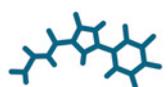




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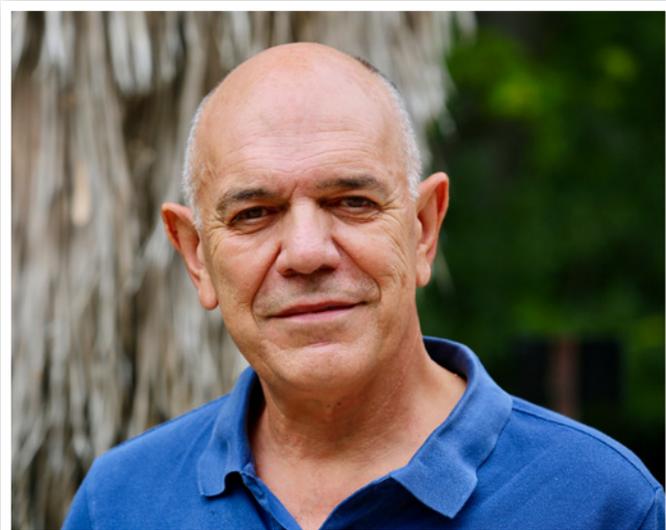
No. 26



ICIQ
Institut
Català
d'Investigació
Química



Antonio M. Echavarren's second ERC Advanced Grant

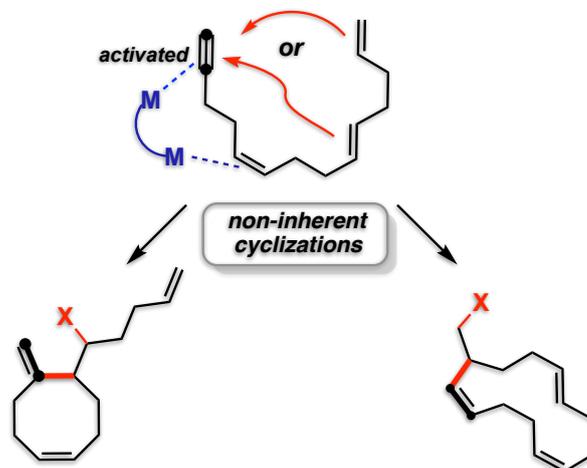


Antonio M. Echavarren, ICIQ group leader, has obtained a new Advanced Grant of € 2.5 million from the European Research Council (ERC) to develop new types of catalysts inspired by natural cyclase enzymes. His previous Advanced Grant (2013-2018) had focused on the discovery of new catalytic gold chemistry. On top of that, he has just been awarded an ERC Proof of Concept grant for the development of efficient routes for the synthesis of polyacenes.

His ERC Advanced Grant project, entitled Catalytic Metallofoldamers of biological inspiration (Foldmetcat), aims to design and develop catalysts (molecules that intervene in the chemical reaction, increasing their speed without being consumed) that transform linear organic molecules into cyclic structures in a single step. The project has the potential to make more efficient the manufacture of drugs such as the anti-tumor taxol.

■ Natural inspiration

"Nature is very wise, but that's because it has had millions of years to optimize its processes. We intend to do something similar in five years," smiles Echavarren. The project has a double objective. On the one hand, develop new types of artificial catalysts (polymetallic catalysts) that mimic the functions of the cyclase enzymes and obtain structurally complex molecules in a precise manner – in a single chemical transformation, as nature does. On the other hand, the research group wants to understand how to control cyclization processes to end up creating molecules with new architectures, which are not found in nature.



The research group will use the economic endowment to provide itself with the most advanced equipment for the analysis of complex mixtures, as well as for the computational work required for the design of artificial catalysts. "If this new strategy works, we will obtain artificial molecules [that are not found in nature] with the potential to develop new and more powerful drugs," explains Echavarren.

With the new project, ICIQ adds a total of 19 ERC projects – seven currently in force.

Profs. Pericàs and Galán-Mascarós honoured by the RSEQ

ICIQ group leader and director, Miquel A. Pericàs has received the Gold Medal of the Spanish Royal Society of Chemistry (RSEQ) as recognition to his professional career – the highest distinction given by RSEQ to scientists carrying out research in the field of chemistry since 1958. “I believe any prize given to people working at ICIQ is a recognition to the institute as a whole. I’m very grateful for this award which also acknowledges the work of colleagues and collaborators!” says Pericàs.



