

ICIQ<sup>B</sup>

Institut  
Català  
d'Investigació  
Química

2021

research  
collaborations  
with  
industry



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# 1 the institute

The Institute of Chemical Research of Catalonia (ICIQ) started its research activity in 2004. During its first 15 years, the Institute has become an internationally recognized leading institution in the field of chemistry, committed to promoting and conducting high-quality research.



ICIQ's research activities focus on two main fields: **Catalysis of Chemical Processes and Renewable Energy.**

Our research in Catalysis of Chemical Processes aims at developing processes and products that employ resources more efficiently and minimize waste and energy consumption.

ICIQ's research on the field of Renewable Energy aims at contributing to the development of new energy solutions that represent viable alternatives to fossil fuels: the generation of hydrogen from water through sustainable processes, the development of novel solar cells, the conversion of CO<sub>2</sub> into liquid fuels and feedstock for the chemical industry, and development of new materials and processes for energy storage.



**Our goal is to contribute to building a more sustainable economy and improve quality of life through chemical research.**



ICIQ hosts 16 research groups, each led by a Group Leader with specific expertise in the research areas of the Institute. The Institute has received 21 ERC Grants, including 9 ERC Proof of Concept (PoC) grants focused on turning research outputs into commercial or valuable propositions for our society.

The Institute has two additional objectives:

- Transferring knowledge and technology to the chemical, pharmaceutical and energy industrial sectors.
- Training the future generation of scientists by offering high-quality educational programs to master and PhD students and postdoctoral researchers.



**21** **09**

ERC Grants

ERC PoC





Team

Facilities

Scientific  
core facilities



290

People

58% 42%

227

Researchers

61% 39%



7%

Group  
leaders

24%

Post-doctoral  
researchers

11%

Scientific core  
facilities technicians

10%

Industrial project  
researchers

45%

PhD  
researchers

3%

Laboratory  
engineers

13.000

Sqm of research facilities

26

Research laboratories

6

Technology transfer  
laboratories

6

Scientific core facilities  
laboratories

1

Computational  
laboratory

ICIQ's Scientific Core Facilities provide the scientific instrumental and highly specialized personnel to assist ICIQ's research, including projects undertaken in collaboration with industry.

- High throughput experimentation laboratory
- X-ray diffraction
- High resolution mass spectrometry
- Nuclear magnetic resonance
- Chemical reaction technologies
- Chromatography, thermal analysis and electrochemistry
- Spectroscopy and material characterization
- Photophysics
- Glass blowing workshop
- Mechanical workshop / 3D printing



# collaboration with industry

It is through collaborations with industry that ICIQ's research has an impact on people's quality of life. Industrial partners can develop and market products and services derived from the Institute's knowledge and technologies, increasing their competitiveness and creating new qualified jobs.

Therefore, it is our aim to promote and enhance collaborations with the industrial sector, especially through the transfer of ICIQ's knowledge and technologies to new or existing companies as a mechanism to increase our impact in society.

ICIQ's strategy for collaborating with industry follows several approaches:

- Technology Licensing
- Contract Research Projects
- Joint Units with Industry
- Technology Development Units

## Technology Licensing

We protect those research results of commercial and industrial relevance. The aim is to have strong industrial property rights to facilitate the uptake of the technology by the private sector, either through licensing to third party companies or through the creation of spin-off companies.

ICIQ implements flexible licensing strategies, seeking the joint development of a technology with an industrial partner, with the ultimate goal of making the technology available to society. ICIQ is also active in developing these technologies via its innovation laboratory CSOL.

### • Active licensing opportunities

PCT/EP2021/050751	Photoinitiators of radical polymerization
EP20382665	Oxygen evolution reaction electrocatalysts based on self-supported Ru oligomers
PCT/EP2021/059779	Oxygen evolution reaction electrocatalysts based on metal oxides prepared by self-combustion
EP19382720	Reagent for metal-free photochemical cyclopropanation
US16/387,084 US16/458,657	Polyesters and polycarbonates derived from limonene oxide
US16/320,691	Method of preparation of linear polyacenes and compounds therefor
EP18702738 US16/482,966	Diazomethylation reagents and late stage functionalization
P201431698	Resistive sensor for detecting benzene gas
Copyright registered via i-Depot	ioChem-BD: Software for storage and management of computational chemistry data

### • Transferred technologies and assets

Technology	License
MOFs for use in CO <sub>2</sub> separation	Orchestra Scientific S.L.
Parallel photoreactor	Trellum Technologies S.L.
Molecular receptor for Creatinine	CreatSens Health S.L.
Nickel(0) catalysts . N-heterocyclic carbenes	University of Michigan / STREM Chemicals
Hydrogenation of carbon dioxide to methanol	InnoxNova
Englerin A analogues for cancer treatment	National cancer Institute





## Contract Research Projects

Our contract research projects make use of the expertise of a research group or technology development unit to successfully undertake a research project proposed by industry.

The average project involves one post-doctoral researcher working full-time under the supervision of an ICIQ Group Leader, with full access to ICIQ's facilities.

The research objectives are set by the industrial partner, and 100% of the resulting intellectual property is assigned to the company (unless otherwise agreed).

Examples of contract research projects including experimental and computational research approaches:

➤ **ChemCatChem, 2015, 7, 928-935**

*Collaboration between REPSOL and Prof. N. López*

➤ **Macromolecules, 2015, 48, 8197-8207**

*Collaboration between SABIC and Prof. A. Kleij*

➤ **ACS Catalysis 2019 9 (9), 7708-7720  
Chem. Eur. J. 2020, 26, 16129-16137**

*Collaboration between COVESTRO and Prof. N. López*



## Joint Units with Industry

Open innovation concept enabling a dynamic collaboration between ICIQ and industry with the aim to facilitate technology transfer.

➤ **One laboratory dedicated exclusively to R&D projects for a single company**

➤ **Research team of 6-9 postdoctoral researchers**

➤ **Full access to ICIQ scientific core facilities and services**

➤ **Scientific advice by selected group leaders**

➤ **Unit manager in close contact with the company to ensure optimal technology transfer**

**AICURIS**  
**ICIQ Joint Unit**  
*Since 2020*

**7** researchers working in medicinal chemistry in anti-infective drugs.

**ESTEVE**  
**ICIQ Joint Unit**  
*2009-2020*

**6-7** researchers working in medicinal chemistry in pain-relief medicines.

**HENKEL**  
**ICIQ Joint Unit**  
*2010 - 2019*

**6-9** researchers working in new curing reactions for high performance adhesives.





## Technology Development Units

ICIQ's Technology Development Units provide R&D and analytical services to the industrial sector. Each unit focuses on particular aspects of chemical and pharmaceutical development. Together they offer a wide range of complementary R&D services.

### Crysforma

Crysforma provides complete scientific support for the discovery, analysis and scale-up of polymorphs, salts and co-crystals of active pharmaceutical ingredients or intermediates.

Crysforma has developed its own crystallization screening methodology based on the combination of several crystallization procedures.



### High Throughput Experimentation (HTE) laboratory

ICIQ's HTE laboratory is a powerful synthetic and analytical platform for fast reaction screening and optimization. The platform explores the chemical space around a target reaction in an accelerated way using small-scale 96- or 24- well plates which can be incorporated within in-house developed reactors for high-pressure or photochemical reactions.

Miniaturization saves costs on expensive starting materials, while statistical support is applied for an optimized and cost-effective design of experiments (DoE).

### CSOL

CSOL is ICIQ's innovation laboratory, providing expertise in technology valorization, process optimization and prototyping. In addition to developing ICIQ's own technologies, CSOL combines industrial know-how, including initial process safety and Quality by Design (QbD), to develop optimized and scalable chemical processes. CSOL makes use of the HTE laboratory at ICIQ when it may be advantageous in their process optimization or route scouting projects. The combination of the HTE laboratory and Design of Experiments (DoE) to optimize chemical processes is particularly powerful.



### Ertflow

Ertflow provides research and development services in the fields of catalysis and flow processes.

Ertflow's services include the synthesis of libraries of compounds in continuous flow, the design, development and supply of new catalysts for flow processes, and the development of safer, economical and easily scalable versions of batch processes in continuous flow, as well as new flow chemistry reactions.







## Past and present industrial collaborators


















# 3

# research groups

ICIQ hosts 16 research groups, each one of them led by a Group Leader with specific expertise in the institute's research areas. The institute's research approach combines a theoretical and experimental methodology, with dynamic collaborations between research groups that foster multidisciplinary perspectives when dealing with relevant scientific and industrial problems.



 <p>Prof. <b>Pau Ballester</b></p> <ul style="list-style-type: none"> <li>➤ Sensors</li> <li>➤ Health</li> </ul>	 <p>Prof. <b>Carles Bo</b></p> <ul style="list-style-type: none"> <li>➤ Big Data</li> <li>➤ Fine Chemicals</li> </ul>	 <p>Prof. <b>Antonio M. Echavarren</b></p> <ul style="list-style-type: none"> <li>➤ Health</li> <li>➤ Materials</li> </ul>
 <p>Prof. <b>José Ramón Galán-Mascarós</b></p> <ul style="list-style-type: none"> <li>➤ Hydrogen &amp; Renewable Fuels</li> <li>➤ Materials</li> <li>➤ CO<sub>2</sub> utilization</li> </ul>	 <p>Prof. <b>Arjan Kleij</b></p> <ul style="list-style-type: none"> <li>➤ Polymers</li> <li>➤ Materials</li> <li>➤ CO<sub>2</sub> utilization</li> </ul>	 <p>Prof. <b>Antoni Llobet</b></p> <ul style="list-style-type: none"> <li>➤ Hydrogen &amp; Renewable Fuels</li> </ul>
 <p>Prof. <b>Julio Lloret-Fillol</b></p> <ul style="list-style-type: none"> <li>➤ Hydrogen &amp; Renewable Fuels</li> <li>➤ Fine Chemicals</li> </ul>	 <p>Prof. <b>Núria López</b></p> <ul style="list-style-type: none"> <li>➤ Petrochemicals</li> <li>➤ Hydrogen &amp; Renewable Fuels</li> </ul>	 <p>Prof. <b>Rubén Martín</b></p> <ul style="list-style-type: none"> <li>➤ Health</li> <li>➤ Fine Chemicals</li> <li>➤ CO<sub>2</sub> utilization</li> </ul>
 <p>Prof. <b>Feliu Maseras</b></p> <ul style="list-style-type: none"> <li>➤ Fine Chemicals</li> <li>➤ Health</li> </ul>	 <p>Prof. <b>Paolo Melchiorre</b></p> <ul style="list-style-type: none"> <li>➤ Health</li> <li>➤ Fine Chemicals</li> <li>➤ Materials</li> </ul>	 <p>Prof. <b>Emilio Palomares</b></p> <ul style="list-style-type: none"> <li>➤ Photovoltaics</li> <li>➤ Materials</li> <li>➤ Sensors</li> </ul>
 <p>Dr. <b>Mónica H. Pérez-Temprano</b></p> <ul style="list-style-type: none"> <li>➤ Health</li> <li>➤ Materials</li> </ul>	 <p>Prof. <b>Miquel A. Pericàs</b></p> <ul style="list-style-type: none"> <li>➤ Health</li> <li>➤ Fine Chemicals</li> <li>➤ Process intensification</li> </ul>	 <p>Dr. <b>Elisabet Romero</b></p> <ul style="list-style-type: none"> <li>➤ Hydrogen &amp; Renewable Fuels</li> </ul>
 <p>Prof. <b>Marcos G. Suero</b></p> <ul style="list-style-type: none"> <li>➤ Health</li> <li>➤ Fine Chemicals</li> </ul>		





