newsletter
SEPTEMBER 2018
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ICIQ Institut Català d'Investigació Química
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Fuel for Life

In June 2017 ICIQ's scientific board interviewed five shortlisted candidates for a group leader position within the institute's Starting Career Programme. One year later, the successful candidate, dressed in black, has obtained an ERC (European Research Council) Starting Grant. Her name is Elisabet Romero.

Dr. Elisabet Romero, ERC Starting Grant awardee

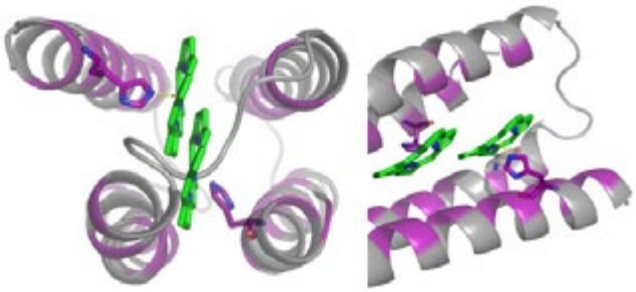
"The ERC Starting Grant is the best funding opportunity an early-stage career researcher could wish for in order to build a competitive research group," says Dr. Romero.

She has now 1.5 M euros and five years to undertake the project entitled 'Engineering Bio-Inspired Systems for the Conversion of Solar Energy to Hydrogen' (BioInspired_SolarH2). A dive into the depths of photosynthesis, chromophore-protein design, and device construction to power the planet.

BioInspired_SolarH2

BioInspired_SolarH2 aims to achieve the efficient conversion of solar energy to hydrogen. The overall objective is to engineer bio-inspired systems able to convert solar energy into a separation of charges and to construct devices by coupling these systems to catalysts in order to drive sustainable and effective water oxidation and hydrogen fuel production.

To this end, Dr. Romero will design and construct robust chromophore-protein assemblies able to exploit coherence to ensure the efficient collection and conversion of solar energy. She will also apply a complete set of steady-state and time-resolved spectroscopic methods to investigate these engineered systems.



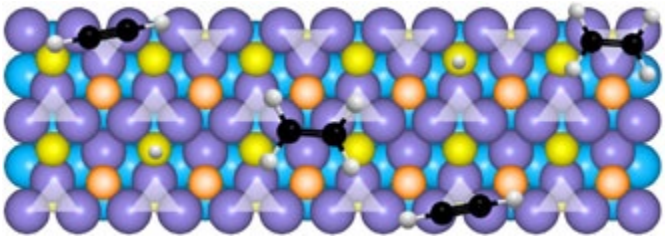
Illustrative chromophore-protein assembly

"We have reached a level of understanding of photosynthesis that is ready to be applied to develop new energy technologies. With the ERC funding, I aim to create a new generation of bio-inspired solar-energy conversion devices based on abundant and biodegradable materials. In this manner, we will contribute to a sustainable future for all," says Romero.

This is ICIQ's sixth ERC Starting Grant of a total of 17 ERC Grants (two Advanced, two Consolidator, six Starting, seven Proof of Concept) obtained since the ERC's grants programme began in 2007.

Selective ensembles in supported palladium sulfide nanoparticles for alkyne semi-hydrogenation

The use of lead-poisoned palladium catalysts, introduced by Herbert Lindlar in the 1950's, still dominates for selective hydrogenations in fine chemical applications. Nevertheless, the search for a more environmentally friendly and efficient catalyst has been a pursued goal in this field.



Now, researchers from ETH Zürich, EMPA and ICIQ (Masoud Shahrokhi and Núria López) have published a paper in *Nature Communications*, presenting sustainable alternatives to catalysts applied to alkyne semi-hydrogenation in industrial organic synthesis. They report a simple and scalable treatment of supported palladium nanoparticles with sodium sulfide, which leads to a crystalline palladium sulfide phase with controlled crystallographic orientation. It exhibits unparalleled performance in the semi-hydrogenation of alkynes in the liquid phase, which is rationalized at the molecular level.

Further information in "Behind the Paper" (Chemistry Community, *Nature*).