Miquel A. Pericàs

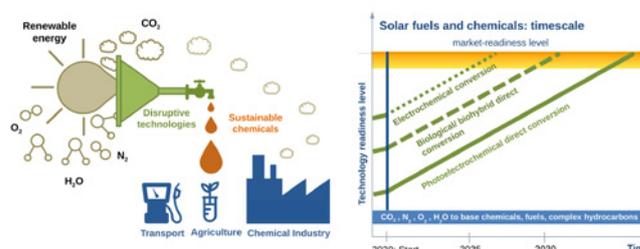


J.R. Galán-Mascarós

José Ramón Galán-Mascarós has been recognised with the RSEQ’s Award to Excellence in Research, given to scientists which during the last years have been doing outstanding research in chemistry. The awards will be given at an official ceremony that will be held in Madrid in November.

SUNRISE: Solar energy for a circular economy

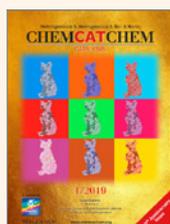
Six CSA projects have been selected for the 2018 call “FETFLAG-01-2018” within one of the three main research areas proposed: Information and communication technology (ICT) and Connected Society; Health and Life Sciences; and Energy, Environment and Climate Change. These actions aim at preparing new European large scale research initiatives to be potentially supported in the next European research and innovation framework programme, Horizon Europe.



SUNRISE, as part of the Energy, Environment and Climate Change area, gathers players from academia, industry, policy-making and society to prepare a strategic long-term research roadmap and a consolidated vision of a future large research project. SUNRISE aims at providing a sustainable alternative to the fossil-based, energy-intensive production of fuels and chemicals, based on solar energy conversion and widely available feedstock (CO₂, H₂O, N₂).

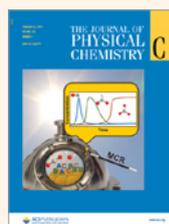
SUNRISE is coordinated by Prof. Huub de Groot from Leiden University (the Netherlands) and brings together a multidisciplinary consortium of 20 partners from 13 European countries, ICIQ among them.

Journal covers



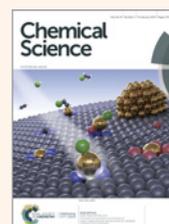
[Ensemble Design in Nickel Phosphide Catalysts for Alkyne Semi-Hydrogenation](#)

D. Albani, K. Karajovic, B. Tata, Q. Li, S. Mitchell, N. López, J. Pérez-Ramírez
ChemcatChem **2019**, 11 (1), 457-464.



[The Active Surface Species Ruling Product Selectivity in Photocatalytic CO₂ Reduction Over Pt- or Co-Promoted TiO₂](#)

M. Borges Ordoño, A. Urakawa
J. Phys. Chem. C, **2019**, 123 (7), 4140–4147.



[Controlling the speciation and reactivity of carbon-supported gold nanostructures for catalysed acetylene hydrochlorination](#)

S. K. Kaiser, R. Lin, S. Mitchell, E. Fako, F. Krumeich, R. Hauert, O. V. Safonova, V.A. Kondratenko, E. V. Kondratenko, S. M. Collins, P. A. Midgley, N. López, J. Pérez-Ramírez
J. Chem. Sci **2019**, 10, 359-369.

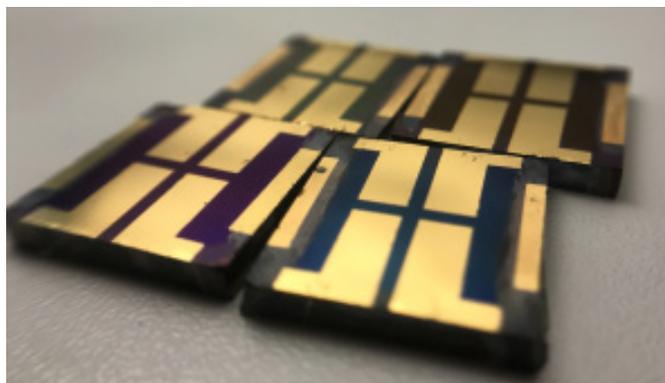
The interface makes the difference

A collaboration led by ICIQ's Palomares group deepens the understanding of the impact that changing the materials in a perovskite solar cell has on its performance. The results, published in the peer-reviewed journal *Energy & Environmental Science*, will help rationalize the design of the components of cells, thus increasing their commercial appeal.