## Prof. Pau Ballester

Prof. Pau Ballester obtained his PhD degree from the Universitat de les Illes Balears (UIB) in 1986. Afterwards, he moved to Pittsburgh University where he was associate researcher and he then held postdoctoral positions at UIB, University of Pittsburgh and the MIT. He held different positions at the UIB from Associate Professor to Vice-dean of the Faculty of Sciences and head of studies of Chemistry.

He was also a visiting scientist at the pharmaceutical company Cubist Pharmaceuticals, Inc. (USA) and spent one year at the Scripps Research Institute (USA) with the rank of Associate Professor of Research between 2002 and 2003.

In 2004, he took a position as ICREA (Catalan Institution of Research and Advanced Studies) Research Professor and he joined the ICIQ as a Group Leader. During his time at ICIQ he has collaborated with Esteve Pharmaceuticals and with Henkel.

➤ SENSORS  
➤ HEALTH

## Functional molecular assemblies for sensor and materials applications

### EXPERTISE

- Molecular self-assembly for the construction of complex architectures (cavitands, rotaxanes, etc)
- Molecular recognition - design and synthesis of molecular sensors for small molecule compounds
- Synthesis of calix[4]pyrroles and calix[4]arenes
- Anion- $\pi$  interactions

### APPLICATIONS

- Detection/quantification of small molecule compounds
- Single-molecule encapsulation

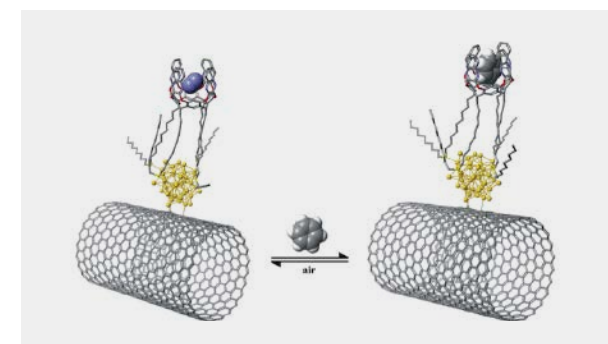
## Research Focus

The Ballester group is working to understand molecular self-assembly processes as a methodology to construct large and functional multimolecular assemblies. A second area of interest for the group resides in the design and application of molecular containers. These are molecules or supramolecules that are sufficiently large to include or encapsulate other molecules. The group investigates the effect that the confinement of molecules in reduced nanoscopic spaces may have in their chemical behavior, as well as develop sensor applications.

## Detection and quantification of small molecule compounds

The Ballester group designs and synthesizes molecular containers that selectively bind a target compound, where this binding event causes a change that can be detected and quantified. Then, in collaboration with other research groups, Ballester's molecular receptors and sensors are integrated into sensing devices. In the last few years the group has developed two commercially relevant sensing applications:

- A resistive sensor for benzene detection in air, which offers high sensitivity and operates in continuous mode, which is not possible with conventional detection methods.



Patent WO2016079356 > resistive sensor for detecting benzene gas and method for the production thereof

- A potentiometric sensor for creatinine in urine and plasma samples. The creatinine sensor, initially developed in collaboration with University Rovira i Virgili (URV), was licensed in 2017 to URV spin-off company CreatSens Health S.L., which is developing a commercial point-of-care product to monitor several biomarkers indicative of a patient's kidney function.

Patent WO2016116175 > selective molecular receptors for creatinine



Moreover, in collaboration with Dr. Claudio Parolo from ICN2, the Ballester group is developing a new fluorescent sensor for monitoring acute kidney injury (AKI), a frequent complication in major surgeries. The new sensor will combine creatinine monitoring using a fluorescent synthetic receptor with the detection of the NGAL protein (biomarker for AKI) using an aptamer-based sensor.

The simultaneous detection of both targets represents a more reliable and superior procedure for the early diagnosis of AKI. The ultimate goal is to produce a portable sensor connected to a urinary catheter that allows healthcare staff to monitor creatinine and NGAL levels with minimal effort.





## Prof. Carles Bo

Prof. Carles Bo received his PhD in Chemistry from the Universitat de Barcelona in 1992.

During his thesis' studies he visited the Laboratoire de Chimie Quantique (Strasbourg, France) several times and carried out research work under the guidance of Profs. Dedieu and Bénard. Later he did a post-doctoral stay at Prof. Baerends' group in VU Amsterdam.

Prof. Bo holds an Assistant Professor position in Physical Chemistry at the Universitat Rovira i Virgili since 1995 and joined ICIQ in 2004 as Group Leader, where he leads a research group on computational chemistry.

- BIG DATA
- FINE CHEMICALS

## In-Silico studies at the service of catalysis

### EXPERTISE

- Computational methods applied to:
  - Homogeneous and enantioselective catalysis
  - Host-guest systems
  - Polyoxometalates (POMs)
- Big data management in computational chemistry

### APPLICATIONS

- In-Silico study and optimization of:
  - Chemical processes (particularly fine chemicals production)
  - Catalysis for energy applications
  - Host-guest systems for detection, quantification and separation
  - Co-crystal formation, other noncovalent interactions

## Research Focus

The Bo group develops and applies computational methods to address chemical reactivity problems, in metal catalyzed reactions, in metal-free organocatalytic reactions, in supramolecular systems, and in polyoxymetallic chemistry. The group uses methods based on functional density theory (DFT) and molecular simulations as basic tools to elucidate reaction mechanisms and properties in solution.

## In-Silico studies in homogeneous and enantioselective catalysis

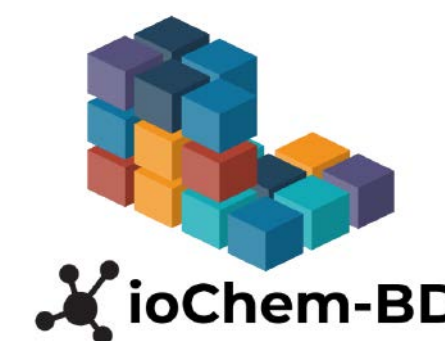
Prof. Bo uses his expertise in computational chemistry to study homogeneous and enantioselective catalysis related issues such as:

- Characterization of reactive intermediates.
- Elucidation of reaction mechanisms.
- Origin of the chemo, regio and enantioselectivity.
- Ligand effects and ligand design.
- Structure-selectivity relationships.

## Big Data management

Realizing the need to have tools able to manage computational chemistry Big Data, the computational groups at ICIQ, together with Universitat Rovira i Virgili (URV) created ioChem-BD in 2015. In 2019, the European Research Council (ERC) highlighted ioChem-BD and included the platform on the Open Research Data and Data Management Plans.

Moreover, the International Journal of Quantum Chemistry, published by Wiley, lists ioChem-BD as one of the solutions to publish computational data, highlighting its versatility to archive data generated with a variety of simulation packages. ioChem-BD is currently distributed in open source to further increase the number of users. In parallel, the Bo group is seeking collaborations with the private sector to develop industry-specific applications built on the platform database and to expand the uptake of the software globally.



## Fine tuning catalysts for clean energy

A collaboration led by Carles Bo and Dr. Haralampos Miras (University of Glasgow), resulted in a new approach to improve molecular catalysts for the Hydrogen Evolution Reaction (HER), in which water is transformed into hydrogen and oxygen.

The combination of theoretical and experimental approaches allowed the scientists to gain mechanistic insights into the Hydrogen Evolution Reaction and explore new catalysts, with the aim of finding cheaper catalysts than the noble-metal based ones currently used.



## Prof. Antonio M. Echavarren

Prof. Antonio M. Echavarren obtained his PhD at the Universidad Autónoma de Madrid (UAM) in 1982. After a postdoctoral stay in Boston College with Prof. T. Ross Kelly, he joined the UAM as an Assistant Professor (1984-86). Following a two years period as a NATO-fellow in the group of Prof. John K. Stille in Colorado State University, he joined the Institute of Organic Chemistry of the CSIC (Spanish Research Council) in Madrid where he stayed until 1992. That year he returned to the UAM as a Professor of Organic Chemistry. He is also Professor of Research at the CSIC since 2004.

In 2004, he joined ICIQ as Group Leader. Prof. Echavarren has been awarded two ERC Advanced Grants for the projects "Advancing Gold Catalysis", in 2013, and "Bioinspired Catalytic Metalofoldamers", in 2019, and the ERC Proof of Concept grant "A new platform technology for the on-demand access to large acenes". During his time at ICIQ he has been involved in research collaborations with the company Esteve Pharmaceuticals.

