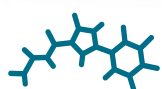




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The Severo Ochoa Accreditation Goes to ICIQ

On July 15th, Dr. Lluís Solà, ICIQ's manager, received the Severo Ochoa accreditation during an institutional event at the Secretary of State for Research, Development and Innovation, in Madrid.



Ms. Carmen Vela, Secretary of State of R+D+I, and Dr. Solà

The Severo Ochoa accreditation will allow ICIQ to develop a strategic project in the area of catalysis. The project deals with the discovery of catalysts for generating fuel (hydrogen) through water splitting using solar energy. It deals also with the discovery of catalysts for converting molecules which have a strong environmental impact (such as CO₂ and fluoroform) or which have low reactivity (such as methane) into molecules of interest for the chemical and energy industry.

ICIQ's 10th Anniversary Celebration



[Symposium's website](#)



[Check the pictures!](#)

ICIQ's Brand New Facility

On July 18th, Andreu Mas-Colell, conseller d'Economia i Coneixement, inaugurated the CELLEX-ICIQ High Throughput Experimentation (HTE) laboratory. This is the only HTE laboratory of this type in Europe. Two other similar laboratories are in the [University of Princeton](#) and [University of Pennsylvania](#).



Andreu Mas-Colell, Carmen Vela (Secretary of State for R+D+I), and Xisco Caldentey, HTE lab. manager

The HTE laboratory provides ICIQ researchers with the instrumentation and know-how to speed up run processes in the development of new drugs and catalysts. The facility offers the possibility to run and analyze a large number of reactions in a very short time, which accelerates the optimization and discovery of new processes. Moreover, the possibility of running many reactions in a short time also allows to follow unexplored ways and to study difficult processes with, a priori, little chance of success.

Fundació Privada
CELLEX

[More info](#)

A Taste of Our Research

Bye Bye Bisphenol A

Plastics have become an indispensable part of our lives. We can find them in food containers, electronic devices, surgical equipment, toys and many other objects. One of the substances widely used for the manufacture of epoxy resins and polycarbonate plastics is bisphenol A [2,2-bis(4-hydroxyphenyl)propane], also known as BPA. The epoxy resins are used as coatings on the inside of almost every food and beverage can and polycarbonate plastics are present in water bottles, medical and dental devices, eyeglass lenses and a long etcétera. BPA could act as an endocrine disruptor and has been shown to cause negative health effects in animals. This has raised concerns about its suitability in certain products such as food containers. Actually, the European Union has banned BPA use in baby bottles and sippy cups and some countries have even more restrictive policies.



At ICIQ, the group of Prof. Arjan W. Kleij is working on alternatives to BPA safer for health. In particular its goal is to replace BPA with limonene, a substance found naturally in citrus fruits. As Prof. Kleij says, “growing concerns about the use of BPA based plastics made us think about the possible alternatives and, more specifically, about polymers that could be derived from renewable natural resources. Limonene (oxide) represents an interesting synthon being abundantly available, but its conversion into copolymers reacting it with CO₂ is a huge challenge. Our recent work has shown that powerful catalysts based on earth-abundant metal complexes may rise to the occasion and provide new technologies for bio-based polymer synthesis”.

The results obtained so far are optimistic and will be published soon.

 [Prof. Arjan W. Kleij group](#)

Collaboration Leads to Success

Collaboration is a key pillar in scientific research. When specialists in different fields join forces usually very interesting and valuable results can be achieved. The ICIQ research groups collaborate frequently with institutions around the world and, sometimes, also with researchers who used to work in the ICIQ and moved to other centers. This is the case of Núria López, group leader at ICIQ, and Javier Pérez-Ramírez, ICIQ's former group leader that now works at ETH (Zurich).



Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Their collaboration started 9 years ago, when they both worked at ICIQ. “From the beginning we knew our strength would be to exploit the complementarity between the experimental and theoretical work collaborating on certain projects”, says Núria. Sometimes this collaboration has been extended to include another group like Dr. Detre Teschner's (Fritz-Haber Institute of the Max Planck Society). In the frame of this collaboration they have also participated in projects with industry (Bayer MaterialScience). Despite the different point of views Javier's and Nuria's groups have got on well along the years. “We are two groups with different backgrounds and it requires an extra effort to make a unique viewpoint that can be transversally understood by our communities. And yet, thanks to the great communication between our students and the confidence to express different views, we have been able to maintain this collaboration over the years with excellent results”. These excellent results have led to the publication of more than 15 papers, one of them published in *Nature Chemistry*. Their latest works have been selected for the cover of *Chemistry A European Journal* and the inside cover of *Angewandte Chemie International Edition*.

