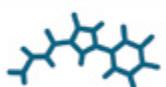




Follow us!

No. 16



ICIQ
Institut
Català
d'Investigació
Química



www.iciq.eu

Julio Lloret-Fillol appointed ICREA Research Professor



The Catalan Institution for Research and Advanced Studies ([ICREA](#)) is a foundation supported by the Catalan Government, which aims to recruit top scientists for the Catalan R&D system. [Prof. Lloret-Fillol](#) joined ICIQ in September 2014 and by being appointed as ICREA Research Professor he enters the group of ICIQ group leaders that are also on the ICREA programme: Professors Vidal, Ballester, Palomares, Melchiorre, Martín, Galán-Mascarós, Kleij and Muñiz.

Prof. Lloret-Fillol focuses his research on the design of new catalysts for a more sustainable chemistry through the use of artificial photosynthetic schemes. He works in the development of new methodologies to employ light as a driving force to produce reductive organic transformations and in the understanding of the reaction of water oxidation, identified as one of the bottlenecks for the production of solar fuels.

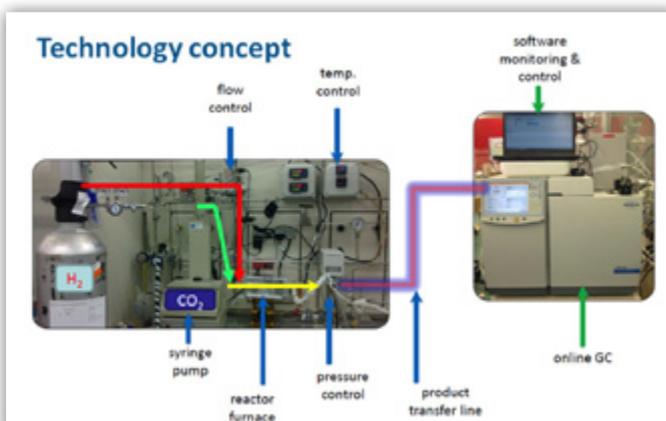
In 2015 he was awarded with an ERC Consolidator Grant for the project "Towards a Greener Reduction Chemistry by Using Cobalt Coordination Complexes as Catalysts and Light-driven Water Reduction as a Source of Reductive Equivalents" (GREENLIGHT-REDCAT).

Patent issued for Urakawa's work on CO₂ conversion to methanol

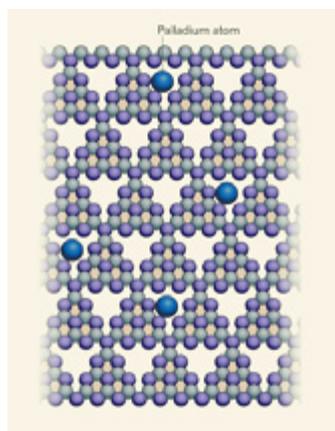
The patent related to the high-pressure hydrogenation of carbon dioxide to methanol and derivatives process developed by [Dr. Urakawa Research Group](#) at ICIQ has been issued by the [United States Patent and Trademark Office](#).

The work published on the [Journal of Catalysis](#) and highlighted in [Science](#), describes a continuous flow process for close-to-quantitative one-pass hydrogenation of CO₂ to methanol where conventional and commercial methanol synthesis catalysts are used.

The process developed by the Urakawa group allows a highly productive conversion of CO₂ to methanol achieving close to full one pass conversion. It also has the advantage that further reactions, such as DME production, can be successfully carried out in the same reactor. Bearing in mind that methanol production worldwide is expected to pass from 40 billion tons per year in 2009 to 80 billion tons/year in 2016, this process is a great step towards the methanol production from non-fossil resources.



Research on palladium catalysts highlighted in Nature



Six-fold cavity in the carbon nitride structure, which is crucial for confining palladium atoms in a stable manner.

The research developed collaboratively by the groups of [Prof. N. López](#) (ICIQ), [Prof. J. Pérez-Ramírez](#) (ETH Zurich) and [Prof. M. Antonietti](#) (Max-Planck institute of Colloids and Interfaces) on anchored palladium atoms acting as catalysts for hydrogenation reactions has been highlighted on the [News & Views section of Nature](#).

The article highlights that isolated palladium atoms on a solid support of carbon nitride can act as catalysts for hydrogenation reactions. The fact that very small amounts of palladium are needed is a crucial issue, since it is a scarce metal whose future availability is a cause of concern.

