ICIQ

Institute of Chemical Research of Catalonia

Research collaboration with industry

Institució CERCA
Centres de Recerca de Catalunya

BIST
Barcelona Institute of Science and Technology

Index

CA *Catalysis*
RE *Renewable Energy*
NM *Nanoscience & Materials*

The Institute of Chemical Research of Catalonia

ICIQ started its research activities in 2004. During its first ten years, the institute has published more than 1400 scientific articles, 90% of them in chemical research journals ranked in the first quartile (the top 25% journals according their impact factor).

ICIQ hosts 19 research groups and up to October 2016, ICIQ has received 14 ERC Grants. In 2014 ICIQ was recognized as a "Severo Ochoa Centre of Excellence" by the Spanish Secretary of State for Research, Development and Innovation.

EXCELENCIA SEVERO OCHOA

ICREA

7 ICREA Research Professors

erc European Research Council

21 ERC Grants

An international leading institution in the field of chemistry committed to performing research at the frontiers of knowledge.

Our goal is to improve quality of life through chemical research.

ICIQ is committed to knowledge and technology transfer of ICIQ's research results to the chemical, pharmaceutical and energy industries. We also prepare the future generation of scientists by offering high-quality training to master and PhD students and postdoctoral researchers. Moreover, we care about engaging youngsters in pursuing chemistry studies.

Collaboration with Industry

13000 sqm
dedicated to R&D

310
PEOPLE

230
RESEARCHERS

- 8 % Group Leaders
- 34 % Postdocs
- 9 % Industrials postdocs
- 43 % PhD students
- 6 % Lab engineers

26 Laboratories

6 Laboratories
dedicated exclusively to technology transfer to industry

1 Computational laboratory

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

1. Joint Units with Industry
2. Contract Research Projects
3. Technology Portfolio
4. Technology Development Units

An essential part of ICIQ's mission is to have a positive impact on quality of life. In order to achieve this goal we collaborate with industry, as it has the power to transform our expertise and results into products and services that can reach society. We are strongly committed to improving the competitiveness of our industrial partners.

Joint Units with Industry

In our joint units with industry, one laboratory is dedicated exclusively to R&D projects for a single company.

ESTEVE-ICIQ Joint Unit

2009-2020
6-7 researchers working in the generation of new scaffolds for medicinal chemistry libraries

HENKEL-ICIQ Joint Unit

2010-2019
6-9 researchers working in new trigger reactions for high performance adhesives.

AICURIS-ICIQ Joint Unit

Since 2020
5 researchers working in medicinal chemistry.

Main characteristics:

- Full access to all ICIQ facilities and services.
- Scientific advice by selected group leaders.
- Unit manager in close contact with the company (or a company employee) to ensure optimal technology transfer.

Contract Research Projects

Our contract research projects are always related to the expertise of a research group or technology development unit in order to maximize added value.

The average project involves one post-doc 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).

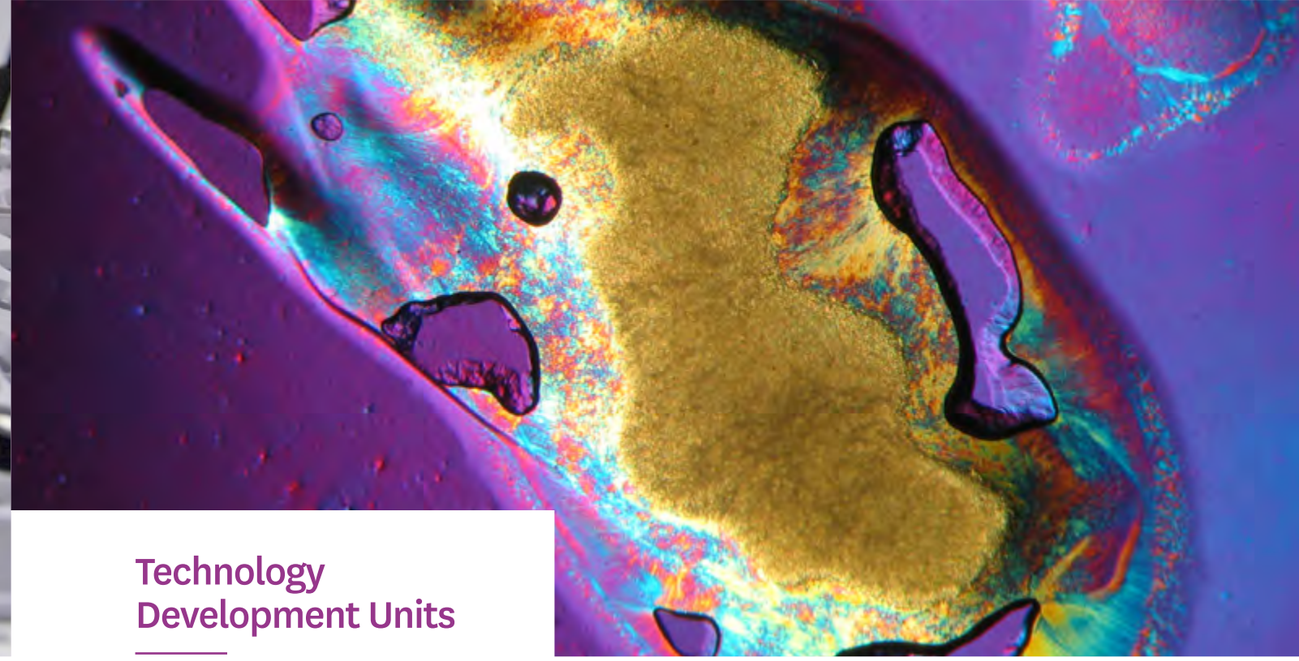
Examples of contract research projects in the fields of pharmaceuticals, bulk chemicals and polymers, including experimental and computational research approaches:

SYNLETT 2010, No. 12, 1873-1877
Collaboration with **ESTEVE**
with Prof. M. Pericàs group

ChemCatChem, 2015, 7, 928-935
Collaboration with **REPSOL**
with Prof. N. López Group

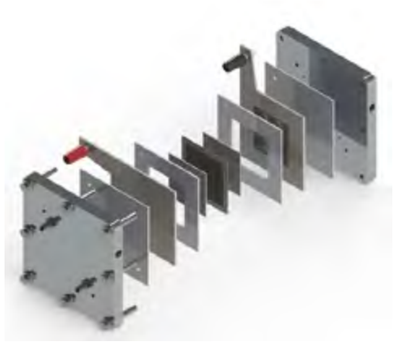
Ind. Eng. Chem. Res., 2012, 51, 16165-16170
Collaboration with **BAYER MaterialScience (now Covestro)**
with Prof. A Vidal Group

Macromolecules, 2015, 48, 8197-8207
Collaboration with **SABIC**
with Prof A. Kleij



Technology Portfolio

We protect those results of industrial interest, in order to have a strong basis for co-development and subsequent license to an industrial partner. Our licensing strategy is flexible and is adapted case to case depending on the technology, the industrial partner's objectives and the main technological/ regulatory milestones in the development process.



