) and nano-interfaces (e.g., metallic nanoparticles or graphene sheets). Next, we use the results to build coarse-grain models for hydration water and explore on larger scales the water contribution to protein folding, protein evolution and design. Next, we employ the outcomes to calculate effective protein-protein and protein-surface interactions to further increase the explored time- and length-scale, focusing on protein self-assembly and crystallization (in bulk and under confinement) and on the kinetics of proteins adsorption on nanoparticles (NP) under physiological conditions. Our research roots on our collaborations with experimental groups and many of our predictions have been successfully verified by independent experimental teams.

SELECTED PAPERS

- *How the stability of a folded protein depends on interfacial water properties and residue-residue interactions.* V. Bianco, N. Pagès Gelabert, I. Coluzza, and G. Franzese. *Journal of Molecular Liquids* 245, 129. **2017**.

- *Role of Water in the Selection of Stable Proteins at Ambient and Extreme Thermodynamic Conditions.* V. Bianco, G. Franzese, C. Dellago, and I. Coluzza, *Physical Review* X 7, 021047. **2017**. Open Acces.

- *Membranes with different hydration levels: the interface between bound and unbound hydration water.* C. Calero, and G. Franzese. *Journal of Molecular Liquids* 273, 488 (2019), published on-line in **2018**.

- *Structural properties of water confined by phospholipid membranes.* F. Martelli, H.-Y. Ko, C. Calero, and G. Franzese. *Frontiers of Physics 13, 136801.* **2018**. Within the 5% most cited article in Physics among those published on the same year (according to https://esi.incites.thomsonreuters.com/BaselineAction.action#).

- *Multi-scale approach for self-Assembly and protein folding.* O. Vilanova, V. Bianco, and G. Franzese, in *Design of Self-Assembling Materials*, I. Coluzza ed. (*Springer International Publishing* AG, **2018**) pag. 107–128. ISBN: 978-3-319-71578-0.

Selected Projects

- Abordaje multiescala de nanobiosistemas hidratados. FIS2015-66879-C2-2-P. PI: G. Franzese. Ministerio de Economía y Empresa & European Regional Development Fund. 2016 - 2019.
- ICREA Acadèmia 2015. ICREA: Institució Catalana de Recerca i Estudis Avançats. PI: G. Franzese. 2017 - 2021.
- 2017 BP 00255. Beatriu de Pinós BP-2017. AGAUR - Agència de Gestió d'Ajuts Universitaris i de Recerca. PI: G. Franzese. 2018 - 2020.

Singular Scientific Equipment

- The group is co-responsible of a remarkable infrastructure dedicated to scientific computing, shared with three other PIs of the UB: the "Laboratorio de Supercomputación en Física Estadística", which is used to run the simulations and numerical calculations necessary for the development of scientific projects. Currently, this laboratory comprises two dedicated computing clusters: one cluster with 64-bit CPU machines, consisting of 30 nodes, for a total of 944 virtual cores working with Hyper- Threading Technology and 844 Gb of RAM; and a second cluster of 6 GPU platforms, with INVIDIA GTX 760, 780, 980 and 1060 cards, for a total value of 170.000€.

International Collaborations

- The group has an extended network of active scientific collaborations with many highly prestigious scientific centers all over the world, such as MIT (US), Princeton University (US), Boston (US), Rockefeller University (US), Imperial College (UK), University of Bristol (UK), IBM (UK), University College Dublin (IE), University of Vienna (AT), Rome La Sapienza (IT), University of Rome Tre (IT), Universidade Federal do Rio Grande do Sul (BR), Peking University (CN).

2.2.44. Supra and Nanostructured Systems Group (SuNS) (NanosMat)

Department of Inorganic and Organic Chemistry, Faculty of Chemistry

Team

- **Laura Rodríguez Raurell (Associate Professor)**
- **Inmaculada Angurell Purroy (Associate Professor)**
- **Francisco Javier Caparrós Rodríguez (Adjunct Lecturer)**
- **Andrea Pinto Martínez (PhD Student)**
- **Ariadna Lázaro (PhD Student)**

Research

The main research lines are:

1. Supramolecular Chemistry: The group is developing luminescent water soluble systems able to give rise to the formation of gels, fibers, vesicles and other kind of supramolecular structures.

SELECTED PAPERS

- *Polarized Supramolecular Aggregates Based on Luminescent Perhalogenated Gold Derivatives.* Gavara R., Pinto A., DonaMaria R., Olmos M.E., López De Luzuriaga J.M., Rodríguez L. *Inorganic Chemistry.* Vol: 56. **2017**.

- *Gold(I)-Complex-Titania Hybrid Photocatalyst for Hydrogen Production.* Aguiló E., Soler L., Casanovas A., Moro A.J., Lima J.C., Rodríguez L., Llorca J. *ChemCatChem.* Vol: 9. **2017**.

- *Aggregation induced emission of gold(i) complexes in water or water mixtures.* Pinto A., Svahn N., Lima J.C., Rodríguez L. *Dalton Transactions.* Vol: 46. **2017.**

The researchers are pioneers in this kind of supramolecules grown from discrete complexes. Applications as sensors, hydrogen production, liquid crystals, nanomaterials and biological properties have been developed.

2. Nanoparticles: Nanoparticles of noble-metals (Pd, Au, Pt, Ru) are prepared and deposited on the surface of supporting materials, mainly magnetite, in order to study their catalytic behaviour in numerous processes, such as hydrogenation reactions, C-C coupling reactions and others. These studies are now being expanded to the formation of SACs (single atom catalyst) that generally are thought to be the best catalysts in terms of effectiveness and economy.

Selected Projects

- Sistemas Supra- y Nanoestructurados para reconocimiento molecular en agua. 2016-2019. Ministerio de Economia y Competitividad. PI: Laura Rodríguez Raurell
- Reference: 2017082311. Alba Synchrotron. Title: Identification of supramolecular gold(I) aggregates involved in biological and molecular recognition purposes. PI: Laura Rodríguez Raurell
- Reference: UC-CLL002537. Title: Effect of aggregation on the photophysical parameters of gold(I) supramolecular aggregates. PI: Laura Rodríguez Raurell. Founding Agency: Unión Europea- CLL-Laserlab Europe

Singular Scientific Equipment

- Spectrofluorimeter to perform measurements for samples emitting at UV-vis and NIR in solution and in solid state, at room temperature, 77 K and variable temperature.
- Fluorescence and Optical Microscopy including polarizers for analysing samples at different polarization light angles.

International Collaborations

- Our department: Dr. Albert Figuerola, Dr. Margarita Crespo, Dr. Ramon Bosque.
- Spanish Universities or Research Centers: Prof. Jordi Llorca (Universitat Politècnica de Catalunya), Prof. Enrique García-España (Universitat de València), Prof. Pau Ballester (ICIQ-Tarragona), Prof. José M López de Luzuriaga (Universidad de La Rioja), Dr. Berta Gómez-Lor (CSIC-Madrid).
- European Universities or Research Centers: Prof. João Carlos Lima (Universidade Nova de Lisboa, Portugal), Prof. Antonella Dalla Cort (Università La Sapienza, Roma, Italy), Prof. Kari Rissanen (University Jyväskylä, Jyväskyla, Finland), Prof. Giulia Licini (Università Padova, Padova, Italy), Dr. Marta Rossell (EMPA, Zurich, Switzerland).