The work was published on *Angewandte Chemie International Edition* and selected for the journal cover.

Japan-Spain symposium on theoretical and computational chemistry

The ICIQ held on November 23-27 the [“ICIQ-FIFC Spain-Japan Joint Symposium on Theoretical and Computational Chemistry of Complex Systems”](#), co-organized between the Institute of Chemical Research of Catalonia and the [Fukui Institute for Fundamental Chemistry](#).



ICIQ-FIFC
Spain-Japan Joint Symposium on
Theoretical and Computational Chemistry of Complex Systems

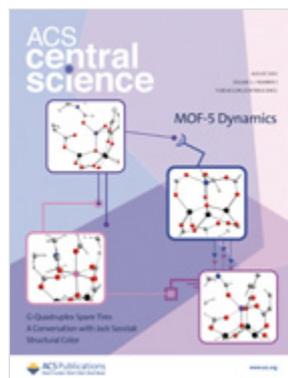
Computational chemistry is applied to the study of a variety of chemical processes with the goal of understanding reaction mechanisms and applying this knowledge to the design of more efficient processes. It can also be applied for predicting the behaviour of molecules or systems that have not yet been prepared in the laboratory and thus assist in more effective design thereof.

Journal Covers



A Stable Single-Site Palladium Catalyst for Hydrogenations

Angew. Chem. Int. Ed., **2015**, 54, 11265-11269. G. Vilé, D. Albani, M. Nachttegaal, Z. Chen, D. Dontsova, M. Antonietti, N. López, J. Pérez-Ramírez



Dynamic DMF Binding in MOF-5 Enables the Formation of Metastable Cobalt-Substituted MOF-5 Analogues

ACS Cent. Sci., **2015**, 1, 252-260. C. K. Brozek, V. K. Michaelis, T.-C. Ong, L. Bellarosa, N. López, R. G. Griffin, M. Dincă



Gold-Catalyzed Reactions via Cyclopropyl Gold Carbene-like Intermediates

J. Org. Chem., **2015**, 80, 7321-7332. R. Dorel, A. M. Echavarren

Many awards to many ICIQ group leaders

Madrid, Nov. 20th- The Spanish Royal Society of Chemistry (RSEQ) bestowed Research Excellence Awards on professors Núria López, Kilian Muñiz and Rubén Martín. They received the *Premio a la Excelencia Investigadora* for their scientific achievements in the last five years.

The RSEQ also awarded Julio Lloret-Fillol with one of the *Premios a Jóvenes Investigadores* for his promising leadership in the field of fuels production and new light-driven catalytic transformations of organic substrates. He received the award during the “Simposio de Jóvenes Investigadores” held in Barcelona on November 3-6, 2015.



From left, professors Pericàs, Muñiz, López and Martín.

Extraordinary PhD students

The *Universitat Rovira i Virgili (URV)* has awarded five ICIQ doctors with the *Premi Extraordinari de doctorat* for the excellent work done during their PhD studies.



Giulia Bergonzini, for her thesis entitled “Assessing the Versatility of Organocatalysis as a Strategy for Enabling Novel Asymmetric Transformations” and developed under the supervision of Prof. Paolo Melchiorre.



Laura Osorio, for her thesis entitled “Rational approaches to the control of molecular function: from catalysis to self-assembly” and developed under the supervision of Prof. Miquel A. Pericàs.

News in brief

Thesis: Drs. Lorenzo Mognon, Andrey Konovalov, Mattia Silvi, Daniel Fernández-Pinto, Xavier Sanz, Xueqiang Wang, José M. Marín Beloqui, Alba Matas, Dolores Melgar, Irina Sagamanova and David Bastida, predoctoral students at ICIQ have defended their PhD thesis. They were all awarded the highest honours for their work.

Honoris Causa Prof. Julius Rebek (Scripps Research Institute and member of the ICIQ Scientific Advisory Board) was invested *Doctor Honoris Causa* by the Universitat Jaume I (Alacant) for his achievements in the field of supramolecular chemistry.



ICREA Conference Professors Pau Ballester (ICIQ) and Chiara O'Sullivan (URV) are leading the organization of the “ICREA Conference on Functional Molecular Nanocontainers”. It will take place at CaixaForum Tarragona from October 17th to the 20th, 2016. We'll keep you posted!