↑ PEM cell (layer by layer) for hydrogen production at high potentials

CSOL

CSOL is ICIQ's valorization unit. Its goal is to further develop our in house technologies and facilitate their transfer to an industrial partner. Development activities include reproducibility and stability studies, initial scale up, etc.

↘ www.catalytic-solutions.com

↓ CSOL also prepares catalysts and reagents developed by ICIQ groups and makes them available to the scientific community and industry.

Technology Development Units

Crysforma

Crysforma provides complete scientific support for the discovery, analysis and scale-up of polymorphs, hydrates, amorphous phases, 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.

↘ www.crysforma.com

Ertflow

Ertflow works in immobilized catalysts and process development to change from batch to flow processes in pharma, biotec and fine chemicals.

↘ www.ertflow.es

CSOL Catalytic Solutions

CRYSFORMA

ERTFLOW

Core facilities

ICIQ's Research Support Area provides the scientific instrumentation and personnel to assist ICIQ research groups, technology development units and joint units in the projects undertaken in collaboration with industry. Our staff members are experts in different characterisation techniques. ICIQ hosts the following dedicated units/laboratories:

- X-ray Diffraction
- High Resolution Mass Spectrometry
- Nuclear Magnetic Resonance
- Chemical Reaction Technologies
- Chromatography, Thermal Analysis & Electrochemistry
- Heterogeneous Catalysis
- Spectroscopy and Kinetics
- Photophysics
- Glass Blowing Workshop
- Mechanical Workshop / 3D Printing

Cutting-edge instrumentation and highly specialised personnel

Research Groups

Research topics

Catalysis

Renewable Energy

Nanoscience & Materials

ICIQ's research groups focus their work on two main areas: **Catalysis**, which aims to discover new and useful chemical processes of industrial interest, shorter and more efficient routes to bioactive substances, and use CO_2 and biomass as feedstock for the chemical industry; and **Renewable Energy** from the chemical point of view, focusing on the generation of renewable hydrogen and other fuels, as well as the development of more efficient thin film photovoltaic devices.

Prof. Pau Ballester

Nanoscience & Materials | Catalysis

EXPERTISE

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

APPLICATIONS

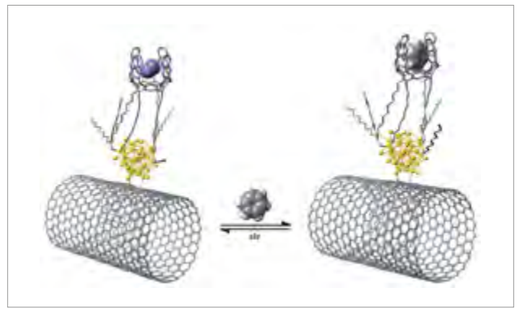
- Detection/quantification of small molecule compounds

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.

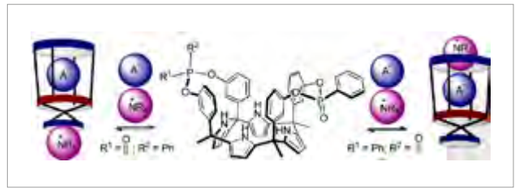
In 2004, he took a position as **ICREA** (Catalan Institution of Research and Advanced Studies) Research Professor and he joined the **ICIQ** as a group leader. During his time at ICIQ he has been involved in research collaborations with the pharmaceutical group **Esteve**.

Detection and quantification of small molecule compounds

We design and synthesize molecular containers that selectively bind a target compound, where this binding event causes a change that can be quantified. Then, in collaboration with other research groups, our molecular receptors are integrated into sensing devices. Two commercially relevant applications that we have developed in the last few years are a resistive sensor for benzene detection in air, which offers high sensitivity and operates in continuous mode (not possible with previous detection methods) and a potentiometric sensor for creatinine in urine and plasma samples.



↑ Benzene sensor based on a resorcin[4]arene molecular sensor, self-assembled onto gold nanoparticles which are attached to the carbon nanotubes that form the electrode.

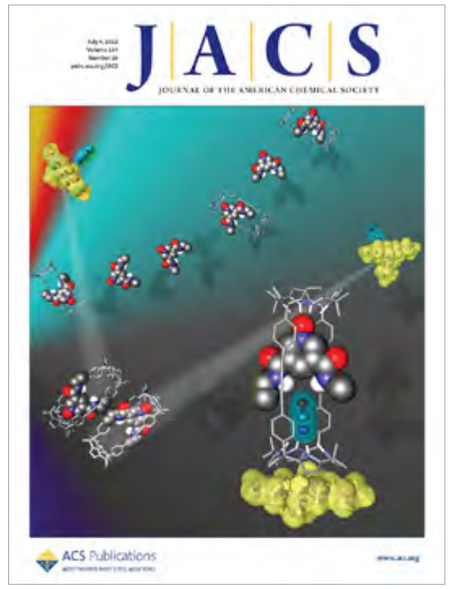


↑ Multitopic receptors for the recognition of ion pairs.

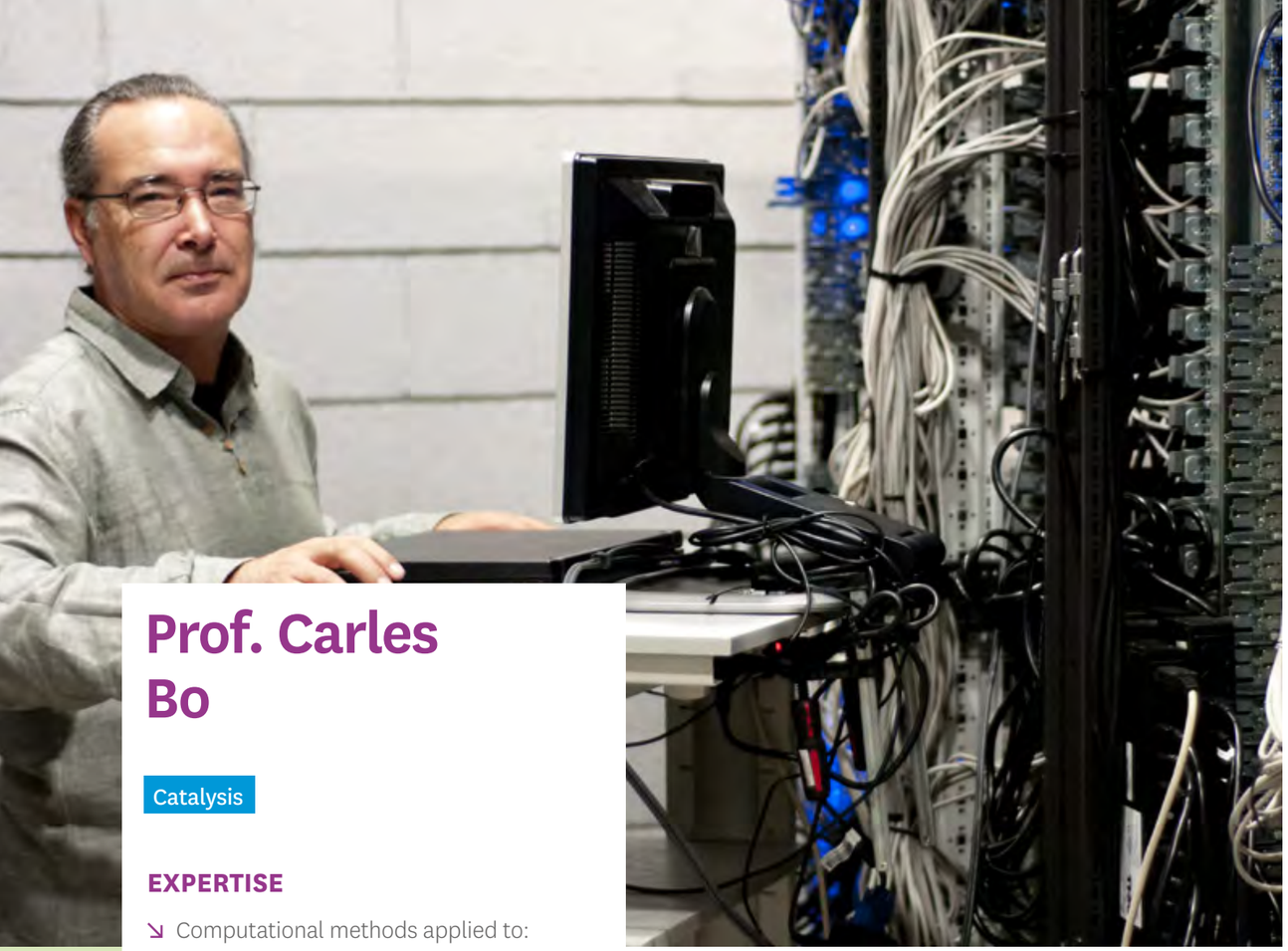
Molecular self-assembly for the construction of complex architectures