➤ HEALTH  
➤ MATERIALS

## Organometallic chemistry for health and material science applications

### EXPERTISE

- New catalytic methods based on the organometallic chemistry of transition metals
- Synthesis of complex natural products
- Synthesis of molecules of interest in molecular electronics
- Gold catalysis

### APPLICATIONS

- Synthesis of natural products for health applications
- Synthesis of polyaromatic carbon compounds for material science applications

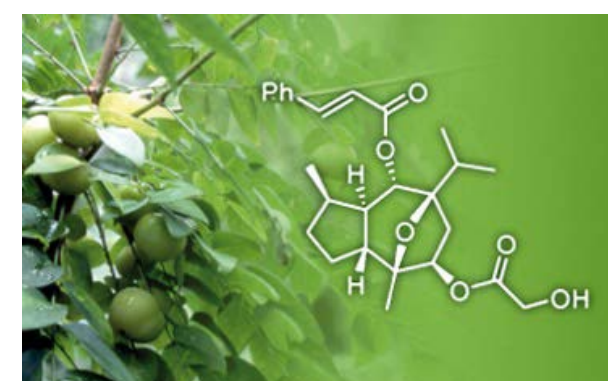
## Research Focus

The group of Prof. Echavarren focuses on the invention of new synthetic methods and on the development of original solutions based on the group's own methodology for the total synthesis of natural and non-natural products.

The most important scientific contributions of the group have been in the field of homogenous gold catalysis, where they have established the mechanistic foundations that have guided the discovery of new transformations and have introduced gold catalysts to the scientific community.


## Gold catalysis applied to natural product synthesis


In the last years, the group has been a leader in the application of gold catalysis for the synthesis of biologically active natural products, having completed the total syntheses of orientalol F, englerin A, schisanwilsonene, epiglobulol, aromadendranediols, rumphellanone A, hushinone, repraesentin F, cannabimovone, nardoaristolone B, lundurines A-C, and seven members of the grandilodine/lapidilectine family of alkaloids.



A success story is the synthesis of (-)-Englerin A analogs as anticancer compounds. Echavarren's group was the first to report a total synthesis of this natural compound, extracted from the stem bark of an African tree, and which presents anti-tumoral activity for renal cancer (tested in collaboration with the National Cancer Institute, USA).

Based on several intermediates in their synthesis they have developed and patented (jointly with NCI) novel analog compounds which present enhanced in vitro activity with respect to the natural product, are active against other cancer types (ovarian and breast cancer, leukemia) and are moreover highly selective, which could potentially result in lower side effects.


 **Patent WO2016168281** > Epoxyazulene derivatives useful for treating cancer and diabetes.

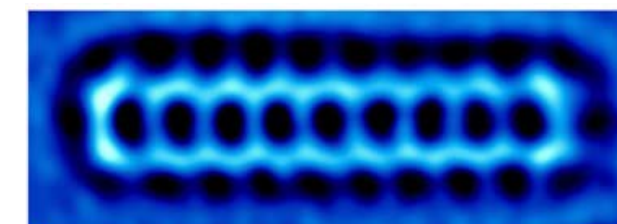
 **Patent WO2019010298** > Englerin derivatives for the treatment of cancer.

## Gold catalysis applied to material science applications

Prof. Echavarren has recently developed a new strategy for the preparation of long linear polyacenes (9, 13, 15 and 17 benzene rings) based on the on-surface, gold and palladium catalyzed, dehydrogenation of a partially saturated linear polyacene compound readily accessible from available raw materials.

Polyacenes are an important class of polycyclic aromatic hydrocarbons constituted by planar sets of linearly fused benzene rings. These compounds exhibit distinctive electronic properties due to their high degree of conjugation and they are appealing materials for the development of the future generation of (opto)electronic devices.

 **Patent US16/320,691** > method for the preparation of a partially hydrogenated polyacene and an intermediate thereof.







## Prof. José Ramón Galán-Mascarós

Prof. José Ramón Galán-Mascarós received his PhD in 1999 at the Universitat de València and then carried out a post-doctoral stay at Texas A&M University, College Station, working on the development of molecule-based magnets and single-molecule magnets. In 2002, Prof. Galán-Mascarós got a Ramón y Cajal Fellowship at the Instituto de Ciencia Molecular (Valencia), where he worked in multifunctional materials with combination of physical properties. In 2009, he took a position as group leader at ICIQ, becoming ICREA Research Professor in 2010. In 2011 he was awarded an ERC Starting Grant to develop his project "Building-up Chemical Complexity into Multifunctional Molecule-based Hybrid Materials" and later three ERC Proof of Concept projects to develop applications based on the most promising results. Since 2016 he is the coordinator of the European project A-LEAF, a H2020-funded consortium for the development of a new device technology for the production of solar fuels. In 2017, Prof. Galán-Mascarós led the entrepreneurial team that launched ICIQ's first spin-off company, Orchestra Scientific S.L.

- HYDROGEN & RENEWABLE FUELS
- MATERIALS
- CO<sub>2</sub> UTILIZATION

## Functional molecular materials for energy, separation and other applications

### EXPERTISE

- Design, synthesis and processing of nanostructured electrocatalysts and electrode materials
- Electrolyzer design and construction
- Highly porous metal organic frameworks (MOFs) and coordination polymers
- Stimuli-reactive materials (sensors, actuators, and molecular memories)

### APPLICATIONS

- Artificial photosynthesis
- Electrochemical production of valuable chemicals (green hydrogen, chloride, methanol, formic acid and acetic acid)
- Separation and capture of target compounds in gas and/or liquid phase (CO<sub>2</sub>/methane; alkanes/alkenes/alkynes; and drugs)

## Research Focus

The team of Prof. Galán-Mascarós is dedicated to the development and processing of hybrid materials with custom properties and controlled dimensionality (at the nanoscale). By means of the suitable design and selection of building blocks, organic linkers and metal centers, they face very different challenges: from intelligent materials for low cost information/separation technologies, to electrocatalysts destined to participate in systems for the production of solar fuels and other electrosynthetic chemicals.

### MOFs for separation applications


The Galán-Mascarós group discovered a new MOF-based material whose nanostructure forms channels that are an excellent match for CO<sub>2</sub> in terms of shape and electronic affinity.

This material can be incorporated in separation modules operated at reduced pressure to efficiently separate CO<sub>2</sub> from a mixture of gases, such as biogas. This affords upgraded gas for pipeline injection and carbon dioxide for other applications.

The technology is being developed into commercial modules and tested in industrial environments by the spin-off company **Orchestra Scientific S.L.** (originated in the Galán-Mascarós team).



In parallel, the group is developing new MOF-based materials to tackle other low-energy separations, including alkanes/alkenes/alkynes; and medical drugs.

 **Patent WO2018073400** > MOFs for separation membranes.

## Reducing the production costs of hydrogen

Avoiding the use of noble metals in water electrolyzers, such as platinum or iridium, is a challenge and a prerequisite to make the hydrogen energy cycle economically viable, since noble metals are expensive and extremely scarce, and their use limits the scaling-up of the technologies for mass production. Instead, scientists are searching for earth-abundant alternatives, which at present are able to offer very good performance in alkaline conditions.

The Galán-Mascarós group, in collaboration with the López group at ICIQ, is working in the discovery of fast and energy efficient alternatives to reduce the costs of current electrolyzer technologies (alkaline, PEM or solid oxide).

Using exclusively non-critical materials, and low cost production protocols, the aim is to incorporate these alternatives into commercially-ready electrolyzers.





## Prof. Arjan Kleij

Prof. Arjan Kleij received his PhD in Chemistry from the University of Utrecht. He worked for three years at Avantium Technologies pharmaceutical branch as a Project Leader.

At a later stage of his career, he worked at Hexion Specialty Chemicals as a Research Scientist in the Epoxy & Phenolic Resins Division, focusing on process optimization of chemical intermediates for coating applications.

In October 2006, he joined ICIQ as a Group Leader and since 2011, he is also an ICREA Research Professor. At ICIQ, Prof. Kleij has been involved in research collaborations with Sabic and Henkel.

- POLYMERS
- MATERIALS
- CO<sub>2</sub> UTILIZATION

## CO<sub>2</sub> valorization and (bio)-renewable building blocks

### EXPERTISE

- Homogeneous catalysis for CO<sub>2</sub> conversion, using cheap and abundant metal complexes (Fe, Al) and organocatalysis
- Biobased polyesters, polycarbonates and polyurethanes
- Use of renewable compounds such as terpenes and fatty acids

### APPLICATIONS

- Monomers, polymers, bulk and fine chemicals incorporating CO<sub>2</sub> and/or biomass
- Functional coatings, composite and polymeric materials

## Research Focus

The group of Prof. Kleij focuses on the catalytic valorization of small molecules, such as CO<sub>2</sub>, into heterocyclic compounds for the synthesis of fine chemicals and pharmaceutical products. In addition, bio-derived compounds such as terpenes are used to design novel types of functional polyesters, polycarbonates and polyurethanes with properties of potential industrial interest.

## CO<sub>2</sub> as carbon feedstock

The Kleij group designs new catalysts for chemical reactions that use CO<sub>2</sub> as a building block to obtain polymers and other chemicals of commercial interest, such as pharmaceutical intermediates or gasoline additives:

- Polycarbonates, polyesters and other CO<sub>2</sub> based polymers (including those obtained from bio-based monomers)
- Cyclic organic carbonates, oxazolidinones
- Lactones, lactams

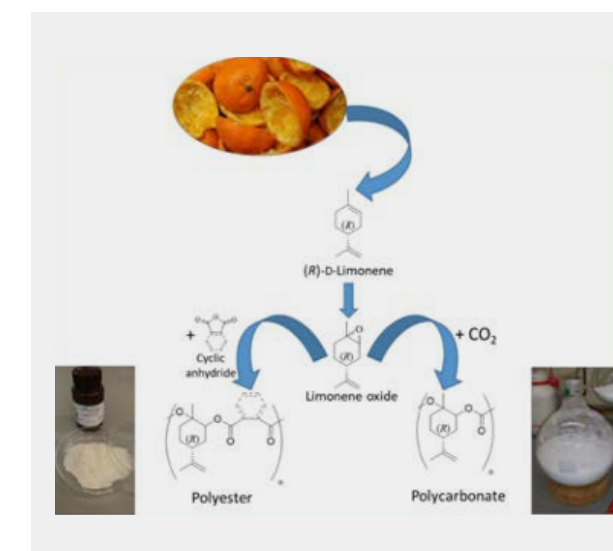
Prof. Kleij aims at using cheap metal complexes under mild reaction conditions for these transformations.

## Polymers incorporating monomers derived from biomass

A key objective of Prof. Kleij is the use of monomers and building blocks derived from biomass, such as limonene which is extracted from the peel of citrus fruit (a waste product from the juice industry) or β-elemene (a by-product from the industrial fermentation of ginger root).