Carlo Cassani, for his thesis entitled “Aminocatalytic Functionalization of Carbonyl Compounds: A Powerful Strategy for Enantioselective Reaction Development” and developed under the supervision of Prof. Paolo Melchiorre.



Laia Pellejà, for her thesis entitled “Exploring Novel Dye Concepts in Dye Sensitized Solar Cells” and developed under the supervision of Prof. Emilio Palomares.



Sara Goberna, for her thesis entitled “Novel Molecular Catalysts for Water Oxidation: Towards Artificial Photosynthesis” and developed under the supervision of Prof. Jose-Ramón Galán-Mascarós.

Face to Face with Ana Moore



Ana Moore is Regents Professor at the Arizona State University. Her research interests center on artificial photosynthesis with an approach that is mimicry of the steps used by nature to convert solar energy into chemical potential. Prof. Moore was one of the invited speakers of 'Lights on Chemistry' -the symposium organized at ICIQ last October- when we had the occasion to interview her.

■ **When did you decide to become a scientist and why?**

I realized I liked sciences when I was in school. Then, in college I discovered organic chemistry and I loved it. At 19 I worked as assistant teacher in the laboratory and I also loved it so, I kept that way.

■ **What do you like and enjoy the most in your job?**

What I like most of the research is to do things that nobody has done before. I could retire but I love working on research. I love it when I raise a hypothesis with the students and when we go to the lab we found that it works. It doesn't happen always but when it does it is very satisfying.

■ **Which are the greatest achievements in your career so far?**

I especially remember when I was in Paris working on the building of artificial photosynthetical reaction centers. When the one I had prepared worked as we had expected I was very satisfied. I think that it was probably the first of these systems that worked properly.

■ **From your point of view, what are the most important areas in which funding should be spent on?**

I could not choose between basic or applied research because without the former it is not possible to reach the second. Nowadays it is difficult to finance a project that has no connection with the industry. But we have to keep in mind that most of the times it is not possible to make an immediate transition.

■ **Could you give a piece of advice to young researchers who want to become excellent researchers in their fields?**

They have to find something they really like and think they are going to spend their life working on it. There are many things to do and the work never ends. So, it is very important to work on a field of research you like.

■ **We see many women studying chemistry at University; however, we do not see that many women working as researchers or academics. Why do you think that happens?**

There are several reasons but I think the most important are children, the difficulty of reconciling work and family life. It becomes easier if the partner contributes 50% of the time, but research centres also have to do their part. Facilities such as daycare centres would help.

■ **What do you do in your spare time (if you have any)?**

Taking care of my dog and reading are my hobbies.

Proust Questionnaire

A chemical element: *Silver.*

Favourite scientist: *Linus Pauling, for obvious reasons.*

Your favourite invention: *Computers.*

If you had not been scientist... *I would have been a teacher.*

Favourite destination: *The mountains.*

A book: *One hundred years of solitude.*

A movie: *The African Queen.*

A dream: *I wish I had more time to see more of my grandchildren.*

Science is... *knowledge and a way to provide a good life for people and help preserve the planet.*

Stand-up chemistry

Ignacio Funes, PhD student in the Maseras group, won the first prize of the “*Vols saber què investigo?*” (Want to know what I’m investigating?) contest organized by the Universitat Rovira i Virgili (URV). The contest was held at Teatre Bartrina (Reus) on November 17th, and it counted with the participation of six other contestants. Ignacio did not only win the jury’s 1st Prize (€700) but he also received the audience’s 1st Prize.



Ignacio receives the diploma from the Rector of the URV

Ignacio delivered a real funny 5-minute monologue entitled “*Rompamos el agua*” (Let’s split water”) to enlighten the audience about the importance of catalysts to split the water into oxygen and hydrogen and then use the H₂ as a fuel. After his monologue the jury complimented him: “You have no shame” and “If you were a better reggaeton dancer you would get extra points!” What was clear is that Ignacio honoured his surname.

[Video of Ignacio’s monologue](#)

Career development

As part of the Research Support Area training programme, Dr. Jordi Benet-Bucholz delivered the seminar “Crystallization Protocol to Obtain Single Crystals” on December 1st, ICIQ Auditorium. The aim of this seminar was to explain different techniques to obtain single crystals of the compounds. At the end of the seminar a few crystallization experiments were performed. More than 100 PhD and postdoctoral researchers were there!