Other topics of interest

We also investigate the changes in the chemical behaviour of catalysts encapsulated within molecular containers (supramolecular catalysis). Another topic of interest is molecular machines, in particular rotaxanes, where two interlocked molecules (rotor + axis) present a translational movement of the rotor molecule along the axis molecule.



↑ Journal cover: "Polyatomic Anion Assistance in the Assembly of [2] Pseudorotaxanes" J. Am. Chem. Soc., 2012, 134, 10733-10736.



Prof. Carles Bo

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:
  - Homogeneous and enantioselective catalysts
  - Host-guest systems for detection, quantification and separation
  - Co-crystal formation, other non-covalent interactions

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** (Strasboug, France) several times and carried out research work under the guidance of Profs. Dedieu and Bénard. Later he spent 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 where he leads a research group on computational chemistry.

Homogeneous catalysis

We use our 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.

As an example we have presented a new QSAR method for correlating structure-activity aimed at predicting the enantiomeric excesses and absolute configurations of transition metal catalysed reactions. We applied this method to correlate activities and predict enantiomeric excesses (e.e.'s) in the asymmetric hydroformylation of styrene by Rh-diphosphane complexes.

↑ Journal cover: "SPOs as new ligands in Rh(III) catalyzed enantioselective transfer hydrogenation" Catal. Sci. Technol., 2011, 1, 401-407

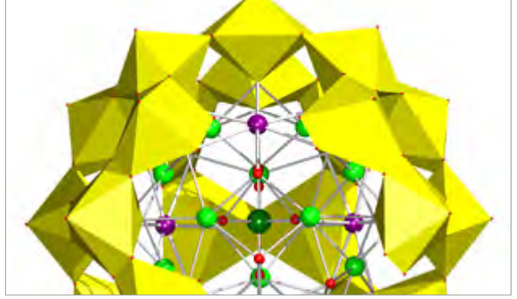
Big data management

Together with other ICIQ's computational groups, we have developed a new web interface, www.iochem-bd.org, designed to manage computational chemistry results and to facilitate data treatment, hierarchical storage and data mining.

In-silico studies at the service of catalysis

Polyoxometalates (POMs)

Using multi-scale computational protocols we have evaluated the electronic properties of POMs adsorbed on metal surfaces. We have also studied a new class of recently discovered Uranium derived POMs (Uranyl-peroxides).



↑ View of U28 with encapsulated $[Ta(O_2)_4^{3-}]$

Host-guest systems

These systems are very interesting for their sensing and separation properties, distinctive reactivity, etc. We applied DFT methods for determining structures, spectroscopic properties and reaction mechanisms within the host-guest complex. As an example of the latter, in collaboration with Ballester's group (ICIQ) we predicted that $[Rh(nbd)_2]^+$ (Nbd=Norbornadiene) could be encapsulated inside a resorcin[4]arene-based host, which modifies the normal outcome of nbd hydrogenation.

Prof. Antonio M. Echavarren

Catalysis

EXPERTISE

- Gold catalysis
- New catalytic methods based on the organometallic chemistry of transition metals
- Efficient synthesis of complex polycyclic molecules
- Gold-catalyzed cyclization of enymes

APPLICATIONS

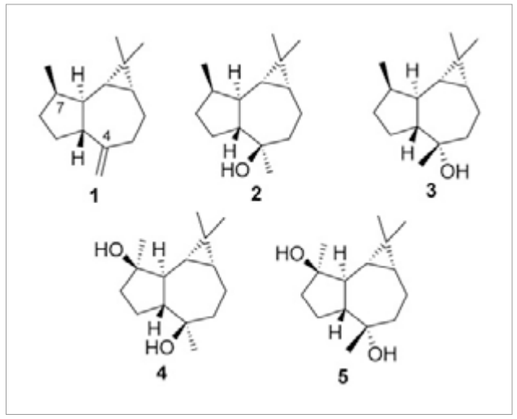
- Synthesis of natural products for health applications
- Synthesis of nanographenes for material science applications

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 of the **CSIC** since 2004.

In 2004, he joined **ICIQ** as Group Leader. In 2013 Prof. Echavarren was awarded an **ERC Advanced Grant** for the project "CATGOLD: Advancing Gold Catalysis. During his time at ICIQ he has been involved in research collaborations with the pharmaceutical group **Esteve**.

Gold catalysis applied to natural product synthesis

As part of our programme on the synthesis of natural products by gold(I)-catalyzed cascade processes, we completed the shortest total synthesis of three aromadendranes from a single precursor by means of a stereodivergent process. Aromadendranes are a family of natural compounds named after the main component in the essential oil from Eucaliptus trees. These compounds are widespread in plant species and are of interest because of their antifungal, antibacterial, cytotoxic and other biological activity.

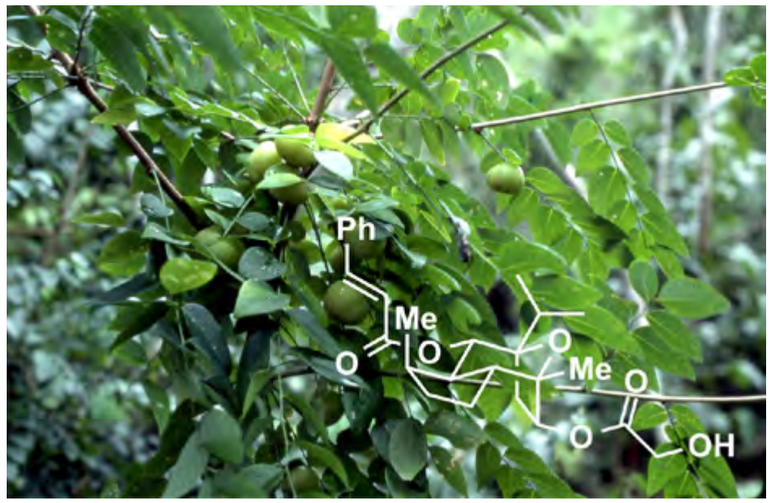


↑ Naturally occurring aromadendranes (-)-epiglobulol (3), (-)-4α,7α-aromadendranediol (4) and (-)-4β,7α-aromadendranediol(5) have been synthesized with 12, 17, and 15 % overall yields, respectively, from (E,E)-farnesol.

