newsletter
DECEMBER 2018
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ICIQ Institut Català d'Investigació Química
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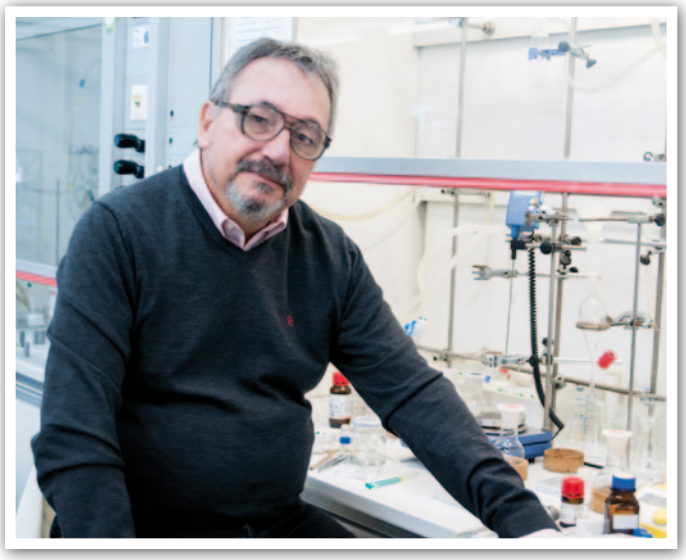
15 Years Already

"I was a player and now I'm also the coach," says Miquel A. Pericàs, ICIQ Director and Group Leader.



He has an office for each role. Today we are in his director's office, where a two-seater sofa, a metal coffee table with a few books on chemistry and architecture and a simple armchair create a warm space for a friendly chat. The space is dominated by a large colorful oil painting of an ICIQ laboratory to remind us that research in chemistry is the reason we are all here.

"When I was a child I wanted to be a doctor, a medical doctor. But when I realized that it could be a hard thing to endure when things go wrong, I decided to study chemistry. I ended up studying Chemical Engineering at Institut Químic de Sarrià and Chemistry at the University of Barcelona," he says.

As a player, he has devoted his efforts at developing a complete toolkit of polymer-supported and magnetic nanoparticle-immobilized catalysts. He wants to develop single-pass, catalytic and enantioselective flow versions of the most relevant processes for organic synthesis, contributing in this manner to a more sustainable practice of chemical synthesis.

"Flow chemistry is a very promising field of research," he says. "In fact, we created Ertflow, an ICIQ technology development unit, that based in flow processes is providing knowledge and technical support to many companies. This is an example of a successful knowledge transfer to industry. I'm happy and proud of the results so far."

Next year ICIQ celebrates its 15th anniversary. Since ICIQ started its research activities in 2004 the path has been one of growth. Highly regarded scientific papers, European projects (17 ERC grants received), research contracts and collaborations with various companies, and the institute's unique and successful formula of ICIQ-industry joint units.

But this year, ICIQ faced a disappointment when it did not obtain the critical 4M Euro Severo Ochoa grant.

"We're in a difficult situation now. We deserve better funding according to our capabilities and excellent performance throughout the years. Our model is based on having exceptional scientists and professionals, and this needs a proper budget," insists Pericàs. "One of the institute's programmes I'm most proud of is the Starting Career Programme. We have helped brilliant young researchers start an independent research career. This task is crucial for our science system."

As a coach, Professor Pericàs is optimistic about ICIQ winning this game.

"We have a scientific team of very good players. I must admit that team management is one of the most difficult tasks I've encountered as a director. Sometimes you make a decision you think is the right one and it is not understood. But I have confidence in ICIQ researchers and all of the staff pushing to keep ICIQ at the top. And we must not forget that when you're playing well, you end up scoring."

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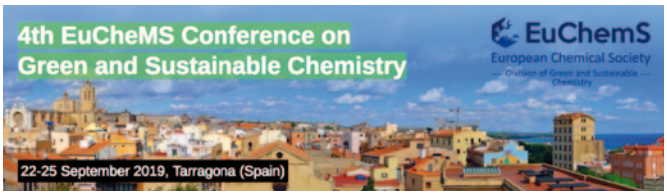
ICIQ to host EuCheMS conference

The 4th EuCheMS Conference on Green and Sustainable Chemistry will be held at ICIQ from 22nd to 25th of September 2019. This conference continues the successful meetings held in Budapest (2013), Lisbon (2015) and York (2017) and offers opportunities to discuss the latest developments in green and sustainable chemistry, to create new partnerships and to expand existing networks between academia and industry.