Young researchers

They are young and chemists. A bond that augurs a promising future. More than 140 PhD and postdoctoral students and researchers gathered in Barcelona in the frame of the “[Young Researchers Symposium XII of the Spanish Royal Society of Chemistry – Sigma Aldrich](#)” (November 3-6, 2015). A conference for researchers under 40 years-old representing all areas of the chemistry spectra.

ICIQ has contributed a great deal to the organisation and development of the symposium. Prof. Julio Lloret-Fillol was member of the symposium’s scientific committee, and his PhD students Carla Casadevall and Arnau Call, were part of the organizing committee. As for the symposium’s programme, Prof. Lloret-Fillol and Prof. Ruben Martin, both ICIQ group leaders, delivered a lecture; Arnau and Carla gave oral communication; Cayetana Zárata, received the Suschem-JIQ award and Prof. Lloret-Fillol got the Premio Sigma-Aldrich a Jóvenes Investigadores RSEQ.



Family picture of the organising committee

IoChem-BD

Moisés Àlvarez and Stefano Serapian (Bo group) presented the ioChem-BD platform to potential users in the framework of the ICIQ-FIFC Spain-Japan Joint Symposium on Theoretical and Computational Chemistry of Complex Systems.

The [ioChem-BD platform](#) is a multi-headed tool aimed at managing large volumes of computational chemistry results from a diverse group of already common simulation packages.



Moisés Àlvarez (right) and Stefano Serapian during the presentation.

Mónica Pérez-Temprano, ICIQ group leader



Dr. Pérez-Temprano (center) with Dr. Sara Martínez de Salinas (postdoc) and Jesús San José (PhD student).

■ How have been these first two months in the ICIQ?

Intense, very intense. There are many things to bear in mind: finding the right people, setting up a laboratory, writing projects. When you're doing research you're too focused on your training but when you're a group leader there are many other things to do. It's very exciting but it's necessary to find the balance.

■ What are your expectations?

To do a good job and teach students everything I can. It is one of my objectives, prepare them for the next step, which I think is very important and in general is a step that is overlooked. Here we are in a privileged place and it's important to take advantage of what we have. The goal is to do our best and match the trust we have been given.

■ Which research will you do at ICIQ?

So far I've been very focused on basic science but I think after the postdoc I'm prepared to go a step further. I'm very influenced by the research I have done but I want to leave my comfort zone and go further. I want to carry out two major projects. One is based on bimetallic catalysis and the other in the activation of C-H bonds using earth-abundant transition metal. The main goal is to obtain fundamental knowledge for the rational development of new catalytic processes.

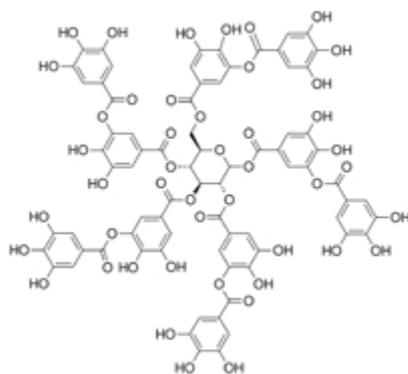
■ How do you see the relationship between science and society?

The perception of science is very different in Spain than in countries such as Germany or USA. In those countries science is seen as an important part of life, something that helps to improve our lives and also scientists are seen as intelligent and hardworking people that work to improve our lives. From my point of view in Spain there are two factors that penalize scientists: One is related to chemistry in particular, people associate chemistry with negative things such as bombs or toxicity and the other is that people don't value the effort you do. They think that it isn't worth working so much. It is not valued.

■ What do you think should be done about it?

We should give more importance to communication and outreach. In the USA many scientists go to schools, they do interviews in non-specialist magazines, etc. We need that visibility and show people that we are much more than people locked in a laboratory.

Sustainable preparation of organic carbonates



Chemical structure of tannic acid

Organic carbonates are compounds of industrial interest. In the last decade, highly efficient methods for the preparation of these carbonates using CO₂ as a carbon source have

been developed. These methods most often involve the use of catalysts that include metals, which may represent a health problem in case the presence of traces of particularly toxic metals in the final product exceeds the allowable limits.

In this context, Prof. Arjan Kleij research group has developed a new catalyst system based on a naturally occurring and fairly inexpensive molecule (tannic acid), which shows excellent catalytic reactivity at exceptionally low loadings for the preparation of organic carbonates using CO₂ as a carbon source. The catalyst system represents an attractive and sustainable alternative to the catalysts that incorporate metals in their structure. The work has been published in [ChemSusChem](#) and selected for its cover.