Organometallic chemistry for health and material science applications

Another success story is the synthesis of (-)-Englerin A analogs as anticancer compounds. Our 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 our synthesis we 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, and leukemia) and are moreover highly selective, which could potentially result in lower side effects.

↓ The natural compound (-)-Englerin A is present in the stem bark of the Phyllanthus engleri tree.



Prof. José Ramón Galán-Mascarós

Catalysis | Nanoscience & Materials | Renewable Energy

EXPERTISE

- Design and synthesis of water splitting catalysts
- Metal organic frameworks and coordination polymers
- Organic conductors and semiconductors

APPLICATIONS

- Renewable hydrogen generation from water and sunlight
- CO_2 capture and hydrogenation
- Smart materials for electronics

Prof. José Ramón Galán-Mascarós received his PhD in 1999 at the **Universitat de València** and then he performed 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.

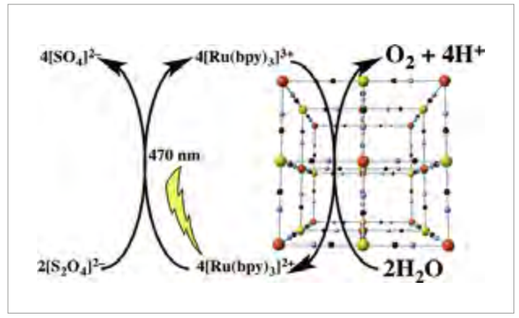
In 2009 he took a position as group leader at **ICIQ** and one year later he became **ICREA** (Catalan Institution of Research and Advanced Studies) Research Professor.

He has been awarded an **ERC Starting Grant** to develop his project "CHEMCOMP: Building-up Chemical Complexity into Multifunctional Molecule-based Hybrid Materials" and an **ERC Proof of Concept** for the project "HYDRER: A Solar-Powered Hydrolizer".

Stable and inexpensive catalysts for water splitting

With the aim of producing solar fuels, in particular hydrogen from water and sunlight, we design, synthesize and study new redox catalysts for water splitting with two main characteristics in mind: the stability and use of inexpensive earth abundant materials. We use two main approaches: catalysts based on polyoxometalates (POMs); and on transition metal hexacyanometalates which are isostructural to the pigment Prussian Blue(PBs). Moreover, we are working towards the integration of these catalysts into a prototype electrolyzers for their combination with renewable energy sources.

← Modified electrode containing the anchored Prussian Blue as WOC in an electrochemical cell for water splitting.



↑ Light-driven water oxidation with metal hexacyanometallate heterogeneous catalysts

Photomagnetic materials and bioinorganic models for energy applications

Composite materials with tailor-made properties

We are developing a variety of new multifunctional materials where the desired properties are incorporated by taking advantage of specially designed molecular building blocks. This powerful approach allows us to combine optical/electrical/chemical/structural/magnetic properties in the search for synergic features. For example, combination of switchable metal complexes with organic conducting polymers yields composite materials where conductivity can be tuned and controlled by external stimuli (light irradiation); or the combination of chiral amino acid derivatives with metal centers yields porous metal-organic frameworks with high porosity and selectivity for CO_2 separation from flue gas.

↓ Suspension of a bistable compound at 80ºC. Left: After heating to 80ºC. Right: After heating above 100ºC and cooling to 80ºC.

Prof. Arjan W. Kleij

Catalysis | Nanoscience & Materials

EXPERTISE

- Polymers, bulk and fine chemicals from CO_2 (CO_2 catalysis)
- Molecular self-assembly
- Use of salen ligands

APPLICATIONS

- Polymers, bulk and fine chemicals incorporating CO_2
- Composite and polymeric materials

Prof. Arjan Kleij received his PhD in Chemistry from the **Unviersity of Utrech**. He worked for more than three years at **Avantium Technologies** as a Project Leader in its pharmaceutical branch. 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 **ICREA** (Catalan Institution of Research and Advanced Studies) Research Professor.

At ICIQ, Prof. Kleij has been involved in a research collaboration with **Sabic**.

CO_2 as carbon feedstock

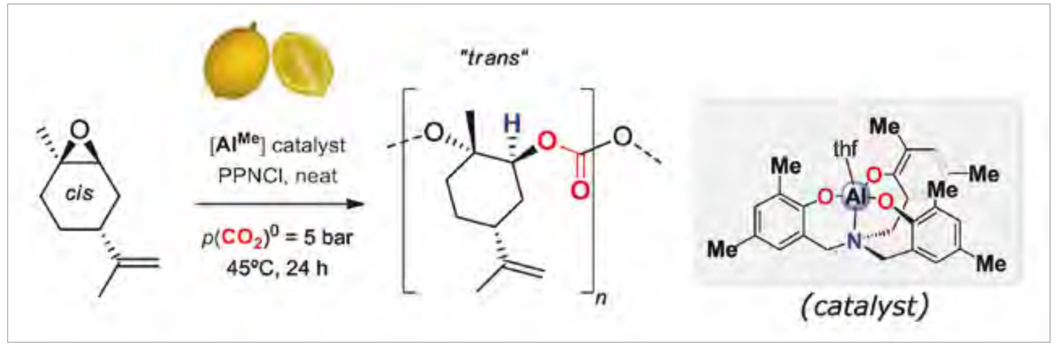
We design new catalysts for chemical reactions that use CO_2 as a building block to obtain polymers and other chemicals of commercial interest, such as pharmaceutical intermediates or gasoline additives:

- Polycarbonates, polyurethanes and other CO_2-based polymers (including with bio-based monomers).
- Cyclic organic carbonates.
- Oxazolidinones.

We aim at using cheap, non-toxic metals and mild conditions for these transformations.

Carbon dioxide valorization catalysis and renewable building blocks

Building blocks from biomass

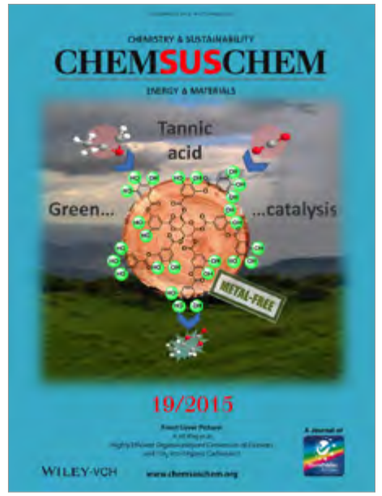


↑ (Bio)Polycarbonates based on Limonene Oxide

In addition to use of CO_2, another key objective of our research is the use of monomers and building blocks derived from biomass. We are particularly interested in using bio-renewable components to substitute Bisphenol A (BPA) in polycarbonates.