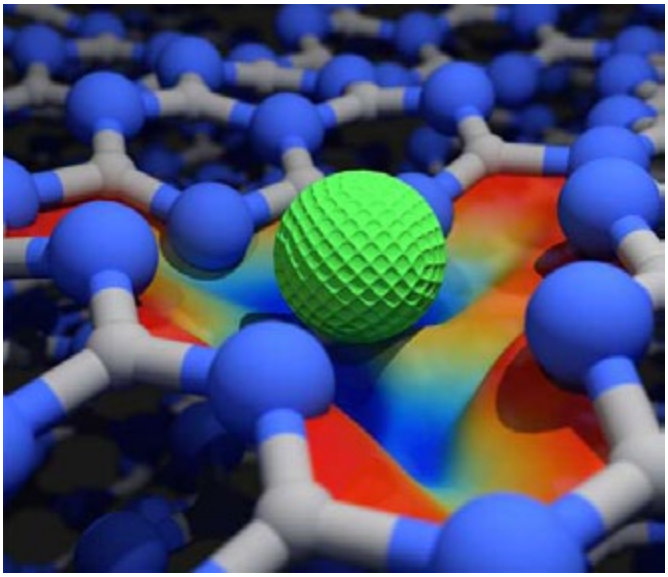
"Selective ensembles in supported palladium sulphide nanoparticles for alkyne semi-hydrogenation"
Davide Albani, Masoud Shahrokhi, Zupeng Chen, Sharon Mitchell, Roland Hauert, Núria López, Javier Pérez-Ramírez
Nature Communications, **2018**,
DOI:10.1038/s41467-018-05052-4

New heterogenous catalyst surpassing homogeneous catalysts in the Suzuki reaction

Edvin Fako, Manuel Ortuño and Núria López are co-authors of a paper published in *Nature Nanotechnology*. The paper reports the development of a new solid catalyst, which surpasses the state of the art of homogeneous catalyst in Suzuki couplings in a cost-effective and eco-friendly way.

The work was coordinated by Prof. Javier Pérez-Ramírez, Professor of Catalysis Engineering at ETH Zürich, who together with ICIQ, Idorsia and the University of Cambridge presents this disruptive technology to immobilize palladium species to mediate Suzuki couplings. This kind of approach is likely viable in other transformations thus avoiding the problems inherent to homogeneous organometallic chemistry.

See the story and an animation about their work here, on ETH's web site.



"A heterogeneous single-atom palladium catalyst surpassing homogeneous systems for Suzuki coupling"
Zupeng Chen, Evgeniya Vorobyeva, Sharon Mitchell, Edvin Fako, Manuel A. Ortuño, Núria López, Sean M. Collins, Paul A. Midgley, Sylvia Richard, Gianvito Vilé, Javier Pérez-Ramírez
Nature Nanotechnology, **2018**,
DOI: 10.1038/s41565-018-0167-2

Mónica H. Pérez-Temprano among the "Talented 12" in chemical research

Chemical & Engineering News "journal of the American Chemical Society" has selected Dr. Mónica H. Pérez-Temprano, an ICIQ group leader, among the 12 talented chemists of 2018. She was recognized for her work on capturing reaction intermediates to design more efficient reactions. Dr. Pérez-Temprano is the first Spaniard to receive this honour.

"I am sure that this international recognition will give great visibility to my group's research, which aims to solve major challenges that are still a mystery for science. It will also help inspire younger generations of chemists," says Pérez-Temprano.

Since 2015, C&EN annually selects 12 promising young chemists working in academia and industry around the world. The names of the winners of 2018 were unveiled yesterday at the ACS meeting in Boston. She had the opportunity to present her research in a TED Talk format during the event.

The "Talented 12" were chosen by C&EN's staff members from a pool of more than 350 nominees. Chemists are selected based on their efforts to seek solutions to the challenges that C&EN describes as "most problematic" within the field of chemical research.

Read Pérez-Temprano's profile in C&EN

Ruben Martin wins the Banc Sabadell Foundation Prize for Sciences and Engineering

"It is very humbling to be the recipient of the 2018 Banc Sabadell Foundation Award for Sciences and Engineering. This award is nothing else but a recognition to the collective effort for all the contributions that my group has made through the years. Their perseverance, diligence and ambition are, beyond any reasonable doubt, key contributory factors for our success. I would also like to thank my wife and two little children for being the pillar of my strength and for their unrestricted support, love and patience."