Perovskite-based solar cells are the fastest-advancing solar technology to date. Since they were first used in 2009, perovskite solar cells have achieved high efficiencies (over 22% under standard solar irradiation) at low production costs. Although most of the perovskite components are optimized, there's still room for improvement. Especially in reference to the Hole Transport Materials (HTMs) employed.

The collaboration, among researchers from ICIQ's Palomares and Vidal groups, the Physical Chemistry of Surfaces and Interfaces group at the [Institut de Ciència de Materials de Barcelona](#) (ICMAB-CSIC)

and [IMDEA Nanociencia](#), sheds light on the reasons behind the differences observed in perovskite solar cells' performance by comparing four different HTMs that present close chemical and physical properties.



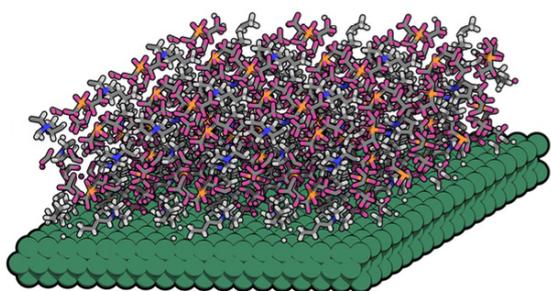
Perovskite solar cells with different materials as HTMs also reflect different colours

[Energy alignment and recombination in perovskite solar cells: weighted influence on the open circuit voltage.](#)

Ilario Gelmetti, Núria F. Montcada, Ana Pérez-Rodríguez, Esther Barrena, Carmen Ocal, Inés García-Benito, Agustín Molina-Ontoria, Nazario Martín, Anton Vidal-Ferran and Emilio Palomares

Energy & Environmental Science. **2019**,12, 1309- 1316.

Diving into ammonia production



Researchers from ICIQ's Lopez group unraveled key molecular interactions involved in the electrocatalytic production of ammonia (NH₃) from nitrogen (N₂). The ICIQ scientists have been able to model a realistic representation of the catalyst-solvent interface at the Density Functional Theory (DFT) level to understand the role of ionic liquids in ammonia synthesis.

Together with collaborators from University of Bonn, and thanks to the computer resources provided by

[HPC-Europa3](#), they simulated a realistic catalyst-solvent model of over 500 atoms to explore the mechanisms of NRR and HER with a metal catalyst. They found that, while the bare metal favours the production of hydrogen, the presence of fluorinated ionic liquid stabilizes key intermediates in NRR, thus driving the reaction towards ammonia production. These features explain the experimental results and could only have been captured by modelling the solvent explicitly.

Ammonia synthesis is the chemical process that feeds the world as it is the main source of fertilizers. Massively obtained through the Haber-Bosch process, the production of ammonia alone is responsible for almost 2% of CO₂ emissions and 1% of the energy consumption worldwide.

["Selective Electrochemical Nitrogen Reduction Driven by Hydrogen Bond Interactions at Metal-Ionic Liquid Interfaces"](#)

Manuel A. Ortuño, Oldamur Hollóczki, Barbara Kirchner, and Núria López

J. Phys. Chem. Lett. **2019**, 10 (3), pp 513-517

Feliu Maseras appointed as Associate Editor for ACS Catalysis



Prof. Feliu Maseras, ICIQ group leader, has been appointed as Associate Editor of the journal ACS Catalysis. He joins a team of eighteen associate editors and will strengthen the journal's expertise in theoretical and computational molecular catalysis.