The Kleij group is particularly interested in using bio-renewable components to substitute bis-phenol A (BPA) in polycarbonates, as well as generating polymers (polyesters, polycarbonates) which provide excellent opportunities for post-synthetic engineering aiming at applications such as functional coatings or composite materials.

The team is involved in a wide range of collaborations with materials experts in academia and industry to characterize the different polymeric materials produced, to develop new applications targeting different industrial sectors (electronics, automotive and construction among others), as well as to create polymers from new biomass-derived building blocks.







## Prof. Antoni Llobet

Prof. Antoni Llobet obtained his PhD at the Universitat Autònoma de Barcelona (UAB) in 1985. After postdoctoral stays at the University of North Carolina at Chapel Hill (USA) and at the University of Sussex-Dow Corning (UK) he became a Scientific Officer for the Commission of the European Communities, based in Brussels, Belgium (1990-1991).

He was appointed Senior Research Associate at Texas A&M University in College Station (USA) from 1992 until 1993, working with the groups of Prof. Arthur E. Martell and Donald T. Sawyer.

From 1993 until 2004 he joined the faculty of the Universitat de Girona where he was promoted to Full Professor in 2000. At the end of 2004 he joined the faculty of UAB also as Full Professor. In 2006, Prof. Llobet joined ICIQ as group leader.

### HYDROGEN & RENEWABLE FUELS

## Inspired by nature: artificial photosynthesis

### EXPERTISE

- Artificial photosynthesis
- Design of molecular catalysts for water splitting and CO<sub>2</sub> reduction
- Redox catalysis using transition metal complexes

### APPLICATIONS

- Generation of hydrogen and other solar fuels
- Photochemical oxidation of organic substrates

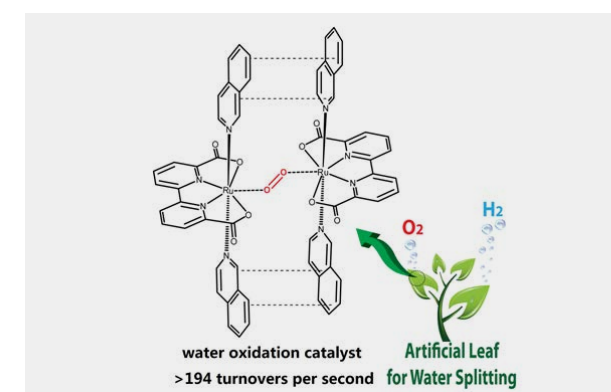
## Research Focus

Prof. Llobet develops research in the field of redox catalysis using transition metal complexes for the oxidation and reduction of organic and inorganic substrates of technological interest. Its general objective is to understand the various factors that affect the efficiency and selectivity of the catalysts, paying special attention to the electronic structure and the spatial arrangement of the transition metals. The group focuses specifically on the catalytic oxidation of water to molecular dioxygen, taking into account the implications of this reaction for new energy conversion schemes based on artificial photosynthesis. The final objective is the generation of clean and renewable fuels with high energy density.

## Water splitting catalysis

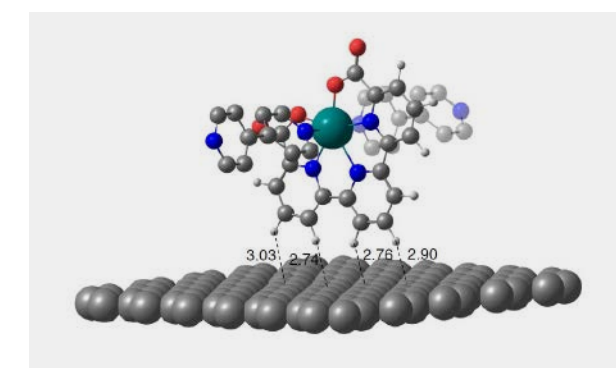
Prof. Llobet has contributed to the development of transition metal complexes as molecular catalysts for redox transformations, particularly for water oxidation, one of the crucial components needed for the generation of solar fuels based on photoelectrochemical cells. His contribution includes a large number of new powerful catalysts based on a bottom up approach. At present, both the fastest and longest lasting catalysts reported in the literature have emerged from his laboratory at ICIQ.

The access of such powerful molecular water oxidation catalysts has allowed him to develop hybrid materials for the preparation of highly performant molecular electro (photo) anodes.




## Solar fuels production based on molecular catalysts

Photoelectrochemical cells that utilize water as a source of electrons and reduce CO<sub>2</sub> to useful products such as MeOH and/or EtOH are one of the most attractive solutions for the replacement of fossil fuels by clean and sustainable solar fuels.



In this respect Prof. Llobet has, recently, developed a highly performant molecular water oxidation electroanode where the catalyst is anchored via multiple CH- $\pi$  interactions into a graphitic surface.

This supramolecular interaction avoids the use of a binder to fix the catalyst to the electrode. The new hybrid material that oxidizes water to dioxygen extremely efficiently, is coupled to the reduction of protons to generate green hydrogen and to the reduction of CO<sub>2</sub> to generate solar fuels via a photoelectrochemical cell.

 **Patent EP20382665** > Catalyst anchoring method and compositions therefrom.





## Prof. Julio Lloret-Fillol

Prof. Julio Lloret-Fillol received his PhD in 2006 at the Universidad de Valencia. Then, he moved to the University of Heidelberg where he stayed two years as a postdoctoral MEyC fellow and two years as a postdoctoral Marie Curie fellow. Since 2010 he has been working as an independent research leader at Universitat de Girona. In 2014 he obtained a position as Young Research Group Leader at the Institut de Química Computacional i Catàlisi at Universitat de Girona.

In November 2014, he started his independent research career at ICIQ within the CELLEX-ICIQ Starting Career Programme. In 2015, he was awarded an ERC Consolidator Grant for the project "Towards a Greener Reduction Chemistry by Using Cobalt Coordination Complexes as Catalysts and Light-driven Water Reduction as a Source of Reductive Equivalents", and he was appointed ICREA Research Professor. In 2020, Prof. Lloret-Fillol was promoted to permanent Group Leader at ICIQ.

- HYDROGEN & RENEWABLE FUELS
- FINE CHEMICALS

## Catalytic transformations promoted by light: solar fuels and fine chemicals

### EXPERTISE

- Water splitting
- Photochemistry

### APPLICATIONS

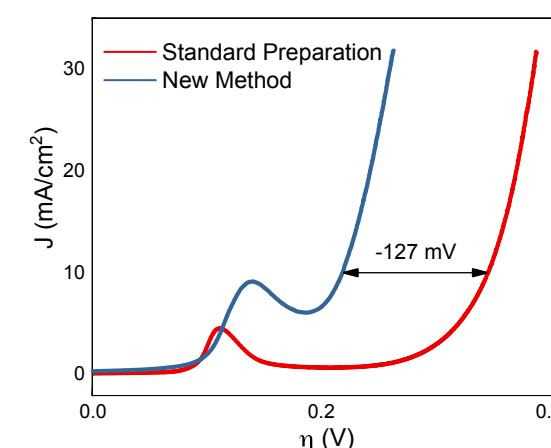
- Renewable fuels
- Fine chemicals from renewable feedstocks
- Parallel reactors for photochemical reactions

## Research Focus

Prof. Lloret-Fillol intends to transfer concepts of artificial photosynthesis to organic synthesis, to carry out endergonic transformations using sunlight as a driving force and to drive the development of new and more environmentally friendly methodologies for the transformation of organic molecules. In this regard, the group has developed biomimetic catalysts based on abundant metals for the reduction of water and CO<sub>2</sub>, catalysts that are also highly active in the photocatalytic reduction of organic compounds as well as in the activation of C-X bonds.


## Nickel based catalytic electrodes for water electrolyzers

The group has developed a new straightforward fabrication method for the production of catalytic electrodes based on inexpensive nickel oxide self-supported on a metal foam. The new method allowed preparing a plethora of catalytic systems, with variable compositions and with superior catalytic performances respect to those reported from classical methods.



Performances can also be improved by introducing metal dopants that modulate the intrinsic catalytic activity of the active phase. The corresponding electrodes revealed huge stability.

The new fabrication method represents a step forward in the production of active and stable electrodes for Anion Exchange Membrane (AEM) water electrolyzers.

 **Patent EP20382294** > Self-supported ultra-active NiO-based electrocatalysts for oxygen evolution reaction by solution combustion.

## Fully controlled parallel reactors for photochemical reactions

Photochemistry, using light to provide the activation energy required to trigger a reaction, can have multiple benefits. In some cases, photochemical reactions are several orders of magnitude faster than their thermal analogues. In other cases, using light to trigger a reaction can enable an otherwise inaccessible reaction path.

Prof. Lloret-Fillol has developed a photo-reactor that allows performing photochemical reactions in parallel under extremely reproducible conditions. It consists of 16 reaction-vials with controlled and stable magnetic stir, temperature-control (with a -40 to 100 °C range) and with independent wavelength customizable LEDs irradiation, allowing to modify the intensity of light for each experiment. The reactors will be commercialized by the spin-off company **Trellum Technologies**.



 **Patent PCT/EP2018/064177** > Photoreactor





## Prof. Núria López

Prof. Núria López obtained her PhD degree in Theoretical Chemistry at the Universitat de Barcelona (UB) in 1999. She then moved to the Center for Atomic Scale Materials Physics (Denmark) for a post-doctoral stage in the group of Prof. Jens K. Nørskov. In 2001, she moved back to the UB as a Ramón y Cajal fellow.

In 2005, she joined ICIQ as Group Leader. In 2010 Prof. López was awarded an ERC Starting Grant for the project “Biomass to chemicals: Catalysis design from first principles for a sustainable chemical industry” and in 2015 an ERC Proof-of-Concept Grant “Big Data for Catalysis.” Prof. López has collaborated with companies such as Repsol and Covestro.

- PETROCHEMICALS
- HYDROGEN & RENEWABLE FUELS

## Computational study of heterogeneous catalysts for chemical and energy production

### EXPERTISE

- **Computational methods applied to:**
  - Heterogeneous catalysis (metals, metal oxides)
  - Metal-organic frameworks (MOFs)
  - Large molecules as substrates (biomass)

### APPLICATIONS

- **Computational screening of heterogeneous catalysts**
- **Rational design of heterogeneous catalysts**
- **Optimization of heterogeneous catalytic processes (including complex substrates: biomass, polymers)**

## Research Focus

The group of Prof. López is dedicated to the study of catalytic phenomena by theoretical means. To this end, they use DFT along with microkinetic models and other continuous equations. The group is experienced in studying complex reaction networks that take place in metals, oxides, individual atoms and any type of material that can serve as a catalyst. Recently, the group has expanded its field of research to include electro and photocatalysis.