These heartfelt words are from Prof. Ruben Martin, ICREA Professor and ICIQ Group Leader, upon receiving the news. The award was officially presented to him at an awards dinner on July 18th, at Banc de Sabadell's premises.

Martin works in the development of new metal-catalyzed methodologies for the activation of CO_2 for the synthesis of relevant molecules such as carboxylic acids. These molecules are fundamental in many pharmaceutical products and other compounds of industrial interest. His work has been published in *Nature*.

The Banc Sabadell Foundation Science and Engineering Award, aims to encourage and reward excellent work in the field of sciences and engineering by Spanish researchers. This award is a collaboration between the Banc Sabadell Foundation and the Barcelona Institute of Science and Technology (BIST) and is accompanied by 50,000 euros.

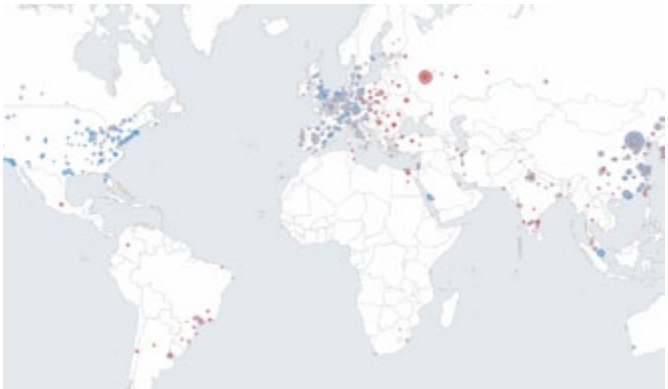
ICIQ's history in EurJOC and EurJIC

ICIQ's director and group leader Prof. Miquel A. Pericàs collaborated in the *European Journal of Organic Chemistry* and the *European Journal of Inorganic Chemisty's* Guest Editorial. As part of the newly introduced section called "Institute Feature", ICIQ's history is outlined from past to present in an issue that also includes articles written by other ICIQ group leaders. The whole piece provides a clear picture of the institute's trajectory, from being a mere project to what it has become nowadays.

At the top

In its fourth release, the web application Mapping Scientific Excellence ranks ICIQ in **first position in "Best Journal Rate"** (ratio of papers published in the most influential journals) **and third in "Best Paper Rate"** (proportion of highly cited papers published by an institution) in the field of Chemistry worldwide.

These results refer to the 2011-2015 time period and to research centers and universities with at least 500 papers published. In the third release for the 2007-2011 time period, the institute ranked second in "Best Journal Rate" and third in "Best Paper Rate."



Journal Covers

Alkali-Driven Disassembly and Reassembly of Molecular Niobium Oxide in Water

D. Sures, M. Segado, C. Bo, M. Nyman

J. Am. Chem. Soc. **2018**, *140* (34), 10803-10813

Organocatalyzed Domino [3+2] Cycloaddition/Payne-Type Rearrangement using Carbon Dioxide and Epoxy Alcohols

S. Sopeña, M. Cozzolino, C. Maquilón, E.C. Escudero-Adán, M. Martínez Belmonte, A.W. Kleij

Angew Chem Int Ed Engl. **2018**, *57* (35), 11203-11207

Synthesis and Reactivity of Copper(I) Complexes Based on C3-Symmetric Tripodal HTIM(PR2)3 Ligands

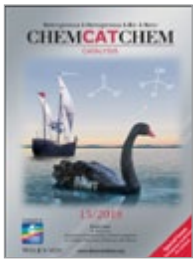
E. S. Smirnova, F. Acuña-Parés, E. C. Escudero-Adán, C. Jelsch, J. Lloret-Fillol

Eur. J. Inorg. Chem. **2018**, DOI: 10.1002/ejic.201800074.