[ACS Catalysis](#) is a peer-reviewed scientific journal established in 2011 by the American Chemical Society. It is an interdisciplinary journal publishing original research on and at the interfaces of heterogeneous catalysis, homogeneous catalysis, and enzymology. The journal is devoted to reports of new and original experimental and theoretical research on molecules, macromolecules or materials that are catalytic in nature.

Paolo Melchiorre joins the journal Chemical Science as an associate editor



Prof. Paolo Melchiorre, ICIQ group leader, has joined the journal Chemical Science as an associate editor. Melchiorre's research focuses on utilising organocatalytic and photochemical processes to develop environmentally respectful reaction processes, aiming to redesign synthetic processes that could find widespread use in organic synthesis.

[Chemical Science](#) is the flagship journal of the Royal Society of Chemistry. It is an open access, weekly, peer-reviewed journal, established in 2010 that covers all aspects of chemistry. Melchiorre will be handling submissions in the area of organic chemistry, photochemistry, asymmetric catalysis and organocatalysis.

Elisabet Romero joins multidisciplinary Q-SPET project



The Barcelona Institute of Science and Technology (BIST) has awarded three outstanding multidisciplinary projects within the BIST Community with grants to continue developing the projects initiated with the [BIST Ignite Programme](#). One of the awarded

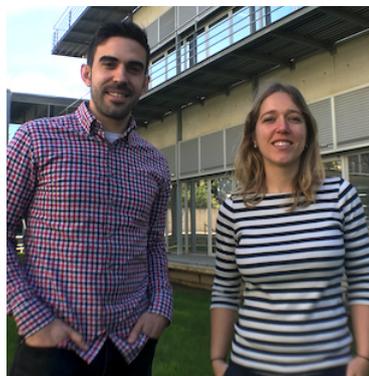
projects, [Quantum-controlled Single Protein Electron Transport \(Q-SPET\)](#), is led by Pau Gorostiza from IBEC, Niek F. van Hulst from ICFO, and Elisabet Romero from ICIQ.

The Q-SPET project will use complementary approaches to study the role of quantum effects in the proteins responsible for transforming sunlight into chemical energy. The scientists will study both natural proteins, isolated directly from plants, and artificial proteins, specifically designed and constructed by the Q-SPET team. The combination of sophisticated ultrafast spectroscopy techniques with high sensitivity photocurrent recordings to measure electron transport at the single molecule level will allow the exploration of the light-to-charge conversion in proteins with unprecedented detail.

"This collaboration is crucial because it will allow us not only to better understand the role of quantum mechanics in biological function but also to develop a new generation of quantum devices, the technology of the future," concludes Elisabet Romero.



Congratulations!



Lilly awards to Ana G. Herraiz and José Enrique Gómez

Two ICIQers have won the [2019 RSEQ-Lilly Awards](#) award: Ana García Herraiz (the Suero group) and José Enrique Gómez (Kleij group), while the third

award goes to Esther Sánchez Tirado, from Universidad Complutense de Madrid.

Ana G. Herraiz works on the development of novel carbon-based reactive species for the discovery of new reactivity at carbon through photoredox catalysis for the modification of feedstock chemicals and medically relevant agents. José Enrique Gómez studies the stereoselective synthesis of sulfones and amino acids from functionalized heterocycles, he is utilizing a catalytic post-modification strategy for the functionalization of organic carbonates into products of pharmaceutical relevance.

As a recognition for the award, the three awardees will present their work in an invited oral presentation during the [XXXVII Biennial Meeting](#) of the RSEQ, which will take place in Donostia in May.



Santiago Cañellas receives the 'Josep Castells' award for best PhD thesis

The Catalan section of the [Spanish Royal Chemical Society](#) (RSEQ) has granted one of the 'Josep Castells' awards 2018

to Santiago Cañellas, postdoctoral researcher in Prof. Miquel Pericàs group who started as a PhD student in the same group with a MINECO FPI-Severo Ochoa Grant. The Josep Castells award recognizes the two best PhD theses of the Catalan section of the RSEQ. The awardees will receive 500€ each and a diploma.

Dr. Cañellas will receive his award and give a short talk at the official ceremony happening in June at the Autonomous University of Barcelona (UAB). The ceremony will also celebrate the work of Michela Milan (University of Girona), co-recipient of the Josep Castells 2018, and Marc Vendrell Escobar (University of Edinburgh), winner of the 2018 Marcial Moreno-Mañas Lectureship.