## Designing new methods to tackle the complexity of biomass

Biomass molecules are big. With complex molecular structures, there are many reaction sites to be considered when biomass interacts with a catalyst. A relatively small molecule, such as a C<sub>6</sub>, could present a reaction network of about 500.000 reactions, making it too time and resource demanding to study using current models.

Prof. López group developed a new computational method that facilitates the rational design of heterogeneous catalysts able to transform the non-edible fraction of biomass into valuable chemical products. The procedure reduces the number of calculations by a factor of 20 while retaining error bars comparable to Density Functional Theory (DFT).

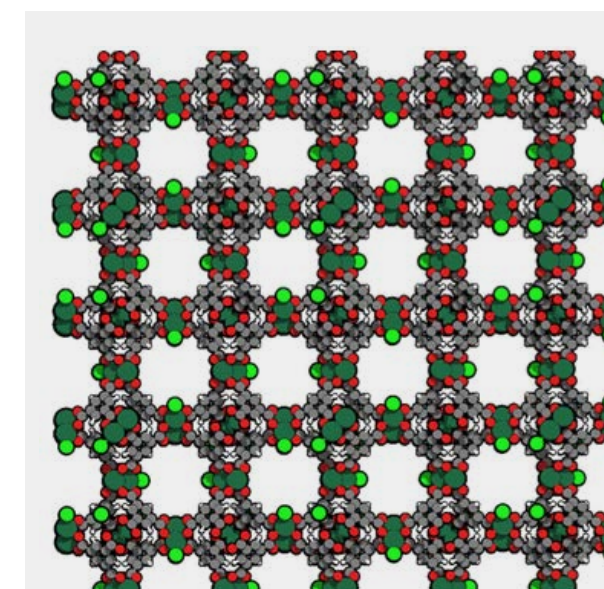
The researchers applied a Machine Learning technique that allowed them to elucidate, for the first time, an interpretable model in heterogeneous catalysis. That is, they have been able to interpret in physical terms the parameters of the equation, which allows them to go further and expand the model.

## MOFs for robust and selective heterogeneous catalysis

The production of 1-butene via ethylene dimerization is one of the few large-scale industrial processes that employs homogeneous catalysis due to its high selectivity, despite the massive amounts of activators and solvent required.

The López group collaborated with University of the Basque Country (UPV/EHU) and RTI International to develop a more sustainable alternative via metal organic frameworks (MOFs), a family of porous materials formed by metallic nodes connected through organic ligands. The resulting MOFs catalyze the reaction with high selectivity and stability, avoiding the need for activators and solvent. These results open new avenues to develop robust heterogeneous catalysts for a wide variety of gas-phase reactions.

The key was to engineer defects in the MOF without compromising the framework structure. The researchers in the López group were able to simulate realistic MOF systems, characterize the defects and elucidate the reaction mechanism. They found that unsaturated metal centers induced by defects drive activity, while the bimetallic nature of the node controls selectivity.







## Prof. Rubén Martín

Prof. Rubén Martín received his Ph.D in 2003 at the Universitat de Barcelona. In 2004, he moved to the Max-Planck-Institut für Kohlenforschung as a Humboldt postdoctoral fellow with Prof. Alois Fürstner, and in 2005, he undertook further postdoctoral studies at the MIT with Prof. Stephen L. Buchwald. He joined ICIQ in 2008, and in 2013, he was promoted to permanent Group Leader and became ICREA Research Professor.

In 2013, Prof. Martín was awarded an ERC Starting Grant for the project "Chasing a Fundamental Challenge in Catalysis: A Combined Cleavage of Molecules" and, in 2019, an ERC Advanced Grant for the project "Escaping from Flatland by 'de novo' Catalytic Decarboxylation Techniques."

He has also been awarded with two ERC Proof of Concept Grants in 2015 and 2016. At ICIQ, Prof. Martín has been involved in industrial research collaborations with Esteve Pharmaceuticals, as well as with other companies in the fields of fragrances & flavours and pharmaceuticals.

- HEALTH
- FINE CHEMICALS
- CO<sub>2</sub> UTILIZATION

## New catalytic methods for the synthesis of relevant molecules through valorization of chemical feedstock

### EXPERTISE

- Selective activation of strong sigma bonds (C-C, C-H, C-O and CO<sub>2</sub>)
- CO<sub>2</sub> as a building block for fine chemicals
- Nickel catalysis

### APPLICATIONS

- Synthesis of bioactive compounds and fine chemicals
- Use of CO<sub>2</sub> as chemical reagent

## Research Focus

Prof. Martín's group is mainly focused on the metal-catalyzed, selective activation of relatively inert entities of great significance, such as CO<sub>2</sub>, C-H bonds, C-C bonds and C-O bonds, as these motifs rank amongst the most widespread and fundamental linkages in organic chemistry. They are also interested on the design and implementation of metal-catalyzed domino reactions since a high degree of molecular complexity can be achieved in one-step, hence allowing a rapid access to key backbones occurring in many natural products.

## Photocatalytic $\alpha$ -arylation of ethers

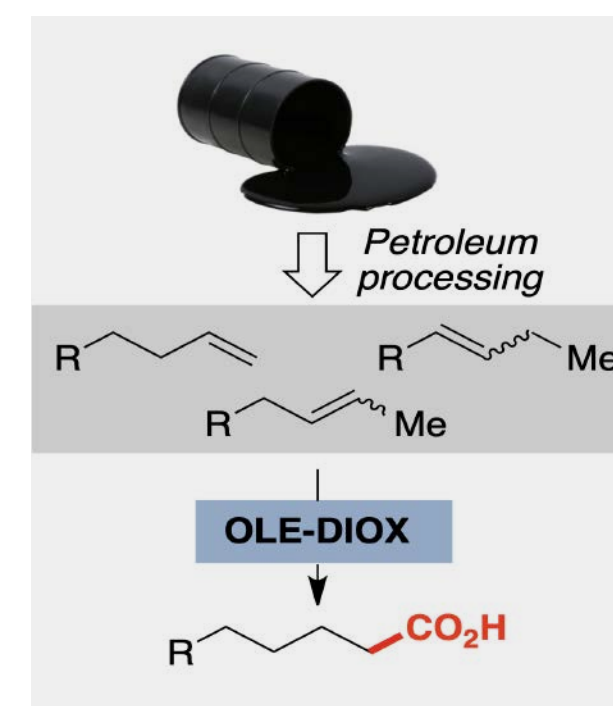
The group has reported a photocatalytic method using blue light irradiation for the direct regioselective C-H arylation of ethers in alpha position starting from aryl bromide derivatives. This application is useful to introduce a broad range of aromatic or heteroaromatic moieties in a given position of a molecular scaffolds, and may therefore find applications in medicinal chemistry and in the development of active fine chemicals ingredients, such as fragrances.

The method was successfully applied in the synthesis of cotinine (a potential therapeutic agent against Alzheimer's disease) and in the functionalization of Ambroxide (key ingredient in the fragrance industry). The developed methodology uses specific benzophenone derivatives as photosensitizers in combination with nickel catalysis in mild reaction conditions, thus avoiding the use of costly noble metal photocatalysts.

## Direct preparation of fatty acids from saturated and unsaturated hydrocarbons

Prof. Martín has described a catalytic technology capable of fixing carbon dioxide in saturated and unsaturated hydrocarbons to prepare fatty acids, key building blocks in the manufacture of polymers, detergents, cosmetics and pharmaceutical products. This nickel catalytic method is capable of promoting carboxylation reactions at remote and unfunctionalized aliphatic sites with CO<sub>2</sub> at atmospheric pressure.

The reaction occurs via selective migration of the Nickel catalyst along the hydrocarbon side-chain with excellent regioselectivity and chemoselectivity. Raw materials, obtained in bulk from petroleum processing, such as alkenes and unrefined mixtures of olefins, can be used as substrates for the synthesis of fatty acids. A single fatty acid is obtained when using mixtures of olefins as starting materials.





## Prof. Feliu Maseras

Prof. Feliu Maseras obtained his doctoral degree in Chemistry at the Universitat Autònoma de Barcelona (UAB). After long post-doctoral stays in the groups of Keiji Morokuma and Odile Eisenstein, he worked as Associate Professor in the group of Agustí Lledós in UAB, from where he moved to his current position at the Institute of Chemical Research of Catalonia (ICIQ) in 2004. He was mentioned on the Nobel Foundation's website as one of the important contributors to the development of multiscale methods, which were the subject of the 2013 Nobel Prize in Chemistry. At ICIQ, Prof. Maseras has been involved in research collaborations with Pfizer and Henkel.

- FINE CHEMICALS
- HEALTH

## Improvement of the efficiency of catalytic processes by computational methods

### EXPERTISE

- DFT and DFT/MM methods
- Computational chemistry applied to:
  - Homogeneous and enantioselective catalysis
  - Reproduction of full catalytic cycles with microkinetic models
  - Mechanochemical processes

### APPLICATIONS

- Reaction optimization

## Research Focus

The Prof. Maseras group applies computational chemistry to the study of homogeneous catalysis. Some of the reactions in which they have achieved most relevant results are in cross-coupling and the activation of C-H links. Recent years have seen an increased interest on less usual processes such as host-guest catalysis, photocatalysis and single electron transfer. New research lines have also started in mechanochemistry and the identification of hidden descriptors for chemical processes. There is an ongoing collaboration with other computational research groups at ICIQ and URV in the development of a repository of computational result.

## Applications in chemical synthesis

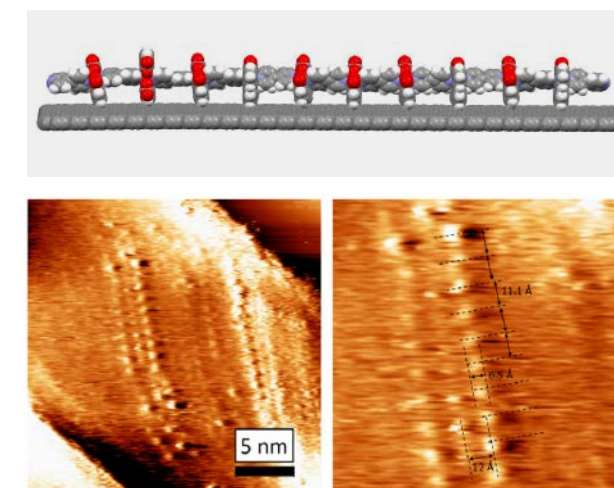
One of the focuses of the group is C-C bond formation. They study the mechanisms of cross-coupling reactions by using computational tools in order to understand and elucidate the effects governing their different steps. This mechanistic elucidation provides an opportunity to further expand these reactions to new substrates and to refine selectivity.