New vistas in transmetalation with discrete "$AgCF_3$" species: Implications in Pd-mediated trifluoromethylation reactions

S. Martínez de Salinas, A. Mudarra, J. Benet-Buchholz, T. Parella, F. Maseras, M. H. Perez-Temprano

Chem. Eur. J **2018**, DOI: 10.1002/chem.201802586.



Manganese N-Heterocyclic Carbene Complexes for Catalytic Reduction of Ketones with Silanes

M. Pinto, B. Royo, S. Friães, F. Franco, J. Lloret-Fillol

ChemCatChem **2018**, DOI: 10.1002/cctc.201800241.

Broadening the Scope of the Gold Catalyzed [2+2] Cycloaddition: Synthesis of Vinylcyclobutenes and Further Transformations

E. de Orbe, A.M. Echavarren

Eur. J. Org. Chem. **2018**, DOI: 10.1002/ejoc.201800170.

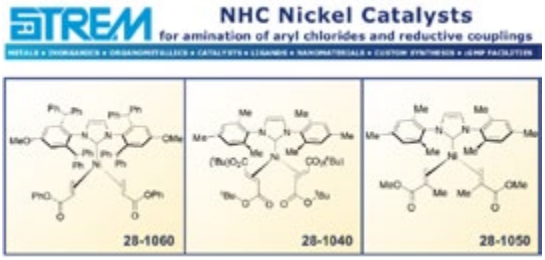
Orchestra Scientific grows

Orchestra Scientific S.L. has signed a capital increase to issue shares to its new partner InnoEnergy, a Knowledge Innovation Community (KIC) that works to build long-lasting integration frameworks among industry, research, and higher education within the energy sector. The new agreement will allow InnoEnergy to join and participate in Orchestra Scientific S.L., while the company will take advantage of InnoEnergy's experience and partners network.

Orchestra Scientific S.L. is an ICIQ-participated spin-off created with the aim of developing and bringing to the market patent inventions by ICIQ's Galán-Mascarós group. Over two years ago, ICIQ researchers disclosed a novel metal-organic framework (MOF) with high selectivity to recognize CO_2 molecules, which can be particularly useful for the separation of carbon dioxide in a mixture of gases.

Nickel goldilocks

A joint collaboration between the John Montgomery's Group at the University of Michigan and an ICIQ researcher (Santiago Cañellas, Pericàs'group) has resulted in the development of a new class of Nickel (0) catalysts, which will expedite a broad range of organic reactions.



These new compounds, published in the American Chemical Society journal, *ACS Catalysis* (patent pending), provide rare examples of Nickel (0) complexes that tolerate air exposure while maintaining high catalytic activities for the construction of strategic bonds in medicinal chemistry. This feature eliminates the need to use an inert atmosphere glovebox, making their use more sustainable and user-friendly. Three of these catalysts can be now purchased from *Strem* Chemicals, Inc.

News in brief

Thesis: Drs. Eloísa Serrano, Belén García and Elena de Orbe, predoctoral students at ICIQ defended their PhD thesis. Congrats!!!

Suschem award to Dr. Francisco Juliá Francisco Juliá, postdoctoral researcher in Prof. Ruben Martin's group, received the Postdoc-Mestralab SusChem award for the best 2017 scientific publication in chemistry. The jury decided to unanimously recognise Francisco for being co-author of the paper "Remote carboxylation of halogenated aliphatic hydrocarbons with carbon dioxide" published in *Nature*.

Beatriu de Pinós: Dr. Manuel Ortuño, working in the López group and Dr. Parijat Borah, who will join the Pericàs group soon have been awarded a Beatriu de Pinós grant. These grants are a COFUND postdoctoral programme co-funded by the EC and AGAUR.

BIST updates

BIST Mothers of Science

Twelve BIST researchers (ICIQ's Dr. Carolina Gimbert among them) were awarded BIST Mother of Science grants. The winners are all exceptional scientists, with the ambition and potential to reach a leading position in research. At the same time as performing cutting edge research in their respective fields, they are also fulfilling maternity responsibilities.

BIST-UPF Master of Multidisciplinary Research in Experimental Sciences (MMRES):

On September 12th, BIST and the Pompeu Fabra University (UPF) organized an MMRES event at the Fundació Catalunya-La Pedrera to recognize and celebrate the 14 graduates of the MMRES class of 2018 and to welcome the incoming 27 students of the MMRES class of 2019. The event's programme included an inspirational keynote speech by ICIQ Group Leader, Elisabet Romero.