- *The Important Role of the Nuclearity, Rigidity, and Solubility of Phosphane Ligands in the Biological Activity of Gold(I) Complexes.* N. Svahn, A.J. Moro, C. Roma-Rodrigues, R. Puttreddy, K. Rissanen, P.V. Baptista, A.R. Fernandes, J.C. Lima, L. Rodríguez. Chemistry. *A European Journal*. **2018**. 24, 14654-14667. Front Cover.

- *Reversible Self-Assembly of Water-Soluble Gold(I) Complexes.* E. Aguiló, A.J. Moro, R. Gavara, I. Alfonso, Y. Pérez, F. Zaccaria, C. Fonseca Guerra, M. Malfois, C. Baucells, M. Ferrer, J.C. Lima, L. Rodríguez. Inorganic Chemistry. **2018**. 57, 1017–1028. *Editor's Choice Article.* Invited Front Cover.

2.2.45. Supramolecular Systems in Nanobiomedicine (NanoPharmaMed)

Department of Pharmacology, Toxicology and Therapeutic Chemistry, Faculty of Pharmacy and Food Sciences

Team

- **M. Lluïsa Pérez Garcia (Associate Professor)**
- **David Limon Magaña (Adjunct Lecturer)**
- **Sandra Giraldo Clemente (PhD Student)**

Research

The Supramolecular Systems in Nanobiomedicine group is interested in the design and evaluation of gold nanoparticles with different conjugates for the treatment of cancer and inflammatory skin diseases. Main research lines are:

- Supramolecular chemistry
- Template synthesis and self-assembly in organic synthesis
- Supramolecular hydrogels for drug delivery
- Functionalisation of micro/nanoparticles for tagging and actuate in living cells
- Nanobiosensors
- Nanoparticles for drug delivery
- Nanomaterials for photodynamic therapy
- Molecular machines and switches

Selected Projects

- *(Bio)funcionalización de Micro- y Nano-Herramientas en suspensión para aplicaciones en células vivas*. TEC2014-51940-C2-2-R. IPs: Perez Garcia, M. Luisa and Gomez Valentín, Elvira. Ministerio de Economia y Competitividad. 2015-2017.
- *(Bio)funcionalización de Suspensiones de Micro- y Nanoherramientas Avanzadas para Aplicaciones Intra- y Extracelulares*. TEC2017-85059-C3-2-R. IPs: Perez Garcia, M. Luisa and and Gomez Valentín, Elvira. Ministerio de Economia y Competitividad. 2018-2020.
- *Functional molecular-based materials and applications at the nanoscale*. 20017SGR1277 Projectes de recerca per potenciar els grups de recerca consolidats. Agència de Gestió d'Ajuts Universitaris i de Recerca. Generalitat de Catalunya. AGAUR. 2017-2019.
- *Collaborating at Wireless communication with cells towards bioelectronic treatments of the future.* EP/R004072/1. EPSRC Healthcare Technologies Challenge Awards. Engineering and Physical Sciences Research Council (EPSRC). 2018-2022.

SELECTED PAPERS

- *Gemini pyridinium amphiphiles for the synthesis and stabilization of gold nanoparticles for drug delivery.* Alea-Reyes M.E., González A., Calpena A.C., Ramos-López D., de Lapuente J., Pérez-García L. *Journal of Colloid and Interface Science.* Vol: 502. **2017**.

- *Water soluble, multifunctional antibody-porphyrin gold nanoparticles for targeted photodynamic therapy.* Penon O., Marín M.J., Russell D.A., Pérez-García L. *Journal of Colloid and Interface Science.* Vol: 496. **2017**.

- *Microscale coiling in bis-imidazolium supramolecular hydrogel fibres induced by the release of a cationic serine protease inhibitor.* Limón D., Jiménez-Newman C., Calpena A.C., González-Campo A., Amabilino D.B., Pérez-García L. *Chemical Communications.* Vol: 53. **2017**.

- *Synthesis and in vitro phototoxicity of multifunctional Zn(II)meso-tetrakis(4-carboxyphenyl)porphyrin-coated gold nanoparticles assembled via axial coordination with imidazole ligands.* Alea-Reyes M.E., Penon O., García Calavia P., Marín M.J., Russell D.A., Pérez-García L. *Journal of Colloid and Interface Science.* Vol: 521. **2018**.

- *Multifunctional Serine Protease Inhibitor-Coated Water-Soluble Gold Nanoparticles as a Novel Targeted Approach for the Treatment of Inflammatory Skin Diseases.* Limón D., Fábrega M.J., Calpena A.C., Badia J., Baldomà L., Pérez-García L. *Bioconjugate Chemistry.* **2018**.

Singular Scientific Equipment

- Diamond Light Source Harwell Campus, Didcot, Oxford (UK)

International Collaborations

Prof. Fraser Stoddart

- Northwestern University, Chicago (US)
  Prof. David Russell/Dra. Mª J. Marin
- School of Chemistry, University of East Anglia, Norwich Research Park, Norwich (UK)
  Dr. Frankie Rawson
- School of Pharmacy, University of Nottingham (UK)
  Dr. David Scurr
- School of Pharmacy, University of Nottingham (UK)
  Prof. Rasmita Raval
- School of Chemistry, University of Liverpool (UK)
  Dra. Maria Luisa Garduño
- Facultad de Químicas, Universidad de Morelos (Mexico)

2.2.46. Surface Engineering. Thin-layer Lab (NanosMat)

Department of Applied Physics, Faculty of Physics

Team

- **Arturo Lousa Rodríguez (Associate Professor)**
- **Joan Esteve Pujol (Emeritus Lecturer)**

Research

The main research of the group is hard coating:

- Vacuum technology applications
- Sputtering PVD of nanometric multilayer coatings
- Cathodic arc PVD of hard coatings
- Plasma polymerization CVD of protective coatings
- Microwave plasma assisted CVD of diamond coatings
- Plasma surface treatments
- Tribological characterization of coatings
- Mechanical properties characterization through nanoindentation

Selected Projects

- *Innovación en recubrimientos avanzados para aplicaciones biomédicas obtenidos mediante técnicas de deposición en vacío asistidas por plasma.* MAT2015-67103-C4-1-R. IP: Lousa Rodriguez, Arturo. Ministerio de Economia y Competitividad. 2016-2018.

SELECTED PAPERS

- *Ultra low nanowear in novel chromium/amorphous chromium carbide nanocomposite films.* Yate L., Martínez-de-Olcoz L., Esteve J., Lousa A. *Applied Surface Science*. Vol: 420. **2017**.
- *Mechanical strength of ground WC-Co cemented carbides after coating deposition.* Yang J., Odén M., Johansson-Jõesaar M.P., Esteve J., Llanes L. *Materials Science and Engineering* A. Vol: 689. **2017**.
- *Chemical and mechanical stability of air annealed cathodic arc evaporated CrAlON Coatings.* Almandoz E., Fuentes G.G., Fernández J., de Bujanda J.M., Rodríguez R.J., Pérez-Trujillo F.J., Alcalá G., Lousa A., Qin Y. *Surface and Coatings Technology*. Vol: 351. **2018**.
- *Low Wear and Low Friction DLC Coating With Good Adhesion to CoCrMo Metal Substrates.* Cano D., Lousa A., Esteve J., Ferrer-Anglada N. *Physica Status Solidi* (B) Basic Research. Vol: 255. **2018**.