Other areas of expertise

We have also used our capabilities in catalysis, supramolecular chemistry and the use of salen ligands for other applications such as organocatalysis, synthesis of polymers from bio-renewable sources, stereoselective conversions and design of colorimetric methods to detect the presence of a target compound.



→ Highly Efficient Organocatalyzed Conversion of Oxiranes and CO_2 into Organic Carbonates. ChemSusChem 2015, 8, 3248-3254

Prof. Antoni Llobet

Renewable Energy | Catalysis

EXPERTISE

- Artificial photosynthesis
- Design of catalysts for water splitting (mainly Ru complexes)
- Redox catalysis using transition metal complexes
- Mechanistic understanding of reactions involving multiple e^-/H^+

APPLICATIONS

- Generation of renewable H_2 from sunlight
- Photochemical oxidation of organic substrates

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 and **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 till 1993, working with the groups of Prof. Arthur E. Martell and Donald T. Sawyer. From 1993 till 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.

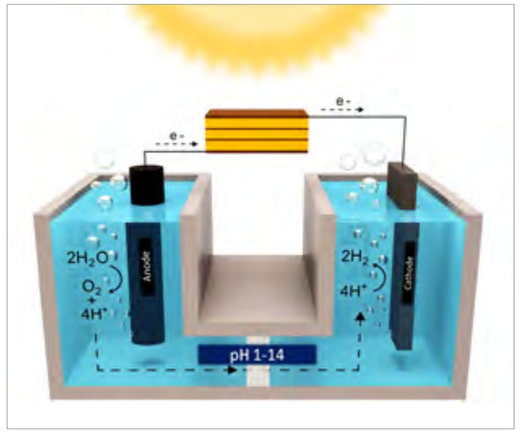
In 2006, Prof. Llobet was appointed as group leader at **ICIQ**.

Water splitting catalysts

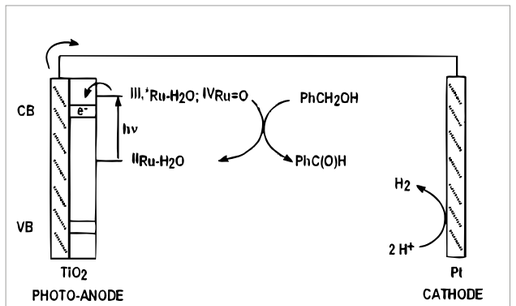
We are particularly interested in the catalytic oxidation of water to molecular dioxygen. The final objective of this route is the photoproduction of hydrogen from water and sunlight. Our main expertise is the design, synthesis and characterization of ruthenium complexes for artificial photosynthesis, although we are also working in other complementary approaches such as substituting Ru by Mn and modifying the ligands accordingly.

↑ Molecular ruthenium catalyst with water-oxidation activity comparable to that of photosystem II

Inspired by Nature: Artificial photosynthesis



↑ Water splitting device scheme



$$PhCH_2OH \xrightarrow{h\nu} PhC(O)H + H_2$$

← Proposed photo-oxidation scheme for organic substrated based on Ru complexes

Other topics of interest

We are applying our expertise in organometallic redox catalysts to the photochemical oxidation of organic substrates, selective chemical oxidation of organic substrates under mild conditions, or combining oxidative catalysis with molecular recognition in a supramolecular catalysis approach.

Prof. Julio Lloret-Fillol

Renewable Energy | Catalysis

EXPERTISE

- Artificial photosynthesis
- Water splitting

APPLICATIONS

- Renewable fuels
- Fine chemicals from renewable feedstocks

Prof. Julio Lloret-Fillol received his Ph.D 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 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**.

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** and he was appointed **ICREA** Research Professor.

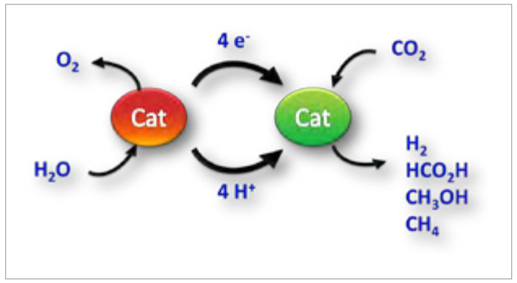
Artificial photosynthesis

Our group focuses its research on the design of new catalysts for a more sustainable chemistry through use of artificial photosynthesis schemes. The use of high throughput experimentation is integral to our research.

- Development of new methodologies to employ light as the driving force in reductive organic transformations, including synthetic methods to transform renewable feedstocks into elaborated chemical structures.
- Understanding the reaction of water oxidation, identified as one of the bottlenecks for the production of solar fuels.

Solar fuels production and new light-driven catalytic transformations of organic substrates

↓ Use of light as energy source to produce solar fuels.



← Light-driven organic transformations.

Prof. Núria López

Catalysis

EXPERTISE

- Computational methods applied to:
  - Heterogeneous catalysis
  - Metal-organic frameworks (MOFs)
  - Nanoparticles

APPLICATIONS

- Computational screening of heterogeneous catalysts
- Rational design of heterogeneous catalysts and optimization of heterogeneous catalytic processes
- Surface behavior simulation

Prof. Núria López got 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 her post-doc 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** to carry out the project "Bio2chem-d: Biomass to chemicals: Catalysis design from first principles for a sustainable chemical industry". In 2015 she got an **ERC Proof-of-Concept Grant** to develop the project "BigData4Cat: Big Data for Catalysis". At ICIQ Prof. López has been involved in research collaborations with industrial companies such as **Bayer MaterialScience** and **Repsol**.

Heterogeneous catalysis

The search for more active, selective, cheap and environmentally friendly heterogeneous catalysts has traditionally been performed by means of trial-and-error methods, which are time-consuming and expensive. Due to the evolution of computational methods, nowadays it is possible to obtain accurate models based on atomistic first principles to determine descriptors that control the relevant chemical properties, and use them to carry out a computational screening of potential heterogeneous catalysts, reducing enormously the amount and cost of the subsequent experimental research.

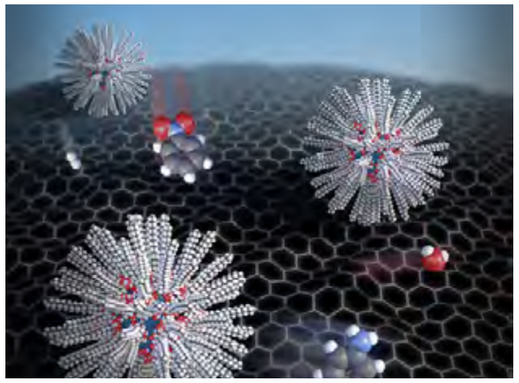
Both the analysis of reaction networks, activity and selectivity issues as well as the final tests on the stability of potential catalysts are fundamental to computationally screen potential heterogeneous catalysts for a given transformation.