Controversy over molecular- ularity of catalysts solved



Collaborative research between ICIQ's Lloret-Fillol group and the Costas group from the Institute of Computational Chemistry and Catalysis (IQCC) of the University of Girona, has shed light on a long controversy over the molecular nature of the catalysts involved in water oxidation. Water oxidation is the conversion of water into oxygen, protons, and

electrons, and can be considered as one of the most important reactions on earth since triggers natural photosynthesis – the reaction where plants take CO₂, water and sunlight and transform them into sugars and oxygen – and thus, sustains life on earth.

“This work provides the strongest case possible for the real nature of active species in water oxidation, validates the reaction mechanism, and will hopefully serve as inspiration for other studies and catalysts design,” explains co-author Julio Lloret-Fillol, ICIQ group leader and ICREA research professor.

[Design of Iron Coordination Complexes as Highly Active Homogenous Water Oxidation Catalysts by Deuteration of Oxidation-Sensitive Sites](#)

Z. Codolà, I. Gamba, F. Acuña-Parés, C. Casadevall, M. Clémancey, J.M. Latour, J. M. Luis, J. Lloret-Fillol, M. Costas

J. Am. Chem. Soc. **2019** DOI: 10.1021/jacs.8b10211.

Face to Face with Atsushi Urakawa



Atsushi Urakawa is from Japan, he obtained his PhD from ETH Zurich (Switzerland), where he worked as a Senior Scientist and Lecturer until he joined ICIQ in 2010. After nine years at ICIQ, he will continue his research as a professor at Delft University of Technology (The Netherlands).

■ Why did you become a scientist?

I never thought I'd be a scientist, or that I'd go into academia. But I've always studied the subject that fascinated me the most: catalysis. During my study in Japan, I read a magazine titled "Trigger" that explained heterogeneous catalysis and photocatalysis. The paper showed the beauty of it, and especially the use of photocatalysis in toilet cleaning! I was triggered!

■ How important do you think it is for scientists in academia to collaborate with industry?

To me, it's extremely important. Heterogeneous catalysis is the field where you always have to think of application... just because it's useful! As scientists in this field, it's our duty to transfer our know-how and skills back to industry so that society can benefit. If we collaborate with industry and we are successful, that's the fastest way to give back to society. That's one of the reasons why I enjoy this kind of collaboration. Unfortunately, there're many gaps in this communication. I've been in contact with many companies and collaborated with them. What I've realized is that typically, scientists in academia don't know how to talk to people in industry – and vice versa. I think this comes from a different perception of priorities and it's something I want to bridge. Academia needs to be in contact with industry to learn what they exactly need and identify how we can work together.

■ What would you do to help close the gender gap in science?

In my opinion, gender shouldn't play a role in selection processes. Female scientists should have the same opportunities as their male counterparts – there's no discussion there. I think it's important to be aware of the unconscious gender biases and if somebody gives negative judgement because of maternity leaves etc. Such behavior should be punished. Mechanisms should be put in place too at the evaluation level: only women can have babies, so we should support and not punish them for it.

■ What's next for you?

The general direction is the same: rational catalyst design. I wish to do it massively, so I'll need to develop new technologies. I want to collaborate with many companies to demonstrate rational catalyst design, accelerate tech transfer and develop innovative technologies for the benefit of society and environment protection. In Delft, a lot of time will be spent on education also – it's a university professor position and I know how serious education is there because that's where I studied my masters. I'm excited about educating the next generation and motivate them to be scientists, educators, and leaders in different fields.

Proust Questionnaire

A chemical element: *silver, it always comes back to me! Throughout my research experience, it's always there, I think I still need to discover something with silver.*

A scientist: *Einstein, because he developed many amazing theories.*

An invention: *CO₂ to methanol at high pressure.*

If you had not been a scientist... *a flamenco guitar player.*

A destination: *Sedona, Arizona.*

A book: *The Alchemist, Paulo Coelho.*

A movie: *Pulp Fiction by Quentin Tarantino.*

A dream: *since I was small I wanted to have a café and offer the best coffees.*

Science is... *creativity to find simplest governing logics*

[Full interview here](#)

1st prize!