2.2.47. Theoretical physics of Nanoscopic Systems (NanoMet)

Department of Quantum Physics, Faculty of Physics

Team

- **Martí Pi Pericay (Full Professor)**
- **Manuel Barranco Gómez (Full Professor)**

Research

Through time-dependent density functional approach we have study the collision of different impurities against a 4He nanodroplets and we have compared the results with available experimental data.

Selected Projects

- DGI, Spain: FIS2014-52285-C2-1-P and FIS2017-87801 (AEI/FEDER, UE).

International Collaborations

- Laboratoire des Collisions, Agrégats, Réactivité, IRSAMC, UMR 5589, CNRS et Université Paul Sabatier-Toulouse.
- Physikalisches Institut, Universität Freiburg, 79104 Freiburg, Germany.
- Department of Chemistry and Biochemistry, California State University at Northridge, Northridge, California 91330, USA.
- Dipartimento di Fisica e Astronomia "Galileo Galilei" and CNISM, Università di Padova, via Marzolo 8, 35122 Padova, Italy.
- Instituto de Física Fundamental (C.S.I.C.), Serrano 123, E-28006 Madrid, Spain.
- Department of Physics and Astronomy, Aarhus University, Ny Munkegade 120, Aarhus 8000 C, Denmark.

SELECTED PAPERS

- *Density functional theory of doped superfluid liquid helium and nanodroplets.* Ancilotto, Francesco; Barranco, Manuel; Coppens, Francois; Eloranta, Jussi; Halberstadt, Nadine; Hernando, Alberto; Mateo, David; Pi, Marti . *International Reviews in Physical Chemistry*. Volume: 36, 621, Published: August. **2017**.
- *Onset of nanoscale dissipation in superfluid He-4 at zero temperature: Role of vortex shedding and cavitation.* Ancilotto, Francesco; Barranco, Manuel; Eloranta, Jussi; Pi, Marti. *Physical Review* B. Volume: 96, 064503, Published: August. **2017**.
- *Capture of Xe and Ar atoms by quantized vortices in He-4 nanodroplets.* Coppens, Francois; Ancilotto, Francesco; Barranco, Manuel; Halberstadt, Nadine; Pi, Marti . *Physical Chemistry Chemical Physics*. Volume: 19, 24805, Published: August. **2017**.
- *Spinning superfluid He-4 nanodroplets.* Ancilotto, Francesco; Barranco, Manuel; Pi, Marti. *Physical Review* B. Volume: 97, 184515, Published: May. **2018**.
- *Self-bound ultradilute Bose mixtures within local density approximation*, By: Francesco Ancilotto, Manuel Barranco, Montserrat Guilleumas, Martí Pi. *Physical Review* A. Volume: 98, 053623, Published: November. **2018**.

2.2.48. Thin Layer Stuctures for Spintronics (NanoMagnetics)

Team

- **Manuel Varela Fernández (Full Professor)**
- **César Ferrater Martorell (Associate Professor)**
- **M Carmen Polo Trasancos (Associate Professor)**

Research

- Deposition of epitaxial thin layers and heterostructures by pulsed lasers and catholic spraying
- Structural, chemical and functional characterization of the deposited materials
- Thin layers and epitaxial hetero-structures of functional materials based on oxides for magnetoelectronics and communications devices
- Magnetic, ferroelectric and multifilic materials

Selected Projects

- *Nuevos Materiales para una electrónica no disipativa.* MAT2014-56063-C2-2-R. IP: Varela Fernandez, Manuel. Ministerio de Economia y Competitividad. 2015-2017

SELECTED PAPERS

- *Epitaxial Growth of SrTi03 Films on Cube-Textured Cu-Clad Substrates by PLD at Low Temperature Under Reducing Atmosphere.* Padilla J.A., Xuriguera E., Rodríguez L., Vannozzi A., Segarra M., Celentano G., Varela M. *Nanoscale Research Letters.* Vol: 12. **2017**.
- *High-temperature Magnetodielectric Bi (Fe0.5Mn0.5) 03 Thin Films with Checkerboard-Ordered Oxygen Vacancies and Low Magnetic Damping.* Coy E., Fina I., Załęski K., Krysztofik A., Yate L., Rodriguez L., Graczyk P., Głowiński H., Ferrater C., Dubowik J., Varela M. *Physical Review Applied.* Vol: 10. **2018**.

2.2.49. Thin-film and Nanostructure electrodeposition group (NanosMat)

Department of Ciència de Materials i Química Física, Faculty of Química

Team

- **Elvira Gómez Valentín (Full Professor)**
- **Elisa Vallés Giménez (Collaborator)**

Research

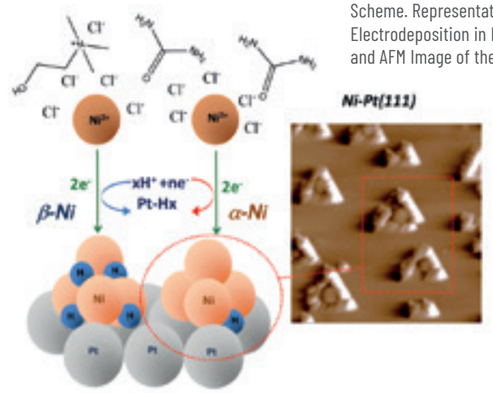
Thin Film and Nanostructure electrodeposition group (Ge-CPN) has wide experience in the electrodeposition processes, both in the analysis of the first stages, as in the material preparation. Catalytic, magnetic and magnetoresistive materials are developed for implementation in sensors, devices, electro- or photocatalysts.

For some time now, ionic liquids (RTIL and DES) have been incorporated, totally or partially, as solvents in electrodeposition processes, expanding the interest to new effects derived from the ionic liquid-electrode interactions, which significantly could affect the early stages of electrodeposition processes. Taking advantage of these new solvents, for different interests, nanostructures have been prepared in a wide type of substrates (ITO, carbon, metals, Si/seed layer, free-standing MWCN structures, and well-ordered Pt or Au monocrystals). These new solvents minimize, in some cases, undesirable processes occurring in aqueous media.

Main research lines are the following:

SELECTED PAPERS

- *Silver nanoparticles/free-standing carbon nanotube Janus membranes.* Ibáñez D., Galindo M., Colina A., Vallés E., Heras A., Gomez E. *Electrochimica Acta.* Vol: 243. **2017**. 339-356.
- *Janus electrochemistry: asymmetric functionalization in one step.* D. Ibáñez, E. Vallés, E. Gómez, A. Colina, A. Heras. *ACS Applied Materials & Interfaces,* Vol: 9. **2017**. 35404-35410.
- *Copper underpotential deposition at gold surfaces in contact with a deep eutectic solvent: new insights.* P. Sebastián, E. Gómez, V. Climent, J.M. Feliu. *Electrochemistry Communications,* Vol: 78. **2017**. 51-55.