The leading topics of this conference will focus on green/bio-polymers, photochemistry and catalysis, electrochemistry and catalysis, carbon dioxide valorization and biomass conversions. Prof. Arjan Kleij, ICIQ group leader, is acting as the chair of the EUGSC-4.



You can have a first look at the speakers participating in EUGSC-4 visiting the web page.

ICIQ-Intecat School

Researchers from ICIQ, Universidad de Huelva, Universidad de Valladolid, Universitat Rovira i Virgili, Universidad de Zaragoza gathered at Montbrió del Camp (Tarragona) to participate in the ICIQ-INTECAT School.

The School is one of the activities included in the RedIntecat project (CTQ2016) funded by the AEI/ Ministerio de Ciencia, Innovación y Universidades. RedINTECAT aims at Facing Societal Challenges through Collaborative Research in Catalysis and builds on an Integrated Approach to Catalysis developed within the INTECAT project. The network has the goal of contributing to the discovery of new chemical processes that make a more rational use of feedstocks, require less energy consumption, and take place without the generation of environmentally harmful by-products.

Von Humboldt award to Prof. Antoni LLobet

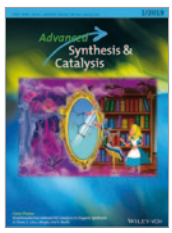
Prof. Antoni Llobet

Antoni Llobet, ICIQ group leader, has been awarded the Alexander von Humboldt Prize – J.C. Mutis Research Award, granted by the Alexander von Humboldt Foundation (Germany), in recognition for his research career.

The award, a recognition of prestige at the European level, consists of an allocation of 60,000 euros to encourage scientific collaboration at the highest level between German and international researchers. The winners receive the award from the President of the Federal Republic of Germany, Frank-Walter Steinmeier, in Berlin during the annual meeting of the von Humboldt Foundation, which will be held next summer.

"As a researcher, I am always looking for synergies," says Llobet, who since joining ICIQ in 2006, has received several awards for his research in the area of catalysis and solar fuels. Inspired by nature, Llobet designs transition metal catalysts that carry out processes efficiently and selectively.

Journal Covers



Enantioselective Iodine(I/III) Catalysis in Organic Synthesis

A. Flores, E Cots, J. Bergès, K. Muñiz

Adv. Synth. Catal. **2018**, DOI: 10.1002/adsc.201800521.

An Electrophilic Bromine Redox Catalysis for the Synthesis of Indole Alkaloid Building Blocks by Selective Aliphatic C–H Amination

J. Bergès, B. García, K. Muñiz

Angew. Chem. Int. Ed. **2018**, DOI: 10.1002/anie.201808939.

2-(4′-Pyridyl-N-oxide)-Substituted Hemithioindigos as Photoresponsive Guests for a Super Aryl-Extended Calix[4]pyrrole Receptor

G. Moncelsi, L. Escobar, H. Dube, P. Ballester

Chem. Asian J. **2018**, *13* (12), 1632-1639, DOI: 10.1002/asia.201800463.

Unveiling intermediates

As important as knowing where you want to go, is it to know how to get there. A collaboration among ICIQ groups Bo, Urakawa and Kleij, has pinpointed the elusive intermediates that precede cyclic carbonate formation from an epoxy alcohol through the catalytic conversion and activation of CO_2. The results, published in *Nature Catalysis*, could be used as blueprints to determine similar catalytic reaction mechanisms.

The ICIQ researchers have unveiled an unknown reaction mechanism that provides a new and more sustainable synthesis route to produce cyclic carbonates – highly relevant products for the polymer and pharmaceutical industry. "This paper increases the potential of using CO_2 as feedstock, making cyclic carbonates derived from CO_2 economically more attractive," explains ICIQ group leader and ICREA professor Arjan Kleij.

To determine the reaction mechanism, the researchers have combined computational as well as experimental approaches such as substrate labelling, X-ray diffraction, and infrared spectroscopy among others.

Read more

"Deciphering key intermediates in the transformation of carbon dioxide into heterocyclic products"

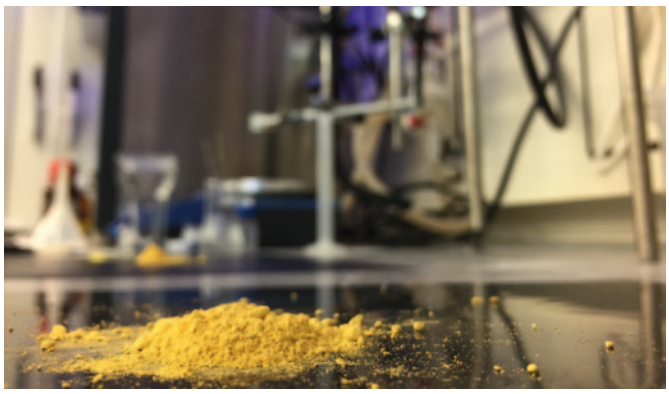
R. Huang, J. Rintjema, J. González-Fabra, E. Martín, E. C. Escudero-Adán, C. Bo, A. Urakawa, A. W. Kleij

Nat. Catal. **2018,**
DOI: 10.1038/s41929-018-0189-z.