Moreover, the Maseras group works extensively in enantioselective catalysis, carrying out studies in a wide range of chemical reactions in collaboration with other theoretical and experimental groups. The analysis of the results provides key information on different aspects such as the role of the substituents in the outcome of the overall catalytic process or the observed regioselectivity for thermodynamic products, and allows for the identification of key interactions responsible for chiral discrimination.

## Energy applications- Water splitting

The Maseras group carried out DFT/molecular mechanics (MM) calculations to characterize hybrid materials for water oxidation electrocatalysis invented by Llobet's group at ICIQ (ruthenium coordination oligomers adsorbed on multiwall carbon nanotubes, the subject of patent application EP20382665).

These calculations analyzed the interaction of the oligomer with the graphitic surface. This is a key aspect of the technology, since the functionality that links the catalyst to the surface is a critical parameter for predicting and understanding performance, and because the process used to anchor the catalyst deviates from standard methods. The structure obtained by DFT/MM is in very good agreement with scanning tunneling microscopy (STM) results, and its analysis allows the rationalization of the binding model and opens the way for design of alternative systems.







## Prof. Paolo Melchiorre

Prof. Paolo Melchiorre received his PhD in Chemistry in 2003 at the Università di Bologna working in the area of asymmetric catalysis. In 2002, he spent a period in Denmark working with Professor Karl Anker Jørgensen at the "Center for Catalysis", Århus University, where his studies centred on asymmetric organocatalysis.

In 2003, Prof. Melchiorre worked as a postdoctoral associate with Professor Giuseppe Bartoli, at the Industrial Chemistry Faculty of the Università di Bologna. In October 2007, he took a permanent position as Assistant Professor at the Università di Bologna.

In 2009, Prof. Melchiorre joined ICIQ as group leader and ICREA Research Professor. In 2011, he was awarded an ERC Starting Grant for the project "Chemical Reactivity with Organocatalysis". In 2016 he received an ERC Consolidator Grant for the project "Light-Driven Asymmetric Organocatalysis". He was also awarded an ERC Proof of Concept Grant in 2019.

- HEALTH
- FINE CHEMICALS
- MATERIALS

## Discovery of new enantioselective organocatalytic and photochemical processes

### EXPERTISE

- Organocatalysis
- Photochemistry
- Radical Chemistry

### APPLICATIONS

- Synthesis of chiral compounds of high molecular complexity
- Photoinitiators for radical polymerizations

## Research Focus

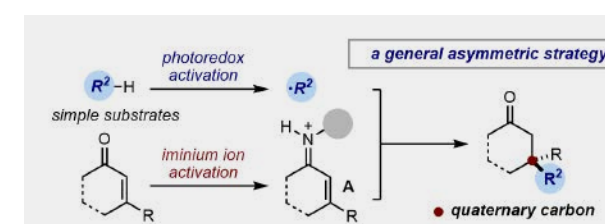
Prof. Melchiorre aims to connect two areas of molecular activation, photochemistry and organocatalysis, to provide new frameworks for chemical reactivity for the development of asymmetric transformations. He has shown that the synthetic potential of organocatalytic intermediates is not limited to the fundamental state, but can be expanded by exploring their photochemical activity.

By bringing an organocatalytic intermediate to an electronically excited state, light excitation opens the door to different reaction pathways to the conventional organocatalytic pathways of the fundamental state, providing new synthetic routes for the preparation of chiral molecules that can not be achieved with the traditional methodologies.

## Radical route for the synthesis of chiral molecules

Visible light photocatalysis and metal-free enantioselective organocatalytic processes are powerful strategies of modern chemical research with extraordinary potential for the sustainable preparation of chiral organic molecules. Prof. Melchiorre has developed a new methodology for the selective formation of chiral molecules under very mild reaction conditions combining enantioselective iminium ion chemistry and photoredox catalysis.

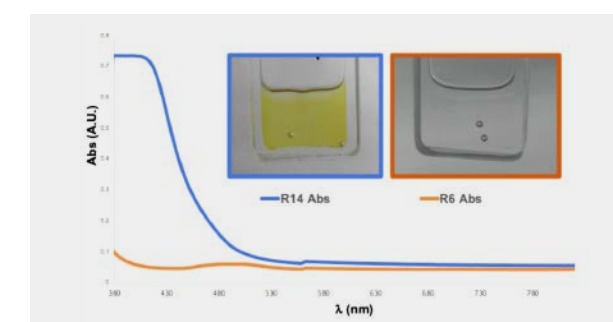
The methodology allows conjugate additions to  $\beta,\beta$ -disubstituted cyclic enones to obtain quaternary carbon stereocentres with high enantioselectivity. Key to success was the design of a chiral organic catalyst which drives the stereoselective interception of photochemically-generated carbon-centered radicals.



## Photoinitiators for switchable controlled polymerization activated by visible light

Photopolymerization is currently used in industry in a broad range of applications such as coating of materials (for example, wood, metal, plastics), decorative paints, binding with adhesives, advanced manufacturing (3D printing) and medical applications (light-curable dental resins).

Prof. Melchiorre has designed proprietary dithiocarbamate compounds useful as photoinitiators for free radical living polymerization. The developed initiator exhibits a good balance between speed of curing under low intensity blue light irradiation and narrow polydispersity. The photoinitiators are cost effective and readily available, operate under visible light, avoiding the problems inherent to the use of UV light, and generate colorless polymers. Moreover, the growth of the polymer can be conveniently controlled by switching on an off the light source.



PCT/EP2021/050751 > Carboxylic dithiocarbamic acid anhydride compounds and compositions thereof



## Prof. Emilio Palomares

Prof. Emilio Palomares received his PhD from Universitat Politècnica de Valencia. He moved to the Centre for Electronic Materials and Devices of the Imperial College (London) where he began his work with molecular and biomolecular devices to obtain renewable energies and obtained a Marie Skłodowska-Curie fellowship.

He returned to Valencia at the Institut de Ciència Molecular of the Universitat de València, he joined ICIQ in 2006 as a Group Leader. In 2007, he was appointed ICREA Research Professor. In 2008, he was awarded an ERC Starting Grant for the project 'Control of the Electronic Properties of Hybrid-Quantum Dot/Polymer-Materials for Energy Production'. In 2015, he received an ERC Proof of Concept Grant for the project 'Ratiometric FRET Based Nanosensors for Trypsin Related Human Recessive Diseases'. At ICIQ, he has collaborated with the companies ACCIONA and Torrecid. In 2020, Prof. Palomares was appointed ICIQ's Director.

- PHOTOVOLTAICS
- MATERIALS
- SENSORS

## Photovoltaics and Photonics

### EXPERTISE

- Synthesis and characterization of (nano)materials and molecules for energy and health applications
- Advanced spectroscopy, device manufacturing

### APPLICATIONS

- Photovoltaics
- Water electrolysis
- (Flexible) light emitting diodes (LEDs) and electronics
- Sensors and diagnostics

## Research Focus

The group of Prof. Palomares works on the synthesis and characterization of materials with optical and electrical properties that they use to manufacture devices for energy applications.

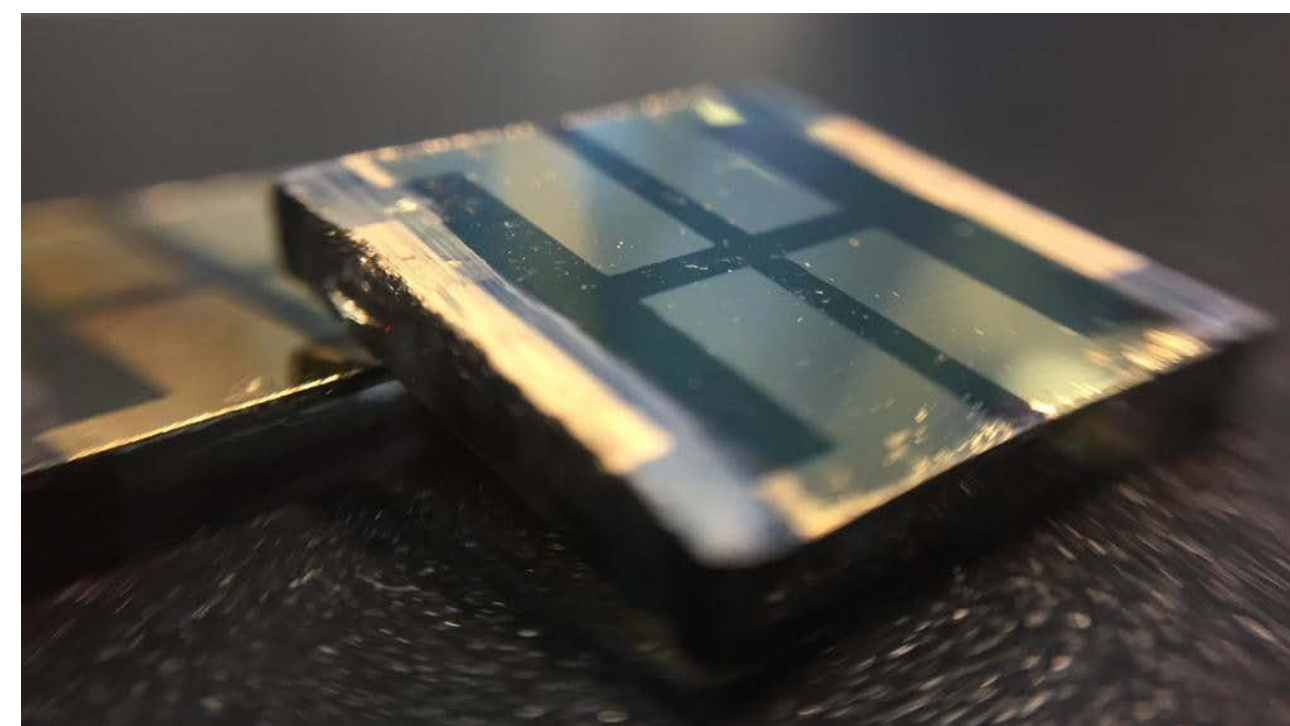
### Improving efficiency in perovskite solar cells

Perovskite-based solar cells are the fastest-advancing solar technology to date. Since they were first used in 2009, perovskite solar cells have achieved high efficiencies (over 25% under standard solar irradiation) at low production costs. Although most of the perovskite components are optimized, there is still room for improvement.