Scheme. Representation of the Ni(II) Electrodeposition in DES on Pt(111) and AFM Image of the Ni Clusters.

- Preparation of thin films, multilayers and composites with embedded micro or nanometric particles, which can contribute to the properties modification of the electrodeposited materials
- Electrochemical preparation of the materials in the micro- and nano-level for the application in sensors or magnetic devices.
- Analysis of the medium influence on well-ordered surfaces using ionic liquids (RTIL, DES). Preparation of multifunctional nanostructures.
- Electrochemical preparation of biocompatible structures for intra-extracellular applications.

Selected Projects

- *(Bio)funcionalización de Micro- y Nano-Herramientas en suspensión para aplicaciones en células vivas.* TEC2014-51940-C2-2-R. IPs: Perez Garcia, M. Luisa and Gomez Valentín, Elvira. Ministerio de Economia y Competitividad. 2015-2017.
- *(Bio)funcionalización de Suspensiones de Micro- y Nanoherramientas Avanzadas para Aplicaciones Intra- y Extracelulares.* TEC2017-85059-C3-2-R. IPs: Perez Garcia, M. Luisa and and Gomez Valentín, Elvira. Ministerio de Economia y Competitividad. 2018-2020.
- Collaborating at: *Preparación en una sola etapa de membranas conductoras tipo Janus formadas por nanoestructuras metálicas sobre películas de nanotubos de carbono monocapa sin soporte físico.* CTQ2014-61914-EXP Program Explora - CTQ - Investigación Química Básica (CTQ-BQU). Ministerio de Economia y Competitividad. COORDINADO Universidades de Burgos y de Barcelona. 2015- 2017. IP: Aranzazu Heras Vidaurre.

Singular Scientific Equipment

- Equipment for basic electrochemical study, electrochemical materials preparation and electrochemical in-situ characterization.
- X-Ray Fluorescence Equipment

International Collaborations

- Dr. Laetitia Philippe and Dr. A. Serrà, Empa.Swiss Federal Laboratories for Materials Science and Technology, Laboratory for Mechanics of Materials and Nanostructures, Thun, Switzerland.
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- Dr. Luca Magagnin.Dipartamento di Chimica, Materiali e Ingegneria Chimica, Politecnico de Milano, Italy.
- Dr. J. Ustarroz. Research Group Electrochemical & Surface Engineering, Vrije Universiteit, Brussel, Belgium.
- Dr. Feliu. Surface Electrochemistry Group. Instituto de Electroquimica. Universidad de Alicante.

SELECTED PAPERS

- *Spectroelectrochemical monitoring of contaminants during the electrochemical filtration process using free-standing carbon nanotube filters.* Ibañez D., Gomez E., Valles E., Colina A., Heras A. *Electrochimica Acta.* Vol: 280. **2018**. 17-24.
- *Use of CO as a cleaning tool of highly active surfaces in contact with ionic liquids. Ni deposition on Pt(111) surfaces in IL.* P. Sebastián, M. Tubodziecki, M.P. Bernícola, V. Climent, E. Gómez, Y. Shao-Horn, J.M. Feliu, ACS *Applied Energy Materials.* Vol: 1. **2018**. 4617-4625.
- *Surface sensitive Nickel electrodeposition in Deep Eutectic Solvent.* P. Sebastián, M.I. Giannotti, J.M. Feliu, E. Gómez, ACS *Applied Energy Materials.* Vol: 1. **2018**. 1016-1028.

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- **IGNES MULLOL, JORDI**
  Associate Professor
  Self-organized complexity and self-assembling materials (SOC&SAM)
- **LÁZARO PALACIOS, ARIADNA**
  PhD Student
  Supra and Nanostructured Systems Group
- **LOUSA RODRIGUEZ, ARTURO**
  Associate Professor
  Surface Engineering. Thin-layer Lab
- **MAESTRO GARRIGA, ALICIA**
  Associate Professor
  Engineering of colloidal systems
- **MARTI GONZALEZ, JOAN**
  PhD Student
  Materials for Energy, Photonics and Catalysis (ENPHOCAMAT)
- **MUSHEGHYAN AVETISYAN, AREVIK**
  PhD Student
  Materials for Energy, Photonics and Catalysis (ENPHOCAMAT)
- **PAGES CASAS, JOSEP MARIA**
  PhD Student
  Self-organized complexity and self-assembling materials (SOC&SAM)
- **PANTOJA SUAREZ, LUIS FERNANDO**
  PhD Student
  Materials for Energy, Photonics and Catalysis (ENPHOCAMAT)
- **PASCUAL MIRALLES, ESTHER**
  Associate Professor
  Materials for Energy, Photonics and Catalysis (ENPHOCAMAT)
- **PINTO MARTÍNEZ, ANDREA**
  PhD Student
  Supra and Nanostructured Systems Group
- **RODRIGUEZ RAURELL, LAURA**
  Associate Professor
  Supra and Nanostructured Systems Group
- **TAHGHIGHI HAJI ALIZADEH, MOHAMMAD**
  PhD Student
  Self-organized complexity and self-assembling materials (SOC&SAM)
- **VELASCO CASTRILLO, MARIA DOLORES**
  Associate Professor
  Organic Materials Unit
- **VIDAL FERRAN, ANTON**
  ICREA Researcher
  Homogeneous Catalysis