↑ Journal Cover: "A Stable Single-Site Palladium Catalyst for Hydrogenations" Angew. Chem. Int. Ed., 2015, 54, 11265-11269

Atomistic simulation addressed to develop more rationalized heterogeneous catalysts

Other topics of interest

Nanoparticles: As catalytic activity in heterogeneous catalysis strongly depends on the number of available active sites, nanoparticles, with their high surface to volume ratio, show an enhanced activity. We study the effects of surfactants on the shape of the nanoparticles and their selectivity as catalysts.



↑ Supported hybrid platinum nanoparticles

Metal Organic Frameworks (MOFs): We also explore the effect of the solvent in complex systems such as Metal Organic Frameworks(MOFs).

Within the framework of the BIGDATA4CAT project, we are developing the io-Chem-BD platform together with other ICIQ's computational groups. A multi-headed tool aimed to parse, organise, publish and analyse results of computational chemistry research projects.

Prof. Rubén Martín

Catalysis

EXPERTISE

- Selective activation of inert bonds (C-C, C-H, C-O and CO_2)
- CO_2 as a building block for fine chemicals
- Transition metal-catalyzed cross-coupling reactions

APPLICATIONS

- Synthesis of fine chemicals
- New scaffolds for medicinal compound libraries

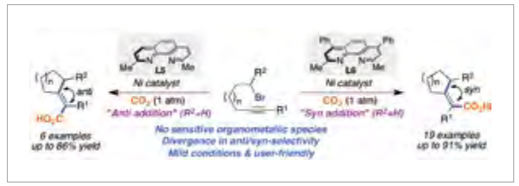
Prof. Rubén Martín received his Ph.D in 2003 at the **Universitat de Barcelona**. In 2004 he moved to the **Max-Planck-Institut für Kohlenforschung** as a Humboldt postdoctoral fellow with Prof. Alois Fürstner, where he worked on the application of novel iron catalysts for cross-coupling and Alder-ene type reactions. In 2005 he undertook further postdoctoral studies at the **MIT** with Prof. Stephen L. Buchwald, where he developed new synthetic strategies for metal-catalyzed C-C and C-N bond-forming reactions.

He joined **ICIQ** in 2008 and in 2011 he was awarded and **ERC Starting Grant** for the project 'FUNCBONDS: Chasing a Fundamental Challenge in Catalysis: A Combined Cleavage of Molecules'. In 2016 he received an **ERC Proof-of-Concept Grant** to develop the project "Catalytic reductive carboxylation of unactivated olefins with carbon dioxide." Prof. Martín is also an **ICREA** Research Professor. At ICIQ he has been involved in research collaborations with the pharmaceutical group **Esteve**.

CO_2 as a building block for fine chemicals

Carbon dioxide is abundant, inexpensive, non-flammable and attractive as an environmentally friendly chemical reagent. Our group is working on Ni-catalyzed CO_2 activation for the preparation of carboxylic acids, a very common motif in bioactive compounds and other compounds of industrial interest.

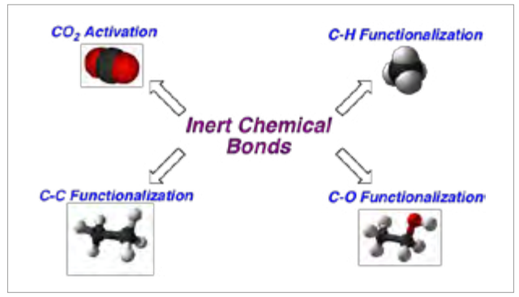
As an example of our work, we have developed a user friendly Ni-catalyzed reductive cyclization/carboxylation of unactivated alkyl halides with CO_2. In contrast to other syn-carbometalation techniques that use stoichiometric, well-defined, and in many cases air-sensitive organometallic compounds, our methods does not require the use of sensitive compounds, while having excellent chemoselectivity profile, and a divergent syn/anti selectivity pattern that can be easily modulated by the ligand backbond or the substrate utilized.



↑ Catalytic cyclization/carboxylation of unactivated alkyl halides with CO_2

Other topics of interest

We are also interested on the metal-catalyzed, selective activation of other relatively inert entities of great significance, such as C-H bonds, C-C bonds and C-O bonds, as these motifs rank among the most widespread and fundamental linkages in organic chemistry.



↑ Selective activation of inert entities of great significance

New catalytic methods for the synthesis of relevant molecules through the activation of inert entities

↑ Journal cover: "Ni-Catalyzed Reduction of Inert C-O Bonds: A New Strategy for Using Aryl Ethers as Easily Removable Directing Groups" J. Am. Chem. Soc. 2010, 132, 17352-17353

Prof. Feliu Maseras

Catalysis

EXPERTISE

- DFT and DFT/MM methods
- Computational chemistry applied to:
  - Homogeneous and enantioselective catalysis
  - Modelling of bioinorganic molecules

APPLICATIONS

- Reaction optimization

Prof. Feliu Maseras obtained his doctoral degree in Chemistry at the **Universitat Autònoma de Barcelona** (UAB). He spent two years working with Prof. Keiji Morokuma at the **Institute for Molecular Science** in Japan and two more working as Research Associate with Odile Eisenstein in **Université de Montpellier**. In 1998 he obtained tenured position as Associate Professor at the **UAB** and in 2004 he moved to **ICIQ** as group leader.

He was mentioned in the **Nobel Foundation**'s website as one of the important contributors to 2013 Nobel Prize in Chemistry for the development of multiscale methods. At ICIQ, Prof. Maseras has been involved in a research collaboration with **Henkel**.

Reactions for C-C bond formation

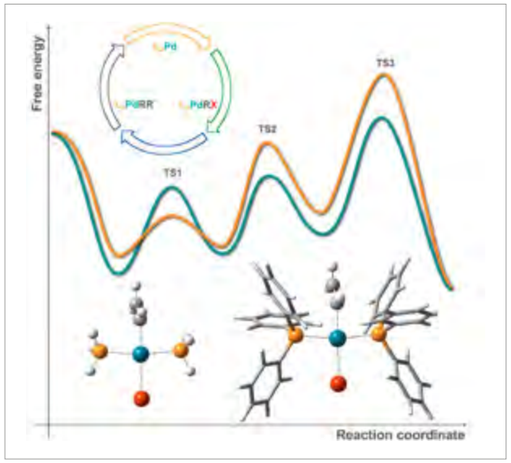
We focus on the study of the reaction mechanisms of cross-coupling reactions by using computational tools in order to understand and elucidate the effects governing their different steps. This mechanistic elucidation provides an opportunity to further expand these reactions to new substrates and to refine selectivity.

Activation of functional groups

Our group aims to study the activation of several functional groups, such as haloalkanes (C-X bonds, X=Cl, Br), amine groups and C-H bonds. Actually, we have contributed significantly to the mechanistic clarification of direct arylation of arenes catalysed by palladium, in collaboration with experimental researchers.

Big Data Management

Together with other ICIQ's computational groups, we have developed a new web interface, www.iochem-bd.org, designed to manage computational chemistry results and to facilitate data treatment, hierarchical storage and data mining.