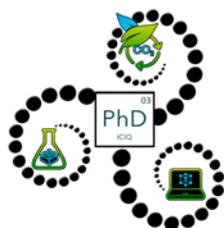


Pablo Bonilla, PhD student in the Melchiorre group, was one of the winners of the science outreach competition “[Somos científicos, ¡Sácanos de aquí!](#).” This 2019 edition took place from April 1st to April 12th. During this time, Pablo

chatted with primary and secondary school students who challenged researchers from a huge variety of fields to answer all sort of questions in an online chat. The students voted for their favourite scientist in the different zones assigned and Pablo got a €500 prize to use in an outreach initiative of his own.

Pablo is the third ICIQ participant in this programme, after Alicia Monleón’s participation in 2017 and Ignacio Funes, who won the ‘Environment’ prize in 2016 – and used his prize money to launch a YouTube channel “[En Cerio o en Bromo](#)”

ICIQ’s PhD Day



ICIQ
III PhD Day
June 6th - 7th 2019

The ICIQ PhD Day (June 6th and 7th at ICIQ premises) is an event designed for and by ICIQ PhD students, featuring interesting invited conferences, flash presentations and poster and networking sessions. In this year’s third edition, the event’s programme includes talks by experts who have followed different chemistry-related careers. Dr. Cristina Sáez de Pipaón, CEO of Orchestra Scientific; Bibiana Campos, Editor in Chief of Chemical and Engineering News and Nessa Carson, chemist at Pfizer and Twitter influencer, among other speakers.

[Full programme here.](#)

News in brief

Thesis: Drs. Cristina García Morales and Franziska Hegner, predoctoral students at ICIQ defended their PhD thesis. Congratulations!



Noah Training School was organized in the frame of Noah (MSCA-ITN). The [meeting’s scientific programme](#) included lecturers such as Prof. Jonathan Nitschke (University of Cambridge), Prof. Michael Schmittel (Universität Siegen) and Dr. Alessandro Aliprandi (Université de Strasbourg). And Prof. Jennifer M. Heemstra (Emory University). The event also featured industry speakers from Leitat, Covestro and Biolitec GmbH.



High Performance Computing: As part of the ELCoREL project meeting, (MSCA-ITN) a [workshop on high performance computing](#) is taking place on June 3rd-5th at Altafulla (Tarragona). ELCoREL aims to train young researchers in all scientific and technological aspects of the storage of renewable electricity into fuels and chemicals.

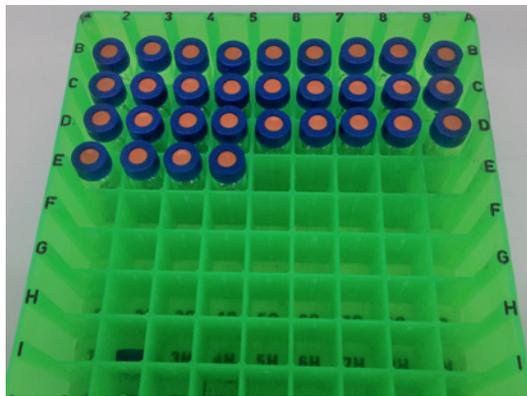
Crysforma: ICIQ’s Crysforma and Technobis, an instrumentation company, organized the workshop “Crystallization: Screening, Applications & Process Development” on April 11th in Barcelona. The workshop was aimed at showing how to solve day to day crystallization challenges and optimize best practices. It counted with 70 participants from the industry sector.

Pint of Science

Tarragona’s second edition of “Pint of Science” has taken place on May 20-22. Several ICIQ people have delivered a talk: Pablo Bonilla (Melchiorre Group), Joan Guillem Mayans (Echavarren Group), Bruna Sánchez (Maseras Group), Angel Mudarra (Maseras and Pérez-Temprano groups), Franziska Hegner (López Group) and Federico Dattila (López Group). Great talks in good company! [“Pint of Science” web page.](#)



ICIQ in green



ICIQ Mountain Group