Face to Face with David Cahen

Prof. David Cahen is Professor at Bar Ilan University's Dept. of Chemistry and at the Department of Materials and Interfaces at the Weizmann Institute of Science in Israel. Cahen's research focuses on exploring chemical means to control the electronic and optical properties of materials.

- **What do you like and enjoy the most about your job?**

Being creative. For a short period, I was a synthetic chemist. I was working in creating materials that no one had ever created. It was a great satisfaction to know you are the first one to make something new. I think the act of creativity is the thing I like the most. The moment you lose that, I don't see why you should continue doing scientific research.

- **Which are your greatest achievements in your career so far?**

Scientifically, I have contributed to the development and application of two types of (now commercial) solar cells by doing basic research. Personally, 45 years ago the Weizmann Institute started a tutoring programme for problematic kids. I helped save one of these kids from a terrible education system that was just going to leave him behind, and he is now my dentist. There're hidden treasures in people and it's a matter of chance that we develop our best qualities.

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

Get students who are smarter than you, because they pull you up. Choose a problem that if you manage to solve, it will matter to you and hopefully somebody else. That's very wise advice, because, especially today, even if you have done something that will be considered brilliant in 20 years from now, the system is not sufficiently patient to wait that long.

- **You do a lot of science communication, why?**

Science is a universal language, you can use it to bridge gaps. It's a good way to start a dialogue because hopefully, scientists can't argue too much about facts in science. After WWII, scientific collaboration is what started the relations between Germany and Israel; that's the perfect example of how science helped bridge the gap between the two countries and made them go forward.

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

I would encourage every country and company to put aside 5 or 10% of their R&D budget for blue sky research. It's extremely important to fund blue sky research because, in the end, it's the crazy ideas that will give us the next stage in technology.

- **We see many women studying chemistry at University including at PhD level; however, we do not see that many women working as researchers or academics. Why do you think that happens and what do you propose to change the situation?**

There's no question there are more social pressures for women than for men, and I have no idea how to fight those, as it is not enough that all the possibilities are open for women like for men. I believe role models can make a difference. There are still few women at the professor level at the Weizmann Institute, but our only Nobel prize awardee is a woman: Ada Yonath!

Proust Questionnaire

A chemical element: *Pb (read the chapter in Primo Levi's "The Elements" on it).*

Favourite Scientist: *Le Chatelier, as his principle explains so many seemingly surprising phenomena.*

Your favourite invention: *bicycle.*

If you had not been a chemist... *I am a hybrid physicist/materials scientist/chemist, but I might have gone into geology if only to be more outdoors, but more seriously because it itself combines so many of the sciences.*

Favourite destination: *Himalaya (trekked there, twice).*

A book: *Guns, Germs and Steel by Jared Diamond.*

A film: *Casablanca.*

A dream: *make artificial photosynthesis a useful reality.*

Science is... *the best occupational therapy I know of.*

Summer Fellows farewell

Summer has come and gone, and so have the Summer Fellows ICIQ has hosted for the last two months. From July until September, ten chemistry undergraduates have joined ICIQ's research groups to have their first approach to research. "It's been very useful to see the research environment outside of university and to see what it is like to work as a researcher. It's been good fun and I have met really good people," explains Amelia Billings from Bristol University, who joined Urakawa's Group.

Summer fellows

The ICIQ Summer Fellowship Programme – funded by Fundació "la Caixa" – has been designed to train the students in the latest research and techniques while providing an insight on research institutions' inner workings. "You can easily tell that everything is well organized and that every department has its responsibilities and takes care of the equipment. If you have a problem there's always someone who will help you solve it," remarks Isabel Arranz, a student from Universidad de Valladolid who has done the summer fellowship in Maseras and Echavarren's laboratories. "ICIQ is very modern, you can see there's a lot of effort invested to make the best science, the labs are very well equipped!" agrees Billings.