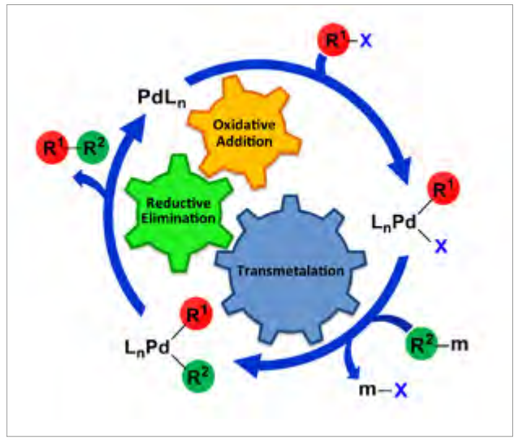
↑ DFT and DFT/MM calculations lead the mechanistic understanding of homogeneous catalysis.

Improvement of the efficiency of catalytic processes by computational methods

Enantioselective catalysis

In collaboration with other theoretical and experimental groups, we have carried out studies on several processes such as copper-catalyzed cyclopropanation, rhodium-catalyzed asymmetric hydrogenation and golden-catalyzed intermolecular hydroalkoxylation of allenes.

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.



↑ Computational chemistry clarifies the mechanism behind cross-coupling.

Prof. Paolo Melchiorre

Catalysis

EXPERTISE

- Organocatalysis
- Photo-organocatalysis

APPLICATIONS

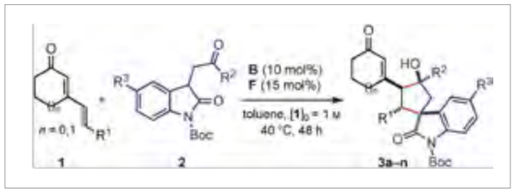
- Synthesis of natural compounds and compounds of high molecular complexity

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 centered 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 an Assistant Professor at the **Università di Bologna**.

In 2009, Prof. Melchiorre joined **ICIQ** as a group leader and an **ICREA** (Catalan Institution of Research and Advanced Studies) Research Professor. In 2011, he was awarded an **ERC Starting Grant** to carry out the project "ORGA-NAUT: Chemical Reactivity with Organocatalysis". In 2016 he received an **ERC Consolidator Grant** for the project "Light-Driven Asymmetric Organocatalysis" (CATA-LUX).

Molecular complexity

Cascade reactions are powerful tools for rapidly achieving molecular complexity since multiple chemical bonds are formed in a single synthetic operation. Their recent marriage to asymmetric organocatalysis has led to highly innovative strategies for one-step synthesis of stereochemically dense molecules. We have reported the first example of vinylogous organocascade catalysis, based on the use of a cinchona primary amine as an organocatalyst, allows the one step preparation of the highly enantio-enriched spirocyclopentaneoxindoles.



↑ Vinylogous cascade reaction

Enantioselective photo-organocatalysis

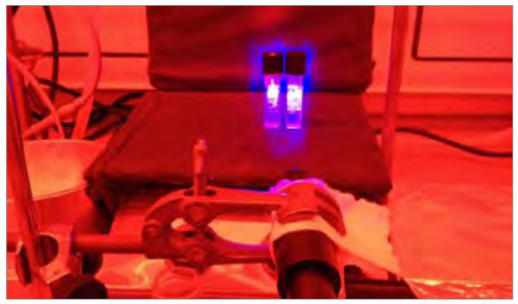
We have started a programme directed toward the use of solar energy to drive synthetic processes. Using light excitation to bring a molecule from its ground state to an electronically excited state can open new synthetic possibilities that cannot be realised using thermal activation.

↑ Asymmetric photochemical α-alkylation of aldehydes under enamine activation. Nature Chem. 2013, 5, 750-756.

→ Photo-Organocatalysis: Measuring the quantum yield.

Discovery of new enantioselective organocatalytic and photochemical processes

↑ Dr. Melchiorre and his team perform a photochemical reaction at the ICIQ rooftop.



Prof. Emilio Palomares

Renewable Energy

Nanoscience & Materials

EXPERTISE

- Design, construction and characterisation of organic and hybrid photovoltaic cells:
  - Dye-sensitized solar cells (DSSC)
  - Perovskite solar cells
  - Solar cells incorporating quantum dots
- Quantum dots (QD) with target properties and multilayered nanoparticles with embedded QD
- Molecular electronics

APPLICATIONS

- Photovoltaics
- Organic and hybrid LEDs
- Health/Diagnostic applications of quantum dots

Prof. Emilio Palomares received his PhD from **Universitat Politécnica de València**. He then enjoyed a postdoctoral stay at 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.

After two years at the Institut de Ciència Molecular of the **Universitat de València**. He joined **ICIQ** in April 2006 as a group leader. In 2007 he was appointed **ICREA** (Catalan Institution of Research and Advanced Studies) Research Professor. In 2008, he was awarded an **ERC Starting Grant** for the project 'PolyDot: 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'.

During his time at ICIQ he has been involved in research collaborations with **ACCIONA**.

Photovoltaic devices

The main interest of our group is the development of light-driven molecular devices (solar cells) where the functionalities of individual molecules are enhanced by their organisation into larger systems, which can be used to convert light into different types of energy sources.

We are also interested in the control of electronic properties in hybrid quantum dots/polymer materials for energy production. In this context we work on the synthesis of new molecular electronic components, such as semiconducting quantum dots and organic semiconductors, the design of self-organizing functional interfaces through supramolecular interactions and the evaluation of these systems for their applications as light-to-energy conversion devices.

Types of PV cells:

- Dye-sensitized solar cells
- Solar cells incorporating quantum dots
- Organic and hybrid photovoltaic devices
- Perovskite solar cells

We also work in the characterization of our in-house developed and third party photonic and photovoltaic devices. We have the capability of designing and assembling our own measuring equipment, which allows us to characterize different properties than those measured with commercial equipment.

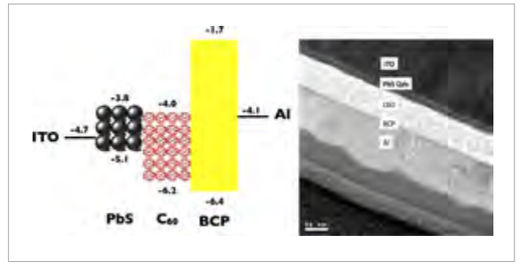
Novel materials for bio-applications

We work on the preparation and characterization of nanomaterials, which can be applied in nanomedicine for diagnosis and theragnosis, focussing our efforts on the synthesis of biocompatible nanomaterials with applications to measure biomarkers. As an example we have recently demonstrated that the rational design of a colour-coded biomarker allows for the accurate measurement of trypsin level in humans, a parameter used in the diagnosis of cystic fibrosis.

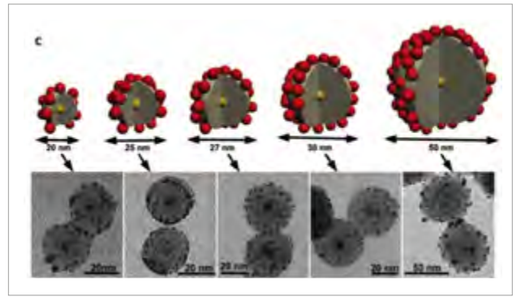
→ Photonic nano-objects for selective detection of bio-analytes composed by CdSe-QD@Si@AuNPs

Development of organic photovoltaic devices and application of quantum dots

↑ Windows of the EPFL's Convention Centre in Lausane. The red coloured glass windows are made with RK1, a new purely organic dye that Palomares' group has studied in the scope of the EU project "ADIOS-Ru" © EPFL/Alain Herzog.