Streamlining radical chemistry

In 1789, Antoine Lavoisier already used 'radical' in his *Traité Élémentaire de Chimie* – although the term had a slightly different meaning back then. Now, ICIQ researchers are still using radicals – molecules that have an unpaired 'valence electron', which makes them very reactive – to bring new synthetic strategies to chemists. "Radical chemistry offers unique ways of making molecules," quips Paolo Melchiorre, ICIQ group leader and senior author of the paper published in *Nature Chemistry*.

The ICIQ researchers have developed a photochemical catalytic strategy that generates carbon radicals from alkyl chlorides – linear organic molecules where all the C-C bonds are single – by exploiting their electrophilic properties. To make the strategy work, the scientists have adorned an organic catalyst with a chromophore unit to make it absorb visible light. The catalyst, by using a fundamental pathway of ionic chemistry, the S_N2 substitution, can generate radical intermediates from a variety of



The new organic catalyst is stable under bench conditions.

chemically interesting molecules. "We can activate molecules that are inert to other strategies. All this is possible because of the catalyst and the mechanisms by which we activate the molecules," explains Bertrand Schweitzer-Chaput, an ICIQ postdoctoral researcher part of the Melchiorre group.

Read more

"Photochemical generation of radicals from alkyl electrophiles using a nucleophilic organic catalyst"

B. Schweitzer-Chaput, M. A. Horwitz, E. de Pedro Beato, P. Melchiorre

Nat Chem **2018,** DOI: 10.1038/s41557-018-0173-x.

Databases catalysing discoveries

ICIQ theoretical group leaders Carles Bo, Feliu Maseras and Núria López have published a comment on *Nature Catalysis* highlighting the role computational results databases can have in accelerating the discovery of catalysts.

The computational studies carried out over the last decades have generated vast amounts of data. Now, several initiatives aim to systematically use the results of these computational simulations to build and maintain databases where scientists will be able to curate, standardize and eventually mine the already generated information. In their comment the ICIQ group leaders give an overview of the situation on the field, citing examples such as the Materials Project, AIIDA NoMaD, the PubChemQC project, or the ICIQ developed Input/Output Chemistry Big Data (ioChem-BD) that allows mapping all reactivity irrespective of the nature of the catalyst.

To the ICIQ scientists, future steps are clear. Computational results should follow the FAIR principles (findable, accessible, interoperable and recyclable) if they need to be combined with machine learning approaches to deliver the next revolution in the discovery of active, selective and stable catalysts.

"The role of computational results databases in accelerating the discovery of catalysts"
C. Bo, F. Maseras, N. López
Nat. Catal. **2018**, DOI: 10.1038/s41929-018-0176-4.

Projects from the "Equipamiento Científico-Técnico 2018"

ICIQ was awarded three projects to install an integral system of time-resolved laser spectroscopy, acquire an X-ray powder diffractometer and renewal the 500 MHz Nuclear Magnetic Resonance (NMR) electronic system for liquid phase samples.

The call was released by the Spanish Ministry of Science, Innovation and Universities (MCIUN) last June. It is part of the European Regional Development Funds (ERDF or FEDER in Spanish) and funds the 50% of activities related with the acquisition, installation and updating of scientific and technological equipment.

BIST updates

3rd Annual Ignite Call: The goals of the BIST Ignite Programme are to promote the initiation of new collaborations among the BIST researchers, facilitate the exchange of knowledge among different scientific fields and explore new approaches to address complex questions. This year, five new collaborative research ideas will be selected by a scientific committee to be funded with 20.000€ each and given eight months to be developed. After these eight months, two of the five projects will be chosen to continue their projects with an additional 50.000€ each.

Training for group leaders: BIST together with ICIQ organized a training course aimed at senior group leaders from BIST centres and other institutes. The course was led by hfp consulting and took place from October 8th to the 10th, in Montbrió del Camp, Tarragona. Participants learned techniques on how to communicate effectively, deal with conflicts constructively, delegate tasks more effectively or set clear goals, among other skills.

Congratulations!

Foto: UBT/Kolb.