3.7. RESEARCH AREA 7. NANOENERGY: PRODUCTION AND STORAGE (NANOENERGY)

Coordination: ***Narcis Homs***

- **ANDREU BATALLE, JORDI**
  Associate Professor
  Solar and Photovoltaic Energy Group
- **ASENSI LOPEZ, JOSE MIGUEL**
  Associate Professor
  Solar and Photovoltaic Energy Group
- **BERTOMEU BALAGUERÓ, JOAN**
  Associate Professor
  Solar and Photovoltaic Energy Group
- **CALVO BARRIO, L.**
  Adjunct Lecturer
  Solar Energy Materials and Systems (SEMS Group)
- **CALVO DE LA ROSA, JAUME**
  PhD Student
  Design and improvement of Processes and Materials (DIOPMA)
- **DÍAZ MARCOS, JORDI**
  Adjunct Lecture
  Design and improvement of Processes and Materials (DIOPMA)
- **FORMOSA MITJANS, JOAN**
  Associate Professor
  Design and improvement of Processes and Materials (DIOPMA)
- **HOMS MARTI, NARCISO**
  Full Professor
  Catalysis and Advanced Inorganic Materials (MATCAT)
- **IZQUIERDO ROCA, VICTOR**
  External Collaborator-Senior researcher at IREC
  Solar Energy Materials and Systems (SEMS Group)
- **MARTINEZ ALANIS, PAULINA RAQUEL**
  Adjunct Lecture
  Catalysis and Advanced Inorganic Materials (MATCAT)
- **MORANTE LLEONART, JOAN RAMON**
  Full Professor
  Nanoenergy and Electronic Materials (M2E Group)
- **PAJARES ROJAS, ARTURO**
  PhD Student
  Catalysis and Advanced Inorganic Materials (MATCAT)
- **PEREZ RODRIGUEZ, ALEJANDRO**
  Full Professor
  Solar Energy Materials and Systems (SEMS Group)
- **PLACIDI, MARCEL**
  External Collaborator-Senior researcher at IREC
  Solar Energy Materials and Systems (SEMS Group)
- **RAMIREZ DE LA PISCINA MILLAN, MARIA DEL PILAR**
  Full Professor
  Catalysis and Advanced Inorganic Materials (MATCAT)
- **SAUCEDO SILVA, EDGARDO**
  External Collaborator-Senior researcher at IREC
  Solar Energy Materials and Systems (SEMS Group)
- **SEGARRA RUBI, MERCE**
  Associate Professor
  Design and improvement of Processes and Materials (DIOPMA)
- **TOM, THOMAS**
  PhD Student
  Solar and Photovoltaic Energy Group
- **WANG, YAN**
  PhD Student
  Catalysis and Advanced Inorganic Materials (MATCAT)
- **XURIGUERA MARTIN, M. ELENA**
  Tenure-Track Lecturer
  Design and improvement of Processes and Materials (DIOPMA)

4. CALLS

4.1. AJUTS A LA RECERCA TRANSVERSAL – ART

Internal call of collaborative Research Projects (Ajuts a la Recerca Transversal – ART). The aim of these calls is to promote transversal an innovative research among the research areas of the Institute between PhD researchers at the beginning of their career.

During this period, 9 ART grants have been awarded. This is the list of the awarded:

- Call 2017 Development Of Oxidized Cellulosic Microfilms As Platforms For Microdevices Applications. Research areas (Faculties) involved: NanoBio (Faculty of Biology and Faculty of Pharmacy and Food Sciences) and NanoEnergy (Faculty of Chemistry).
- Call 2017 Nanoparticle-assisted lab-on-a-chip (LoC) for cancer cell treatment and monitoring. Research areas (Faculties) involved: NanoPharmaMed (Faculty of Pharmacy and Food Sciences) and NanoPhotoElectro (Faculty of Physics).
- Call 2017 Microscopic origin of electrostatic surface potential of phospholipid Langmuir-Blodgett monolayers. Research areas (Faculties) involved: NanoBio (Faculty of Pharmacy and Food Sciences) and NanoMet (Faculty of Physics).
- Call 2018 Liquid crystal Elastomers with programmed magnetic anisotropy for SMart ACTuators (ESMACT). Research areas (Faculties) involved: NanosMat (Faculty of Chemistry) and NanoBio (Faculty of Physics).
- Call 2018 Design of an age-dependent corneal membrane model for *in vitro* interaction studies of biodegradable polymeric nanoparticles. *In vitro/ex vivo/in vivo* correlation. Research areas (Faculties) involved: NanoPharmaMed (Faculty of Pharmacy and Food Sciences) and NanoBio (Faculty of Pharmacy and Food Sciences).
- Call 2018 FESTA: Fe oxidation state role in Alzheimer's disease. Research areas (Faculties) involved: NanoBio (Faculty of Physics) and NanoMet (Faculty of Physics).
- Call 2018 Controlled gas insertion in thermally switchable molecular materials. Research areas (Faculties) involved: NanoMagnetics (Faculty of Chemistry) and NanoPhotoElectro (Faculty of Physics).
- Call 2018 Nanostructured transition metal carbides/semiconductors for photocatalytic hydrogen production: an integrated synthetic process at low temperature. Research areas (Faculties) involved: NanosMat (Faculty of Physics) and NanoEnergy (Faculty of Chemistry).
- Call 2018 "Water-soluble gold nanoparticles for the efficient delivery of DNA in cancer gene therapy. Research areas (Faculties) involved: NanoPharmaMed (Faculty of Pharmacy and Food Sciences) and NanoBio (Faculty of Pharmacy and Food Sciences).

It is to note, that the proposals of 2018 first call have been revised by the external independent agency AGAUR so that these awards could be officially included as merits by the University of Barcelona track system (PDA-Recerca).

4.2. MASTERS FELLOWSHIPS

- IN²UB aims to give financial support to its students, either at the beginning or end of their Master or Doctoral Thesis in Nanoscience Programs. These grants have been published in the frame of "beques de col·laboració amb IN²UB", which have been published during Spring and Autumn 2017 Call. A total of 5 "beques de col·laboració amb IN2UB" have been given.
- IN²UB aims to give financial support to Masters Students working at its groups, through grants. These grants have been published in the frame of *"beques de col·laboració amb IN²UB"*, which have been published during Spring and Autumn 2018 Call. A total of 5 *"beques de col·laboració amb IN²UB"* have been called: one for each faculty in which the Institute has researchers.

4.3. INVITED PROFESSORS

During 2018, the Institute, through an internal call, supports with up to 300€ the visit of invited researchers. The elected invited researchers, which are proposed by professors of the Institute, impart a seminar to the whole IN²UB community. Here, the list of the seminars co-financed:

- *METALLOPORPHYRIN FRAMEWORKS FOR A HYBRID QUANTUM COMPUTATION ARQUITECTURE*
  By **Dr. Olivier Roubeau** CSIC-UZA - Instituto de Ciencia de Materiales de Aragon (ICMA)
  July 2018
- *BIRDS, MAGNETS, SOAP, AND SANDBLASTING: SURPRISING CONNECTIONS IN THE THEORY OF INCOMPRESSIBLE FLOCKS*
  By **John Toner** University of Oregon
  July 2018
- *NEW INSIGHTS INTO STRUCTURE AND ACCESSIBILITY OF THE ALLOMORPHIC FORMS OF CELLULOSE*
  By **Dr. Diana Ciolacu** "Petru Poni" Institute of Macromolecular Chemistry, Iasi, Romania
  November 2018
- *QUANTUM PHENOMENA AND APPLICATIONS OF THERMOELECTRIC MATERIALS FROM NANO TO BULK*
  By **Nicolás Pérez**. IFW-Dresden
  October 2018
- *RECENT ADVANCES ON SPINTRONICS*
  By **Prof. Fèlix Casanova** CIC nanoGUNE (Donostia, Spain)
  April 2018

4.4. FUNDING THE ORGANIZATION OF CONGRESSES

In addition, the IN²UB has cofounded and given support, among others, to the following congresses organized by IN²UB members:

- **11th Spanish Conference on Electron Devices**

  Albert Romano Rodriguez (Conference Chairman)

  For almost 20 years the Spanish Conference on Electron Devices, CDE, has served as the major stage for the examination of current and emerging electron devices and technologies developed by Spanish research groups.

  Venue: Barcelona (Faculty of Physics-UB) / / Date: 8th-10th February, 2017

- **Frontiers in Water Biophysics 2017**

  Giancarlo Franzese (Co-Director)

  The conference offers opportunities for presentation and discussion of the most up-to-date research in the field of water structure and dynamics at the nanoscale and mesoscale, properties which make water a unique molecule in all aspects of human life.