↑ Energy level alignment in PbS/C60/BCP based hybrid solar cells.



Prof. Miquel A. Pericàs

Catalysis

EXPERTISE

- Catalyst design and immobilization
- Asymmetric catalysis in batch and flow
- Continuous flow chemistry
- Photo catalytic processes
- Magnetic nanoparticles: synthetic and applications

APPLICATIONS

- Enantioselective catalysts toolkit
- From batch to flow: thermal, catalytic and photocatalytic processes
- Sequential flow synthesis of libraries of enantiopure compounds
- Nanoparticles for selective trapping, delivery and catalysis

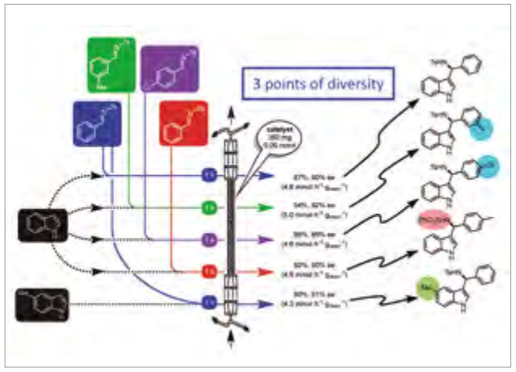
Miquel A. Pericàs obtained his doctorate in 1979 under the guidance of Prof. Fèlix Serratosa at the **Universitat de Barcelona** (UB). After postdoctoral studies at the Spanish research council (**CSIC**) with Prof. Francesc Camps, he joined the **UB** as Assistant Professor in 1980 and was promoted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

In June 2000, he was appointed to found the Institute of Chemical Research of Catalonia (**ICIQ**) where he now serves as Director and Group Leader. Prof. Pericàs is also involved in supporting technological innovation in industry, playing a central role in the creation of the **Centro de Tecnologías Avanzadas en Química Fina i Síntesis Asimétrica** (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** and **Henkel**. He has also promoted the creation of the ICIQ Technology Development Unit **ERTFLOW**.

Green approaches to catalysis for fine chemicals

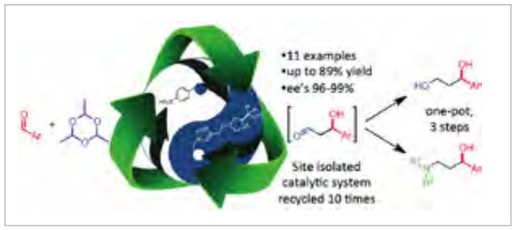
Supported catalysts and flow processes

Considering the inherent advantages of using continuous flow systems such as workup suppression and simplified scale-up, we have extended the applicability of our systems to the preparation of small libraries of enantioenriched compounds.



↑ Supported chiral phosphoric acid: Construction of a library in flow. Enantioselective continuous-flow production of a library of 3-indolylmethanamines. Productivities (mmol $h^{-1}gresin^{-1}$) are shown in parentheses.

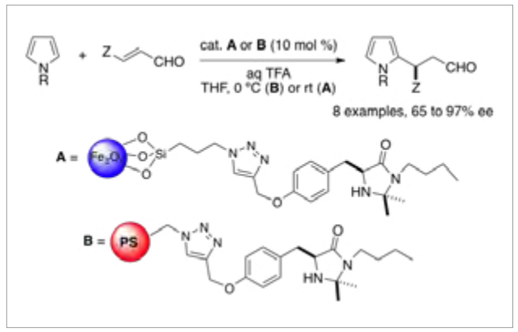
Acidic and basic catalysts (incompatible in solution) can work synergistically thanks to the site isolation conditions generated upon immobilization. This "wolf-and-lamb" dual catalytic system has been applied to the preparation of enantiopure drug precursors showing high reusability (up to 10 times).



↑ Highly enantioselective cross-aldol reactions of acetaldehyde mediated by a dual catalytic system operating under site isolation.

Catalysts anchored on magnetic nanoparticles (MNPs)

Immobilizing a catalyst on MNPs allows its retrieval by simple magnetic decantation. In addition, a synergistic effect has been observed in cases where the nanoparticles and anchored ligand separately did not present catalytic activity. Moreover, we have prepared a toolkit of pre-functionalized MNPs where catalysts or sensors can be easily grafted.



↑ Heterogeneous MacMillan organocatalysts for asymmetric Friedel–Crafts alkylations. The PS-supported catalyst (B) showed higher catalytic activity and enantioselectivity, while the MNP-supported analog (A) showed higher recyclability.

Dr. Marcos G. Suero

Catalysis

EXPERTISE

↘ C-H Activation

New catalytic C–H functionalization strategies for chemical synthesis

Our group explores new reactivity concepts using catalysis and its applications in solving important synthesis problems. Particularly, we aim to develop new carbon-hydrogen bond functionalization strategies using innovative reactivity platforms that are based on the catalytic generation of novel species.

We also explore new functionalization methods of simple building blocks that could be used for the preparation of complex molecules and biologically privileged structural motifs. The intensive use of high throughput experimentation, which enables the rapid discovery and development of new chemical reactions is an integral part of our research.

Dr. 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**.

Dr. Mónica H. Pérez-Temprano

Catalysis

EXPERTISE

↘ C-H Activation

Development of new chemical transformations: From organometallic mechanistic studies to catalysis

We are interested in the fundamental understanding of relevant organometallic processes in the context of bimetallic catalysis and C-H activation using first row metals.

Our long-term goal is to provide critical information for the rational design and development of novel catalytic transformations.

Dr. Mónica H. Pérez-Temprano obtained her PhD in 2011 at the Institute CINQUIMA (**Universidad de Valladolid**). During 2009, she joined the laboratory of Prof. Lutz Gade at the **University of Heidelberg** as a PhD visiting student. After her PhD she moved to the **University of Michigan** to work with Prof. Melanie S. Sanford on the synthesis and reactivity of high-valent organopalladium complexes. During her stay at the **University of Michigan**, she received a two-years postdoctoral fellowship from the **Ramón Areces Foundation**. Dr. Pérez-Temprano joined **ICIQ** in October 2015.

ICIQ

Institute of Chemical Research of Catalonia

Institut Català
d'Investigació Química
Av. Països Catalans 16
43007 Tarragona (Spain)
Phone: +34 977 920 238
Fax: +34 977 920 224
www.iciq.eu

Contact persons:

Dr. Frédéric Ratel, IP Management
fredratel@iciq.es

Irene Puntí, Business Development
ipunti@iciq.es

Trustees:

Generalitat de Catalunya
Departament d'Economia i Coneixement

Universitat Rovira i Virgili

BASF We create chemistry

REPSOL

covestro

ESTEVE

Supported by:

Gobierno de España
Ministerio de Economía y Competitividad

Excelencia Severo Ochoa

Unió Europea
Fons Europeu de Desenvolupament Regional
Una manera de fer Europa

Fundació Privada CELLEX