Dr. Dagmar Scharnagel, a postdoctoral researcher in the Echavarren Group, was awarded the City of Bayreuth prize. On Friday 9th of November during a formal dinner, also known as "President's Dinner," the mayor of Bayreuth recognised the work of three candidates of the Bayreuth University for their excellent thesis. Dr. Scharnagel was honoured for her thesis entitled "Chiral, rigid diamines – from ligands to bispidine alkaloids."

Ana García-Herraiz, PhD student in the Suero group, and Andreu Tortajada Navarro, PhD student in the Martín group, were awarded the 1st and 3rd prize of the Reaxys-RSEQ Early Career Researcher Award. For a second year, Elsevier and RSEQ have organized Early Career Researcher Award. To participate, young researchers have written an essay highlighting how the use of the Reaxys scientific platform has helped them to develop and advance their research projects. García-Herraiz won the 1st prize with her essay "How Reaxys enabled reaction discovery with carbyne equivalents."

Winners of the Reaxys-RSEQ Early Career Researcher Award and members of the committee.

Insights

What follows is a selection of the answers our newly minted doctors gave to the question: **From the lessons learnt at ICIQ, which one do you value the most?**

Sofia Ferrer: During my time at ICIQ I have learnt many things, one of the most valuable was learning about time management. I consider it something really important when you are a researcher.

Pablo Garrido: You need to be passionate about what you are doing! Working in chemistry, doing a PhD is very hard work. From all the things you try out in the lab, only 20% of them work out, so you need to be very passionate about what you are doing because otherwise, you will get upset quite often. You also need to learn from your mistakes.

Luca Buzzetti: What I have learnt is that the key to success is to not expect the same from all the people working with you. Ask people to help you with the stuff they are best at, that's an important lesson.

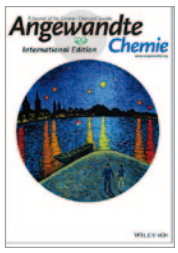
Yuangyuang Shi: The mentoring! Antoni Llobet, my thesis supervisor is a very busy scientist, but he always finds the time to talk with me about the research progress and problems. Talking with him can help me understand experiments and mechanisms deeply, he is so knowledgeable! I also feel very grateful for Dr. Carolina Gimbert, who supervised my work in the lab during my master and PhD studies at ICIQ.

Journal Covers

High-efficiency organic solar cells based on a halide salt and polyfluorene polymer with a high alignment-level of the cathode selective contact

V. S. Balderrama, J. G. Sánchez, G. Lastra, W. Cambarau, S. Arias, J. Pallarès, E. Palomares, M. Estradae, L. F. Marsal

J. Mater. Chem. A **2018**, 22534-22544, DOI: 10.1039/C8TA05778H.



Design of Single Gold Atoms on Nitrogen-Doped Carbon for Molecular Recognition in Alkyne Semi-Hydrogenation

R. Lin; D. Albani; E. Fako; S. K. Kaiser; O. V. Safonova; N. López; J. Pérez-Ramírez

Angew. Chem. Int. Ed. **2018**, DOI: 10.1002/anie.201813083.

Face to Face with Ilan Marek

Ilan Marek is a professor at the Schulich Faculty of Chemistry, at the Technion – Israel Institute of Technology. Marek's group is focused on designing and developing new and efficient stereo- and enantioselective strategies for the synthesis of important complex molecular structures. The group wants to provide an answer to challenging synthetic problems but it has to be coupled with unique efficiency and elegance.

When did you decide to become a scientist and why?

I never actually decided to become a scientist, but I know when I decided to become a synthetic chemist. At university, I studied physics, chemistry, and biology and at some point, I took an organic synthesis class. I immediately fell in love with it: I've only studied this ever since!

What do you like the most about your job?

Organic synthesis is like being an architect at a molecular level. When looking at landmark buildings you can see if they are beautifully built. In synthesis you can see the same, you can tell when something is made in a beautiful manner. There's a lot of room for art in science and I try to do my work as beautifully as I can. There are many ways to build molecules, so I let creativity decide how to build it in the most elegant, beautiful and efficient manner. Let your creativity go!

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

Funding should be spent on good research, no matter the area. I think we should help as much as we can young faculty members to get funding. We need to give the maximum of chances to the new generation of scientist to express themselves. There're a lot of opportunities to help: For instance, a group of chemists in which I belong as well as Antonio Echavarren have created a European workshop for young chemists where they share ideas, present their own work, discuss science and create networks. I think there should always be some funding reserved for new faculty members – based on academic excellence, of course!

Tell me about a time your failed

In science, I fail every day. When one tries to solve important questions, one has to be prepared to fail a certain number of times until he/she finds the key to the problem. It's never easy to fail that much, but the point is to understand why we are failing and to improve ourselves; We learn more from failures than we learn from success. In addition, it puts things in perspective and teaches us to be modest!