  Venue: Erice, Sicily (Italy) / / Date: May 23-28, 2017

- **9th International Conference Engineering of Chemical Complexity**

  Francesc Sagués (Chair of the conference)

  The central aim of the conference is to review current experimental and theoretical progress in the understanding, design, and control of complex physicochemical, soft matter, biochemical and biological systems.

  Venue: Neàpolis Auditorium, Vilanova i la Geltrú (Barcelona) / / Date: 19-22 June, 2017

- **14th International Workshop on Nanomagnetism and Superconductivity**

  Javier Tejada (Scientific Chair)

  Topics include all areas of nanomagnetic and superconducting research: spintronics, novel magnetic and superconducting phases, low-dimensional systems, etc.

  Venue: Comarruga (Tarragona) / / Date: 1–6 july 2018

- **8th International Conference on Spectroscopic Ellipsometry (ICSE8)**

  Oriol Artega (Vice Chair and exhibition)

  An excellent forum for scientists and engineers working in instrumentation, science and applications of spectroscopic ellipsometry and related techniques.

  Venue: Barcelona / / Date: 26 - 31 May, 2019

Moreover IN²UB gives financial support to the following activities:

Since July 2009, the IN²UB is part of the scientific cluster **SECPhO** (Southern European Cluster of Photonics and Optics). The IN²UB collaborates with the costs and activities of the cluster through an annual fee and, when needed, funds attendance to specialized conferences by the cluster members belonging to the IN²UB.

The association **Science²** was founded in April 2017 by 4 chemists from The University of Barcelona, three of which being IN²UB members. The aims of this association are the followings:

- to promote the dissemination of high-quality research without private intermediaries, primarily through the creation of top-level open access journals with low article-processing charges (€500/article + VAT);
- to prioritize standards of excellence and complete transparency in the process of open dissemination of science;
- to promote the training of early career scientists from around the world, prioritizing excellence.

4.5. SCIENTIFIC AND TECHNOLOGICAL EQUIPMENT RENEWAL CALL

In frame of the scientific and technological equipment renewal call by the UB, the IN2UB has participated and been able to cofound a LANGMUIR-BLODGETT – KSVNIMA system. This is a high precision surface tension balance with the ability to extract thin layers of extended molecules at the air-water / other solvents interface (Langmuir-Blodgget system). This equipment is of special interest for researchers at the Institute working on the development of biomaterials, studying amphiphilic interactions with membrane models or interface dynamics. It is to note the versatility of the instrument and of its possible applications, since the system allows from nanoparticle coating and functionalization to the study of interfacial interactions, including the possibility to fabricate surface sensors or the study of polymers.

This equipment has been installed at the Faculty of Pharmacy and Food Sciences, where the Institute also has the Atomic Force Microscope for the analysis of biological samples.

5. EVENTS

5.1. INTERNATIONAL RESEARCH SEMINARS (IRS)

Finally, one of the new actions undertaken during 2018 was the launching of the cycle of International Research Seminars (IRS), in which once a month an international researcher is invited to impart a high level research seminar, covering all subjects areas from the Institute:

- *OPTICAL AND MAGNETIC MOLECULAR SWITCHES: FROM SOLID STATE TO SOLUTION*
  By **Dr. Rodolphe Clérac**
  CNRS-Centre de Recherche Paul Pascal and Université de Bordeaux (France) / / November 2018
- *SENSING THE MATRIX: TRANSDUCING MECHANICAL SIGNALS FROM INTEGRINS TO THE NUCLEUS*
  By **Dr. Pere Roca-Cusach**
  Institute for Bioengineering of Catalonia (IBEC) and IN²UB / / October 2018

5.2. ANNUAL WORKSHOPS

Each year IN²UB celebrates an annual meeting aimed at stimulating collaborations between our researchers.

On 2006, IN²UB was formally constituted, so on January 2017 the Xth Anniversary of IN²UB was celebrated: **2017 Anual Meeting**. During the event, which took place at COMB - Col·legi Oficial de Metges de Barcelona, there were speeches from young researchers representing the 6 research areas of the Institute and from the three **Ajuts a la Recerca Transversal** (2015 and 2016 calls) awardees. There has also been an invited talk from Lorena Redondo-Morata (INSERM-Marseille) and the Plenary Session from Christoph Gerber (Director of scientific communication Swiss Nanoscience Institute. Institute of Physics University of Basel). Prof. Greber is a pioneer in Scanning Probe Microscopy, and he made major contributions to the invention of the Scanning Tunneling Microscope and the Atomic Force Microscope (AFM), he is also a co-inventor of Biochemical sensors based on AFM Technology.

Moreover, a poster session took place, where 29 posters were exposed. Finally, an image competition was also celebrated; 13 original images exposed by researchers were voted and the selected one has been the cover of the 2015-2016 annual activity report.

2017 IN²UB ANNUAL MEETING
BOOK OF ABSTRACTS

The **2018 Annual Meeting** took place on 5th June 2018 at the Paranymph Hall, Faculty of Medicine. There were two invited researcher who did the plenary sessions:

- Prof. Michael J Sherratt. Senior Lecturer in Molecular Biochemistry / Academic Lead for Year 2 PEP / Division of Cell Matrix Biology and Regenerative Medicine / School of Biological Sciences / Faculty of Biology Medicine and Health / The University of Manchester
- Prof. Pere Roca i Cabarrocas. Research Director at CNRS / Director of PICM Laboratory and FedPV / Laboratory of Physics of Interfaces and Thin Layers (LPICM) / L'École polytechnique / Université Paris-Saclay

There were also oral presentations from 2018 ART guarantee and from selected posters. The poster session hosted 42 presentations.

2018 IN²UB ANNUAL MEETING
BOOK OF ABSTRACTS

5.3. IN-HOUSE SEMINARS

After the 2017 Annual meeting event and with the aim to enhance and strength internal collaborations between IN²UB researchers, promoting transversal research among the different Research Areas of IN²UB, a serial of In-house seminars has been initiated, the aim of these is that researchers who presented the poster could have the possibility to explain their research. These seminars take place regularly each fifteen days. The following In-house seminars have taken place:

- *FABRICATION AND CHARACTERIZATION OF OPTO-ELECTRONIC MATERIALS*
  By **Oriol Blázquez**, PhD Student. (Department of Engineering: Section of electronics, Faculty of Physics) // April 2017
- *RHEOLOGICAL STUDIES INSIDE LIVING CELLS WITH OPTICAL TWEEZERS: FROM CALIBRATION-BASED METHODS TO DIRECT FORCE MEASUREMENTS*
  By **Raúl Bola Sampol**, PhD Student. BiOPT: Optical Trapping Lab Grup de Biofotònica (Department of Applied Physics, Faculty of Physics) // May 2017
- *CHOLESEROL-PHOSPHOLIPID INTEGRATION IN MONOLAYERS REVISITED: SURFACE THERMODYNAMICS AND AFM-FS STUDY*
  By **Adrià Botet**, PhD Student al Grup de Nanoestructures en Biomembranes (Department of Pharmacy and Pharmaceutical Technology and Physical-Chemical, Faculty of Pharmacy and Food Sciences) // May 2017
- *NANOPARTÍCULES MAGNÈTIQUES: EINES EN DIAGNÒSTIC I TERAPIA*
  By **Dr. M. Antònia Busquets**. Colloidal Group (Department of Pharmacy and Pharmaceutical Technology and Physical-Chemical, Faculty of Pharmacy and Food Sciences) // June 2017
- *ACTIVIDAD ANTIFÚNGICA DE UNA NANOEMULSIÓN DE CLOTRIMAZOL*
  By **Ivette Camarasa**, PhD Student (Department of Pharmacy and Pharmaceutical Technology and Physical-Chemical, Faculty of Pharmacy and Food Sciences) // June 2017
- *CLUES AND PITFALLS OF ADVANCED TEM IN SOME MATERIALS FOR OPTOELECTRONICS AND ENERGY APPLICATIONS*
  By **Catalina Coll**, PhD Student at Micro-nanotecnologies and nanoscopies for electronics and photonic devices (MIND). (Department of Engineering: Section of electronics, Faculty of Physics) // June 2017
- *INDIVIDUAL GALLIUM OXIDE NANOWIRE AS LOW POWER HUMIDITY SENSOR*
  By **Guillem Domènech**, PhD Student (Department of Engineering: Section of electronics, Faculty of Physics) // October 2017
- *DECONSTRUYENDO LA LIGNOCELULOSA. ENZIMAS MICROBIANAS PARA APLICACIONES INDUSTRIALES Y AMBIENTALES*
  By **Susana V. Valenzuela**, PhD (Laboratory of microbial enzymes for industrial application. Department of Genetics, Microbiology and Statistics. Faculty of Biology) // November 2017
- *TUNING NANOMAGNETS THROUGH NANOSTRUCTURING AND PROXIMITY EFFECT*
  By **Dr. Arantxa Fraile Rodríguez**. (Group of Magnetic Nanomaterials. Department of Condensed Matter Physics, Faculty of Physics) // November 2017
- *ADVANCED TEM IMAGING TOOLS FOR MATERIALS SCIENC*
  By **Dr. Lluís López**. Micro-nanotecnologies and nanoscopies for electronics and photonic devices (MIND) (Department of Engineering: Section of electronics, Faculty of Physics) // November 2017
- *HYALURONAN-BASED MATERIALS AS CONTROLLED DRUG DELIVERY SYSTEM*
  By **Dr. M José García-Celma**. Drug Development in Nanostructured Systems (Department of Pharmacy and Pharmaceutical Technology and Physical-Chemical, Faculty of Pharmacy and Food Sciences) // January 2018
- *NANOMATERIALS: GOOD OR EVIL? ZNO NANOPARTICLES AS AN EXAMPLE*
  By **Dr. Montserrat Mitjans**. Physiology Section (Department of Biochemistry and Physiology, Faculty of Pharmacy and Food Sciences) // January 2018
- *THERAPEUTIC APPLICATIONS OF STIMULUS TRIGGERED DELIVERY SYSTEM*
  By **Dr. M. Carmen Morán Badenas**. Physiology Section (Department of Biochemistry and Physiology, Faculty of Pharmacy and Food Sciences) // February 2018
- *LOW TEMPERATURE INDUCTIVELY COUPLED PLASMA CHEMICAL VAPOR DEPOSITION OF VERTICALLY ORIENTED GRAPHENE NANOWALLS FOR SUPERCAPACITOR APPLICATION*
  By **Arevik Musheghyan**, PhD student. Phyisics and Engineering of amorphous materials and Nanostructures. FEMAN (Department of Applied Physics, Faculty of Physics) // February 2018
- *TRANSPORT AND ASSEMBLY OF COLLOIDS IN LIQUID CRYSTAL*
  By **Josep Maria Pagés**, PhD Student at Self-organized complexity and self-assembling materials (SOC&SAM) (Department of Materials Science and Physical Chemistry, Faculty of Chemistry) // March 2018
- *GROWTH OF CARBON NANOTUBES ON STAINLESS STEEL USING NITRIDED MULTI-LAYER AS DIFFUSION BARRIE*
  By **Luis Fernando Pantoja**, PhD student. Phyisics and Engineering of amorphous materials and Nanostructures. FEMAN. (Department of Applied Physics, Faculty of Physics) // March 2018
- *HYBRID MOLECULAR-INORGANIC MATERIALS: SMMS GRAFTED ONTO IRON OXIDE NANOPARTICLES*
  By **Dr. E. Carolina Sañudo**. Magnetism and Functional Molecules Group (GMMF) (Department of Inorganic and Organic Chemistry, Faculty of Chemistry) // April 2018
- *INTRODUCING NOBLE METHOD OF FABRICATION SERS SUBSTRATE AS A SENSOR TO IDENTIFY AND MEASURE ORGANIC POLLUTAN*
  By **Mohammad Tahghighi**, PhD Student. Self-organized complexity and self-assembling materials (SOC&SAM). (Department of Materials Science and Physical Chemistry, Faculty of Chemistry) // May 2018

5.4. TRANSVERSAL WORKSHOPS

Moreover, a series of workshops has been initiated. The aim of these workshops is that expertise scientists from the Institute in different research fields, meet together and share their research and know-how in order to start collaborative projects or solve questions of mutual interest. The **I Workshop Transversal IN²UB** was in the field of Biomedicine, and took place 26th April 2017 at Faculty of Physics. In this first session, the following researchers from IN²UB shared their investigation:

- **Juan Daniel Prades** (Faculty of Physics)
- **Aurora Hernández-Machado** (Faculty of Physics)
- **Estela Martín** (Faculty of Physics)
- **Albert Romano** (Faculty of Physics)
- **Joan Estelrich** (Faculty of Pharmacy and Food Sciences)
- **Carlos Ciudad** (Faculty of Pharmacy and Food Sciences)
- **Marisa García** (Faculty of Pharmacy and Food Sciences)
- **Patrick Gámez** (Faculty of Chemistry)
- **Gustavo Egea** (Faculty of Medicine)

II Workshop Transversal IN²UB in the field of Nanoenergy (18th January at Faculty of Physics) with the participation of the following researchers from the Institute:

- **Joan Bertomeu** (Faculty of Physics)
- **Enric Bertran** (Faculty of Physics)
- **Narcís Homs** (Faculty of Chemistry)
- **Lorenzo Calvo** (Faculty of Physics)
- **Sergi Hernández** (Faculty of Physics)
- **Dolors Velasco** (Faculty of Chemistry)
- **Alejandro Pérez-Rodríguez** (Faculty of Physics)

III Workshop Transversal IN²UB in the field of Functionalization of Surfaces (2nd February at Faculty of Physics) with the participation of the following researchers from the Institute:

- **Arturo Lousa** (Faculty of Physics)
- **Laura Rodríguez** (Faculty of Chemistry)
- **Carolina Sañudo** (Faculty of Chemistry)
- **M. Elena Xuriguera** (Faculty of Chemistry)