In the case of the Hole Transport Materials (HTMs), the major concern is the materials used. Particularly spiro-OMeTAD, the most widely used HTM, is prone to degradation and expensive to synthesize. Therefore, current research focuses on finding alternatives. Prof. Palomares realized that new molecules with the potential to replace spiro-OMeTAD were selected on the basis of their properties in solution.

However, in functional solar cells, these molecules are prepared in the form of thin films whose surfaces, in turn, are placed in contact with other materials, forming interfaces. These interfaces may confer changes in the properties of the molecules and resulting devices.

In another recent collaboration, the Palomares group demonstrated the potential of using organic molecules that self-assemble in monolayers (SAMs) to simplify the construction of perovskite-based solar cells. The new approach eliminates the need to employ inorganic metal oxides that are processed at high temperatures, which will enable the use of flexible substrates to build solar devices. This approach led to one of the highest solar to energy conversion efficiencies reported to date in inverted-structure solar cells.







## Dr. Mónica H. Pérez-Temprano

Dr. Mónica H. Pérez-Temprano obtained her degree in Chemistry at the University of Valladolid in 2005, and her PhD in 2011 under the supervision of Prof. Pablo Espinet and Prof. Juan Casares.

As a graduate student, she worked in the area of organometallic chemistry, investigating the mechanisms of different palladium-catalyzed processes. In early 2012, she joined the research group of Prof. Melanie Sanford at the University of Michigan where she focused on the synthesis and reactivity of high-valent palladium(IV) complexes.

In October 2015, she began her independent career as Junior Group Leader within ICIQ's Starting Career Programme.

➤ HEALTH  
➤ MATERIALS

### Development of new chemical transformations: from organometallic mechanistic studies to catalysis

#### EXPERTISE

- C-H Activation
- Cobalt coordination chemistry and catalysis
- Mechanistic studies

#### APPLICATIONS

- Synthesis of bioactive compounds and materials

### Research Focus

The group of Dr. Pérez-Temprano uses mechanistic studies as an extremely powerful design tool to detect and solve the obstacles that hinder the efficiency of transition metal catalyzed transformations. This strategy will be decisive for the discovery and optimization of innovative sustainable processes. To develop their research projects, they apply different approaches, from synthetic organic chemistry and ligand design, to mechanistic studies, including the capture and characterization of highly reactive reaction intermediates.

### Homogeneous catalysis using cobalt and first-row transition metals

Cobalt and other first-row transition metals are less expensive and more sustainable than the precious metals, such as palladium, that chemists typically use in synthetic processes.

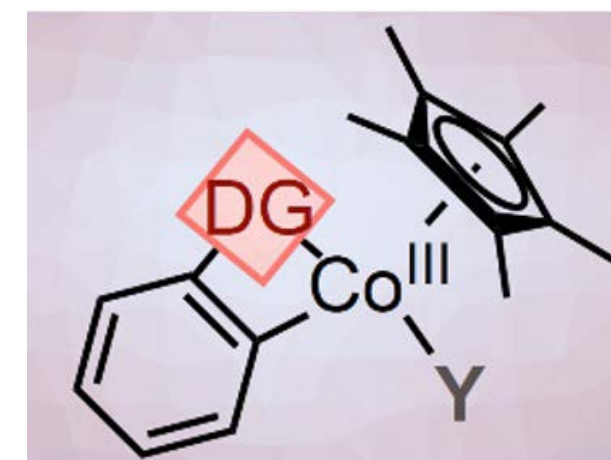
Moreover, catalysts containing first-row transition metals can potentially yield intermediates, and thus products, that catalysts containing precious metals cannot. That variety would be of high interest to synthesize new materials or drug candidates.

However, reaction development for first-row metals is in relative infancy because mechanisms are unclear. The group focuses on capturing intermediates and understanding mechanisms to guide the design of cobalt-catalyzed reactions.

### Understanding Cp\*CoIII-Catalyzed C-H Functionalization

Pentamethylcyclopentadienyl (Cp\*)CoIII catalysts have attracted much attention as an alternative to noble transition metals for C-H activation reactions. However, the fundamental organometallic understanding of these systems is still limited.

The Pérez-Temprano group has developed different synthetic tools for overcoming this challenging situation and capitalize on all the gathered fundamental knowledge for developing mechanism-driven catalytic processes. Over the past years, the group has explored the functionalization of a wide variety of starting materials, including fragments of drug-type molecules, using electrophilic and nucleophilic coupling partners.



In addition, the group has developed a library of metallacyclic Cp\*Co(III) complexes that exhibit interesting catalytic efficiency in different Cp\*Co-catalyzed C-H functionalization reactions. They also found that Cp\*Co species promote cross-coupling reactions of aryl halides. This work opens new avenues for accessing previously inaccessible reactive intermediates in Cp\*Co catalysis and designing novel catalytic systems that could substitute more expensive and scarce alternatives like Rh or Ir.



## Prof. Miquel A. Pericàs

Miquel A. Pericàs obtained his doctorate in 1979 under the guidance of Prof. Fèlix Serratosa at the Universitat de Barcelona (UB). After postdoctoral studies at the Spanish research council (CSIC) with Prof. Francesc Camps, he joined the UB as Assistant Professor in 1980 and was promoted to Full Professor in 1991.

In June 2000, he was appointed to create the Institute of Chemical Research of Catalonia (ICIQ) where he served as Director until 2020. Prof. Pericàs is also involved in supporting technological innovation, playing a central role in the creation of the Centre de Tecnologies Avançades en Química Fina i Síntesis Asimètrica (TECNOQUIRAL), that later gave rise to the spin-off Enantia, S.L.

At ICIQ, he has collaborated with chemical and pharmaceutical companies such as Esteve Pharmaceutical, Henkel and Aicuris. He has also promoted the creation of the ICIQ Technology Development Unit ERTFLOW.

- HEALTH
- FINE CHEMICALS
- PROCESS INTENSIFICATION

## Immobilized catalytic systems for asymmetric processes in continuous flow

### EXPERTISE

- Catalyst design and immobilization
- Asymmetric catalysis in batch and flow
- Continuous flow chemistry

### APPLICATIONS

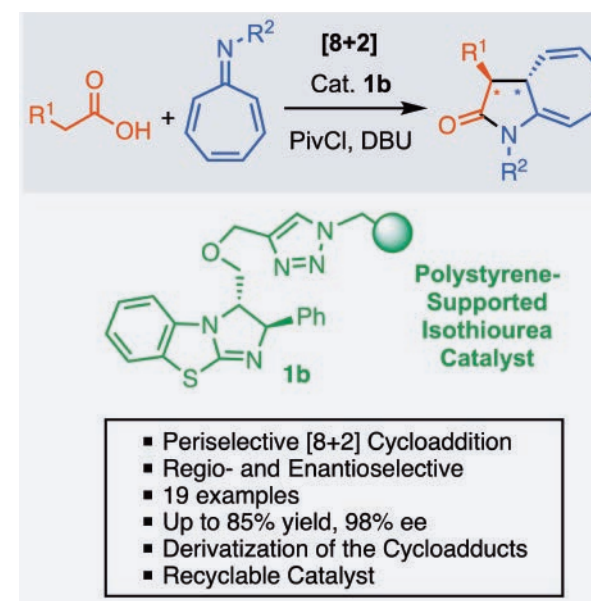
- From batch to flow: thermal, catalytic and photocatalytic processes
- Sequential flow synthesis of libraries of enantiopure compounds

## Research Focus

The group of Prof. Pericàs participates in an extensive research programme aimed at developing a complete set of catalysts immobilized in polymers and magnetic nanoparticles with optimal characteristics in terms of catalytic activity, stereoselectivity and life cycle. The final objective is the development of continuous flow versions of the most relevant catalytic and enantioselective organic synthesis processes, contributing to a more sustainable practice of chemical synthesis. Its current objectives involve the development of commercial solutions for the application of catalytic methodologies in continuous flow to production.

### Supported catalysts with improved performance

Prof. Pericàs' group discovered a recyclable isothiourea catalyst that promotes asymmetric [8+2] annulations. This new reaction combines azaheptafulvalenes and chiral ammonium enolates to yield asymmetric 7,5-fused heterocyclic compounds. Researchers demonstrated the versatility of this procedure synthesizing a wide scope of products with good yields and very good enantiomeric excesses (ee = 90-97%).

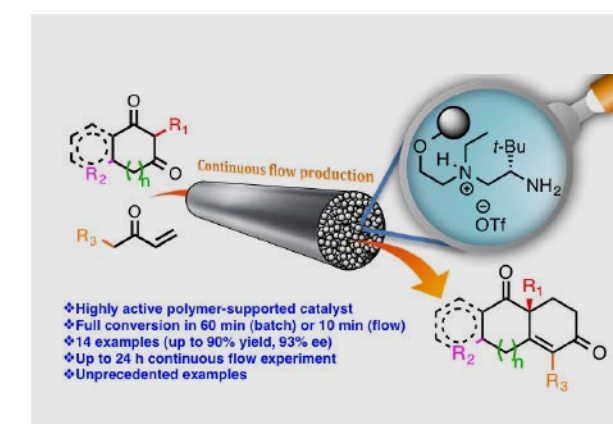


The transformation is catalyzed by an immobilized isothiourea that can be easily recovered by filtration and with a TON almost five times higher than the TON observed in the classical homogeneous approach for asymmetric [8+2] annulations.

## Flow chemistry for the straightforward preparation of libraries of compounds

Considering the inherent advantages of using continuous flow systems such as workup suppression and simplified scale-up, Prof. Pericàs group have extended the applicability of their systems to the preparation of small libraries of enantioenriched compounds. Among others, they prepared a heterogenized organocatalyst based on Luo's diamine and applied it to the asymmetric Robinson annulation reaction.

This polystyrene-supported diamine enables the high-yield, highly enantioselective preparation of a wide scope of chiral bicyclic enones under mild conditions, with reaction times as short as 60 minutes (batch) or residence times of 10 minutes (flow).