Proust Questionnaire

A chemical element: *copper, because it does beautiful transformations.*

Favourite scientist: *can't choose only one, so Albert Einstein, Victor Grignard, and Marie Curie.*

Your favourite invention: *the one that's going to happen in a year or two from now!*

If you had not been a scientist… *I'd be a surgeon, where you use your hands and brain and save lives.*

Favourite destination: *New York, I like the atmosphere and the architecture, it's gorgeous!*

A book: *a thriller, like the ones from Harlan Coben.*

A movie: *Cherry blossoms, by Doris Dörrie, it's an extremely touching movie, I cried like a baby.*

A dream: *to succeed (in part) in my crazy ideas…*

Science is… *creativity and fun, it's a wonderful job!*

She leads

"Científiques: passat i present," ICIQ's new educational programme in collaboration with the URV, wants to introduce the research and findings by female scientists, the pioneers and today's leading scientists working in different research topics (catalysis, crystallography, geometry, light, DNA, radioactivity, programming). To this end we have created class materials for primary school teachers so they can have female references in the world of science.

Our educational material focuses mainly on the scientists' biographies, their research topics and applications, and we have also included experiments to better explain each one of the topics.

Científiques web page: http://cientifiques-stem.cat

Innovative schools

ICIQ has established a Magnet alliance with Pau Delclòs school in Tarragona. Magnet is an educational programme of Fundació Jaume Bofill that aims at helping public schools draw students from their school zone and from other districts by offering a unique curricula.

The alliance between Pau Delclòs School and ICIQ will allow the school to develop an innovative and quality educational project around chemistry. An attractive project that has magnetism and that becomes a reference project in its territory, both for families as for the educational community. The ultimate goal is to attract children of various socio-economic backgrounds, race and academic achievement levels thanks to a challenging scientific project.

Magnet web page: http://magnet.cat

News in brief

Thesis: Drs. Joan González Fabra, Yuanyuan Shi, Sofia ferrer, Marta Borges, Luca Buzzetti, Pablo Garrido, Yangyang Shen, Santi Cañellas and Xiang Yin, predoctoral students at ICIQ defended their PhD thesis. Congratulations!

eScaled meeting: Researchers from across Europe gathered last week at ICIQ for the scientific kick off of the European School for Artificial Leaf Electrode Devices (eSCALED) project. Officially launched on April 2018, eSCALED is a Marie Skłodowska-Curie Action project with a double ambition: to train the researchers of the future and to develop a device able to store solar energy in a chemical form. Prof. Antoni Lobet, ICIQ group leader, is part of the eScaled project.

Sweet chats

We are back with "La Ciència de la Xocolata" workshop series. This time we're programming the different seminars at Biblioteca Pública de Torredembarra. "La Ciència de la Xocolata" consists of nine theoretical-experimental seminars that show the research and knowledge behind chocolate. Female researchers from the URV and ICIQ bring to light the value of research from different perspectives. Both the research they carry out and their life experience are important to inspire the children involved in this project.

See video

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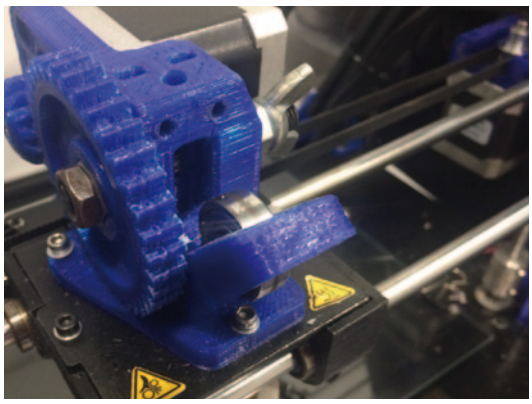
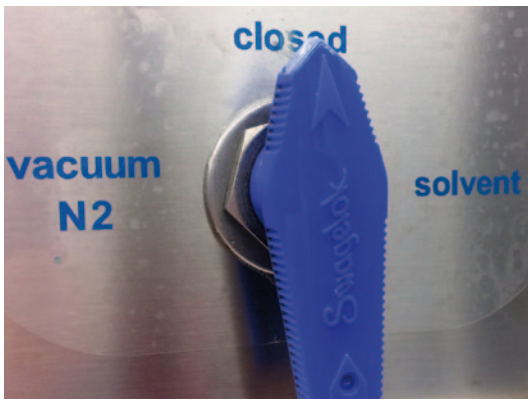



Christmas Lunch