After the two-month experience, the students are moving on to new challenges "I will go to do another fellowship at a company in Oxford. I'm very excited because I really like the project!" quips Arranz. Others will stay closer to home, like Jordi Morales who, after spending his summer doing theoretical chemistry at López's group, will be joining the URV/ICIQ MSc in Synthesis, Catalysis and Molecular Design.

Viro-Flow kicked-off

VIRO-FLOW, ICIQ's first industrial ITN (H2020 Innovative Training Network), held its kick-off meeting on May 22nd and 23rd at ICIQ's premises. The project, a partnership between ICIQ and the German pharmaceutical company AiCuris, obtained €750k to train early-stage researchers and advance the integration of continuous flow chemistry with *in vitro* microfluidic bioassay technologies for the discovery of novel drugs for treatment and cure of HBV (Hepatitis B Virus) infections.

Nit de la Recerca

ICIQ participated in the chemical workshop "Colours" and the afternoon snack "Pa amb oli, sal i xocolata."

5th CHAOS meeting

Scientists from across Europe and North America gathered at ICIQ last week to attend the 5th CHAOS meeting. For three days, the more than 80 attendees have shared research results, discussed projects and found common ground to create fruitful collaborations in the field of Carbon-Hydrogen Activation in Organic Synthesis (CHAOS). CHAOS is part of the European Cooperation in Science and Technology Action programme (COST), a programme created to foster trans-national cooperation among researchers across Europe and beyond by funding networking activities – and the longest running EU funded programme.

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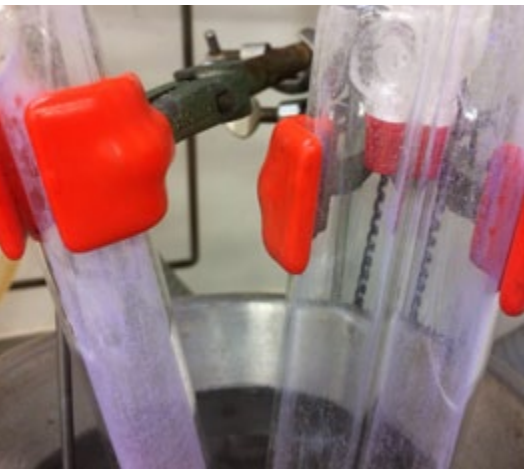
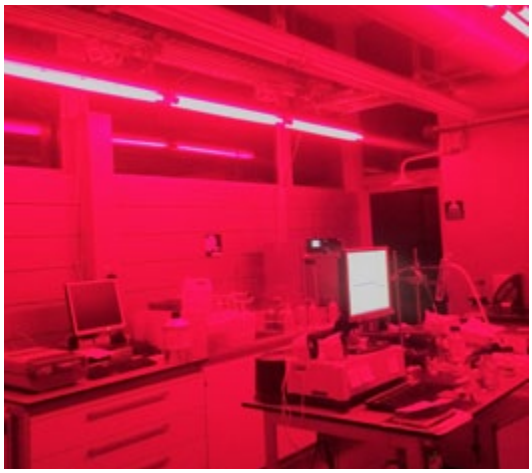
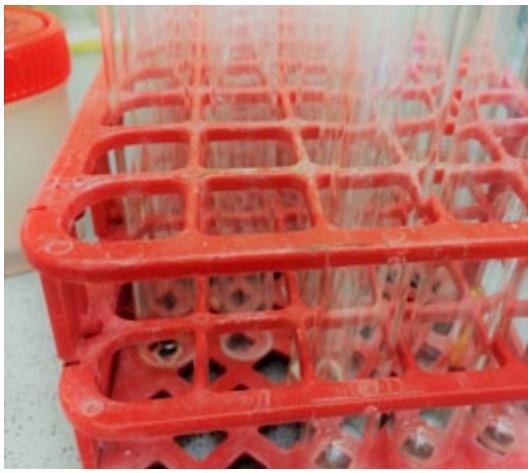
ICIQ in red



ICIQ's Beach Volleyball Championship

Tarragona, September 15th. On a cloudy day 16 teams shined on the sand of the Arrabassada beach. ICIQ's 5th volleyball tournament was courageously played by everyone.

The ExpendaBalls won the championship.