## Dr. Elisabet Romero

Dr. Elisabet Romero graduated in Chemistry in the University of Barcelona in 2003, and obtained a master degree under the supervision of Dr. Lluís Julià at the Institute of Advanced Chemistry of Catalonia. Shortly after, she gained a pre-doctoral Marie Curie fellowship at the Biophysics group led by Prof. Rienk van Grondelle at the Vrije Universiteit in Amsterdam (The Netherlands), where she received her doctoral degree in 2011.

She was then appointed as a postdoctoral researcher to implement a new ultrafast spectroscopic technique (Two- Dimensional Electronic Spectroscopy) at the same university, where she led and coordinated a group of six members, including PhD students and postdocs. In February 2018, she started her independent research career at ICIQ within ICIQ's Starting Career Programme, funded by the "Severo Ochoa" grant. In the same year, she was awarded an ERC Starting Grant for the project "Engineering Bio-Inspired Systems for the Conversion of Solar Energy to Hydrogen."

### ➤ HYDROGEN & RENEWABLE FUELS

## Bio-inspired systems to produce H<sub>2</sub> using solar energy

### EXPERTISE

- Natural and artificial photosynthesis
- Design of bio-inspired macromolecular systems
- Time-resolved spectroscopic characterization of multi-chromophoric systems

### APPLICATIONS

- Generation of hydrogen and solar fuels

## ➤ Research Focus

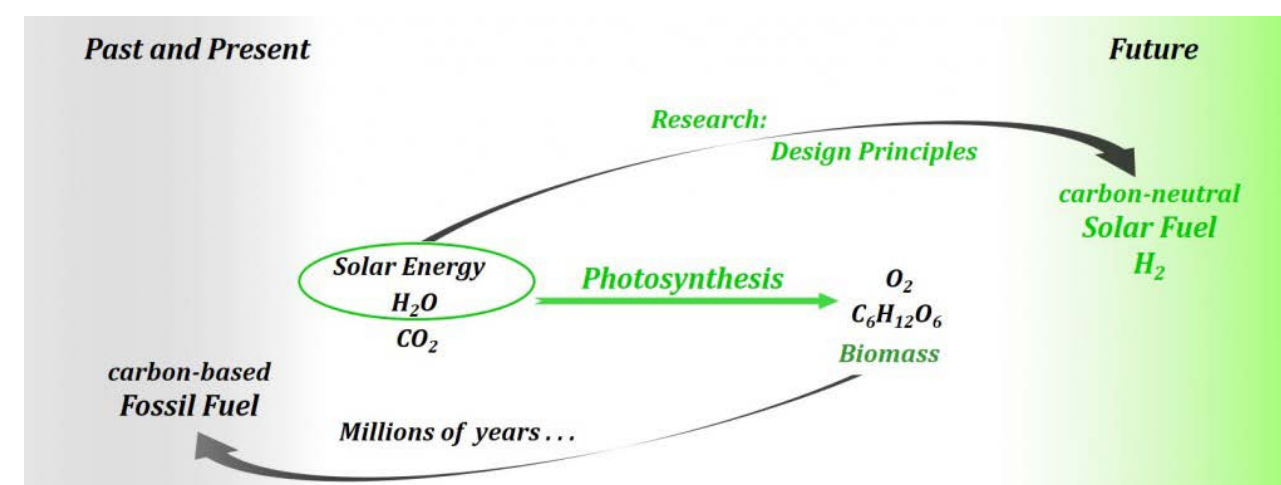
Dr. Romero aims to develop a new generation of bio-inspired macromolecular systems able to convert solar energy to fuels. The group objective is to design and construct chromophore-protein assemblies based on abundant and biodegradable materials with the capacity to absorb, transfer and convert sunlight into electrochemical energy with high efficiency. The resulting energy and electron transfer dynamics in these assemblies will be investigated by ultrafast laser spectroscopy. Ultimately, the optimized systems will be incorporated into devices to provide a renewable, safe and inexpensive energy solution towards a sustainable future.

## Hydrogen generation using bio-inspired macromolecular systems

The efficient and inexpensive conversion and storage of solar energy into fuels remains a fundamental challenge. Currently, solar-energy conversion devices suffer from energy losses mainly caused by disorder in the materials used. The solution to this problem is to learn from nature. In photosynthesis, the photosystem II reaction center (PSII RC) is a pigment-protein complex able to convert solar photons into a separation of charges with near 100% efficiency.

Crucially, the generated charges have enough potential to drive water oxidation and hydrogen production. The Romero Group works to create a new generation of bio-inspired devices based on abundant and biodegradable materials that will drive the transformation of solar energy and water into hydrogen, an energy-rich fuel that can be stored and transported.

In addition, in collaboration with ICFO and IBEC researchers, the Romero group works on the study of both natural proteins (isolated directly from plants), and artificial proteins (specifically designed and constructed), able to convert solar energy into a separation of charges; a necessary step for the transformation of solar energy and water into hydrogen, an energy-rich fuel. The combination of sophisticated ultrafast spectroscopy techniques with high sensitivity photocurrent recordings will allow the exploration of the light-to-charge conversion in these proteins with unprecedented detail.





## Prof. Marcos G. Suero

Prof. Marcos G. Suero received his PhD in 2009 at the Institute of Organometallic Chemistry Enrique Moles (Universidad de Oviedo). During the summer of 2005, he joined the laboratory of Prof. Andrew Myers at Harvard University working on the synthesis of novel tetracycline antibiotics as a PhD visiting student.

In May 2010 he moved to the University of Cambridge to work with Professor Matthew Gaunt on copper(III) catalysis as a Postdoctoral Marie Curie Fellow and in October 2014 he started his independent research career at the Institute of Chemical Research of Catalonia (ICIQ) within the CELLEX-ICIQ Starting Career Programme. In 2020, Prof. Suero was promoted to permanent ICIQ Group Leader.

In 2019, he received an ERC Consolidator Grant for the project "New Carbon Reactivity Rules for Molecular Editing."

➤ HEALTH  
➤ FINE CHEMICALS

## New reactivity rules for molecular editing

### EXPERTISE

- C-H/C-C Activation
- Carbyne chemistry

### APPLICATIONS

- Late stage functionalization of APIs

## Research Focus

The main scientific objective of Prof. Suero is to catalytically generate reactive carbon species not yet explored, and study their behavior towards carbon-hydrogen and carbon-carbon bonds. His goal is to discover new rules of reactivity of carbon, not only for the design and discovery of new chemical reactions, but also for its use to build molecular complexity. The group has been a pioneer in the catalytic generation of diazomethyl radicals as direct equivalents of monovalent carbyne species. This discovery clearly revealed the dual radical-carbene behavior of the carbynes, and allowed the design of different disconnection strategies for the construction of chiral centers.

## Late-stage C-H functionalization reagents for chiral center sequencing

Prof. Suero has developed a new class of hypervalent iodine reagents for the photoredox diazomethylation of (hetero)aromatic substrates through the generation of carbynes, leading to the regioselective introduction of diazo functional groups in the reaction substrate. The diazo group can be further functionalized by using robust and well-known transformations to introduce molecular diversity.

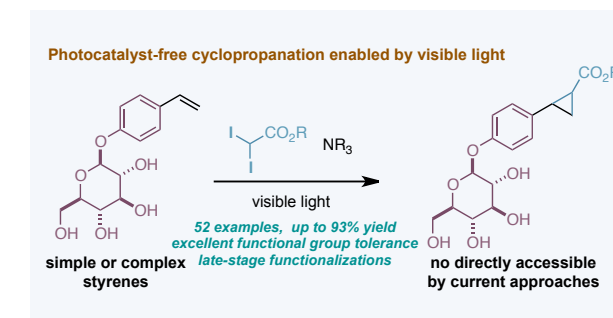
The hypervalent iodine reagents are stable, are suitable for the transfer of the diazomethyl group to an aromatic C-H bond mediated by visible light and a Ru(II) photosensitizer, under mild conditions, with excellent regioselectivity and exceptionally high functional group tolerance.

These features makes the technology tremendously suitable for the late stage functionalization of agrochemicals and drugs.

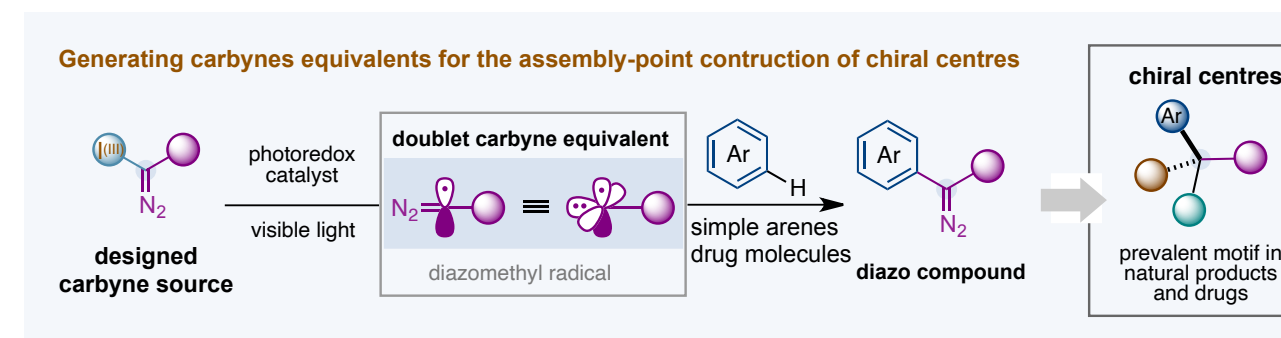
📄 Patents EP18702738/ US16/482,966 (granted): Diazomethylation reagent and process for using it

## Metal-free cyclopropanation reagent

Prof. Suero has developed a shelf-stable solid reagent for the metal-free photochemical synthesis of cyclopropanes from substrates incorporating a double bond conjugated to an aromatic or heteroaromatic group. The cyclopropanation takes place without photosensitizer or metal catalyst, has an excellent functional group tolerance and has a high chemoselectivity. The technology is extremely robust and has been proved on 52 different substrates, including heterocycles and biomolecules, with up to 93% yield for the cyclopropanation product. The reagent is an easily scalable and shelf-stable solid, particularly safe to use.



📄 Patent EP19382720 > Cyclopropanation method and reagent.







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