Little scientists

The “*Química en Família*” workshop gathered children between the ages of 4 and 12 to experience what chemistry is about. The experiments prepared by Dr. Laia Pellejà, science outreach officer at ICIQ, showed how a polymer absorbs water in diapers; how vitamin C is also useful to erase texts written with betadine; why you can't mix water containing different quantities of sugar; and a luminescent reaction performed in our dark lab. There were also two experiments related to the main subject of this year's workshop: Create your own perfume! We are sure everyone around the kids will enjoy their 5 to 10 essences perfumes they brought home.

[Link to video](#)



Experiment with different densities of liquid to make a column of colour.

No signs of recovery from craziness



Some of our “crazy students” in the lab.

The selection process for Crazy about Chemistry 2016 is finished. The 21 high-school students selected to carry out their studies at ICIQ will start coming to ICIQ by the end of January 2016.

“This is going to be the “Bojos” third edition. We are paying special attention to the experimental work and to the learning our students draw from our researchers' experience,” says Dr. Laia Pellejà, ICIQ's science outreach officer. Crazy about Chemistry is a year-long chemistry course funded by [Fundació Catalunya-La Pedrera](#). The course includes a mixture of theoretical lectures and hands-on experimental activities, covering 12 different chemistry topics, including the main chemical reactions.

[Link to video](#)

Journal Covers



Substrate Activation in the Catalytic Asymmetric Hydrogenation of N-Heteroarenes

Eur. J. Org. Chem., **2015**, 5293-5303.

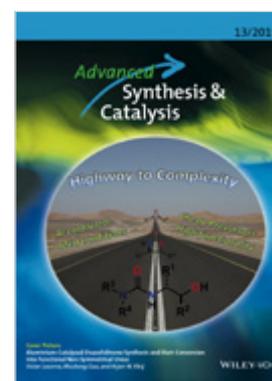
B. Balakrishna, J. L. Núñez-Rico, A. Vidal-Ferran



Highly Efficient Organocatalyzed Conversion of Oxiranes and CO₂ into Organic Carbonates

ChemSusChem, **2015**, 8, 3248-3254.

S. Sopeña, G. Fiorani, C. Martin, A. W. Kleij



Aluminium-Catalysed Oxazolidinone Synthesis and their Conversion into Functional Non-Symmetrical Ureas (*BACK COVER*)

Adv. Synth. Catal., **2015**, 357, 2849-2854.

V. Laserna, W. Guo, A. W. Kleij

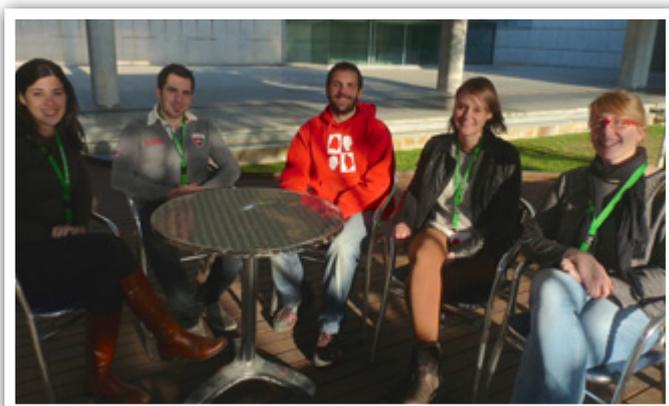
Christmas

Institute of Chemical Research of Catalonia (ICIQ)
 Av. Països Catalans 16, 43007 Tarragona (Spain)
 Phone +34 977 920 200



Happy Holidays!

Empleo Joven



From left, Blanca (Projects Management), Xavier (CELLEX-HTE lab), Dídac (CSOL), Àfrica (Crysforma) and Alba (ERTFlow).

Thanks to the MINECO “Programa Empleo Joven” ICIQ has the opportunity to incorporate five people to the institute who will work during two years in different units while receiving specific training according to the proposals approved.

Picture



From left, Núria, Bea, Paula, Elena and Sara

Why this picture? Because we had a blank spot, it's Friday afternoon and we came up with the idea of taking a picture of the people outside the communications office. They have interrupted the Christmas decoration of their work space to pose for this picture. We thank them for being so helpful (now and always) and nice!