5.5. ORGANIZATION OF SEMINARS

During this period, IN²UB have organized seminars, symposiums and talks of general interest to the IN²UB community:

- *UNIQUE SCIENCE OF SIMPLE OXIDES*
  By **Prof. Ivan K. Schuller** Physics Department and Center for Advanced Nanoscience, UCSD-La Jolla, California 92093, USA // March, 2017
- *ULTRAFAST AND VERY SMALL: DISCOVER NANOSCALE MAGNETISM WITH PICOSECOND TIME RESOLUTION USING X-RAYS*
  By **Prof. Hendrik Ohldag** SLAC National Accelerator Laboratory, Menlo Park, California, USA // June 2017

- *LATERAL DRAG PROPULSION FORCES INDUCED BY ANISOTROPY*
  By **Prof. Dr. Igor Nefedov** Aalto University, Finland // July 2017
- *NANOTECHNOLOGY FOR DRUG AND GENE DELIVERY*
  By **Dr. Uday Kompella** University of Colorado Denver // October 2017
- *PEPTIDE BINDING TO LIPID MONOLAYERS AND BILAYERS: HOW TO GET VALUABLE AND USEFUL INFORMATION*
  By **Prof. Christian Salesse** Centre de recherche du CHU de Québec-Université Laval. Hôpital St-Sacrement. Canada // October 2017
- *FUNCTIONALIZED HYBRID NANOMAGNETS: NEW MATERIALS FOR INNOVATIONS IN ENERGY STORAGE AND MEDICAL THERANOSTICS*
  By **Prof. Michael Farle** IEEE Magnetics Society Distinguished Lecturer 2017. University of Duisburg-Essen, Germany, and Immanuel Kant Baltic Federal University, Russia // October 2017
- *IN²UB - CBNI SYMPOSIUM: A Symposium between researchers from IN²UB and Centre For BioNano Interactions (CBNI), of the University College Dublin about the application of nanotechnology in biological systems from both a practical and a theoretical point of view*
  Speakers: **Prof. Kenneth Dawson** (CBNI), **Prof. Yan Yan** (CBNI), **Prof. Mª Antònia Busquets** (IN²UB), **Prof. Miguel Rubí** (IN²UB) // November 2017
- *DENDRIMER DIRECTED SELF-ASSEMBLY FOR HOGH RESOULTION NANO-LITHOGRAPHY*
  By **Prof. Hee-Tae Jung** Director, KAIST Institute for Nano-century, Kore // December 2017
- *NANOMATERIALS FOR HIGH PERFORMANCE VOC GAS SENSORS*
  By **Prof. Hee-Tae Jung** Director, KAIST Institute for Nano-century, Kore // December 2017
- *IMPROVEMENT OF JEJU BLACK PIG PRODUCTIVITY AND ANIMAL ODOR MEASUREMENT*
  By **Prof. Tae-Sun Min** Director Jeju International Animal Research Center (JIA) Korea) // December 2017
- *MAGNETIC MEMORY IN SINGLE MOLECULES*
  By **Dr. Nick Chilton** Faculty member at Manchester University // January 2018
- *PROGRAMMABLE SELF-ASSEMBLY OF NANOCRYSTALS*
  By **Dr. Alex Travesset** Iowa State University // June 2018
- *MAGNETS SOLVE PROBLEMS*
  By **Dr. Xavier Martí** IGSresearch Enterprise // March 2018
- *NANOSCALE OPTICS AND LASER-BASED 2D AND 3D NANOMANUFACTURING*
  By **Prof. Xianfan Xu** Professor of Mechanical Engineering School of Mechanical Engineering, Purdue University, USA // March 2018
- *NEUROMORPHIC COMPUTING*
  By **Prof. Ivan K. Schuller** University of California San Diego // May 2018
- *SURFING ON ACTIVE CARPETS: NUTRIENTS CURRENTS DRIVEN BY BACTERIAL CLUSTERS AND TURBULENCE*
  By **Dr. Francisca Guzmán Lastra** Physics Department, University of Chile, Santiago // July 2018

6. OUTREACH

In the framework of the events of Woman's Day *Women And Science: Challenges And Perspectives In A Incert Context*

- *ELECTRONIC MICROSCOPY OR WHEN THE DUALITY WAVE-PARTICLE OPENS THE EYES TO SEE THE ATOM*
  By **Dr. Francesca Peiró**
  Full Professor of Electronics and member of the Board of Directors of the IN²UB
  Venue: Aula Magna, Faculties of Physics and Chemistry
  Date: March 8th, 2018 at 9:45h

- *SEMINAR ENGANXA'T A LA NANODIVULGACIÓ*
  A seminar to explain how to divulgate science at nanoscal
  By **Dr. Jordi Díaz**
  Responsable i Tècnic Unitat de Tècniques Nanomètriques i Coordinador Nanodivulga U
  Venue: Faculty of Physics
  Date: October 5th, 2017 at 12h

  IN²UB has given financial and institutional support to this innovative project.

As in the previous editions and together with CCiTUB and Nanodivulga UB, IN²UB has participated at 2017 and 2018 Festival 10alamenos9.es, which aims to share the importance and impact of nanoscience and nanotechnology with society.

7. PhD DEFENDED

It is also to note, that most of IN²UB researchers are involved in the Doctorate of Nanoscience. In fact, theses defended during this period are the following:

7.1. 2017

- Author: **Claudia Patricia Ciurlizza Celis**
  Title: *APORTACIÓN AL ESTUDIO DE PERMEACIÓN TRANSDÉRMICA DE CETIRIZINA*
  Directors: **Ana C Calpena Campmany and Francisco Fernández Campos**

- Author: **Marta Reig Canyelles**
  Title: *CARBAZOLE-BASED MATERIALS FOR ORGANIC THIN-FILMS TRANSISTORS AND ORGANIC LIGHT-EMITTING DIODES*
  Director: **M Dolores Velasco Castrillo**

- Author: **Pau Guillamat**
  Title: *CONTROL OF ACTIVE FLOWS THROUGH SOFT INTERFACES*
  Directors: **F Sagués and J Ignés-Mullol**

- Author: **Elisabet Aguiló Linares**
  Title: *ESTRUCTURAS SUPRAMOLECULARES DE ORO(I) CON PROPIEDADES LUMINISCENTES ESTUDIOS DE AGREGACIÓN Y APLICACIONES*
  Director: **Laura Rodríguez**

- Author: **Joaquim Suñer Carbó**
  Title: *ESTUDI GALÈNIC I BIOFARMACÈUTIC D'EMULSIONS MÚLTIPLES DE CLOTRIMAZOL, ECONAZOL I BIFONAZOL D'APLICACIÓ TÒPICA*
  Director: **Lyda Halbaut Bellowa and Ana Calpena Campmany**

- Author: **Mireia mallandrich Miret**
  Title: *ESTUDIO DE FORMULACIONES DE KETOROLACO DE TROMETAMINA PARA APLICACIÓN SOBRE MUCOSAS Y PIEL*
  Directors: **Ana C Calpena Campmany and Francisco Fernández Campos**

- Author: **Roser Sanz Casañas**
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