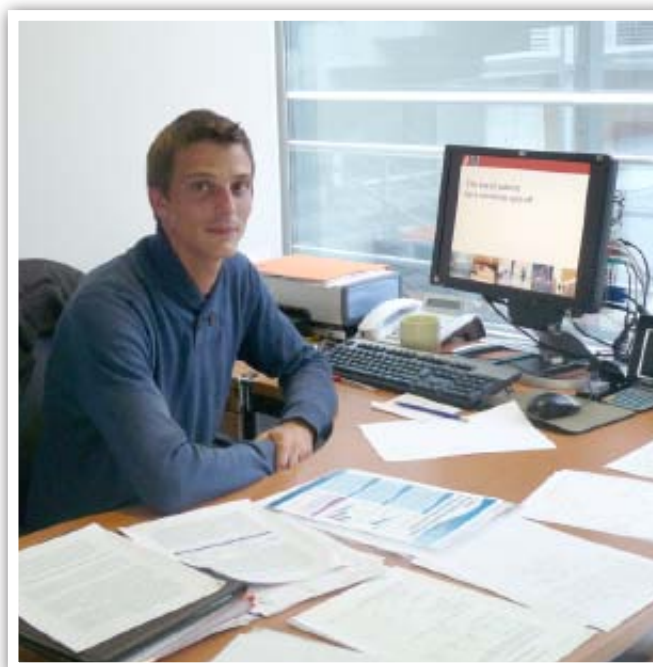
 [Prof. Núria López group](#)

 [Prof. Javier Pérez-Ramírez group](#)

ICIQ's Pushing for Innovation and Entrepreneurship

Dr. Frédéric Ratel has spent most of his career in the ICIQ. He arrived in 2004, when ICIQ first opened its doors, to do a PhD in the group of Prof. de Mendoza. After that, in 2008, he joined the group of Prof. Pericàs to work in the Esteve-ICIQ Joint Unit and, finally, in 2010, he joined the Industrial Property Unit, which now he manages. This unit deals with different aspects of knowledge economy such as collaboration with public and private sectors and technology transfer. Technology transfer is a long process that includes steps such as the evaluation of the commercial potential of R&D results, the legal protection of these results and the development of the technologies, among others.

“We have to identify which technologies developed at ICIQ may have more interest to the industry and get companies interested in them”, says Fred. To help researchers in this area and give guidance and support to entrepreneurship, the ICIQ has developed a series of documents (available on the intranet) that explain the steps to be followed by those

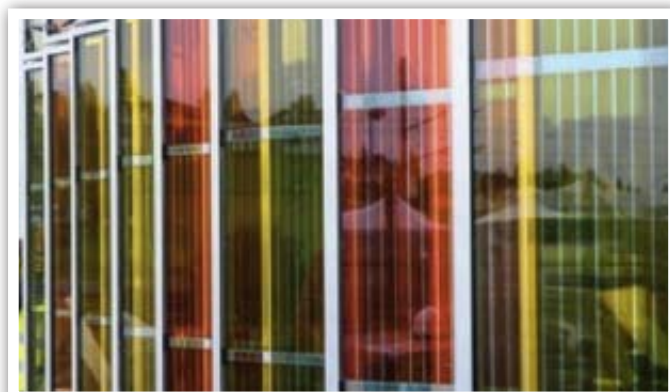


Dr. Ratel, IT Unit manager

who think they have a patentable result or who are considering to create a company. During the month of May Fred has been teaching courses on this topic to clarify any possible doubt.

Pascual Segura, founder and director of Patent Centre (University of Barcelona), came in June to ICIQ to teach a course about ‘Intellectual Property for researchers in Chemistry and related fields’.

Dye-Sensitized Solar Cells (DSC): A Realistic Approach Towards Energy Markets



Windows from EPFL conference centre in Lausanne

The new conference centre at the Swiss Federal Institute of Technology (EPFL) in Lausanne has the world's first solar window, composed of colored solar panels, on the west façade. With a total surface area of 300 m² of DSC, it represents the first application of such technology to a public building and has been done with the participation of ICIQ's researchers. The red colored glass windows are made with RK1, a new purely organic dye patented by CEA (France) that Palomares' group has studied in collaboration with CEA-INAC, Solaronix (Switzerland), KaïronKem (France) and Solarprint (Ireland) in the scope of the EU project “ADIOS-Ru”. RK1 achieves one of the best output power conversion efficiencies and an outstanding long-term stability for a solar cell based on an ionic liquid electrolyte. The synthesis and characterization of RK1 have been published on *Scientific Reports*, an online and open access publication from the publishers of *Nature*.

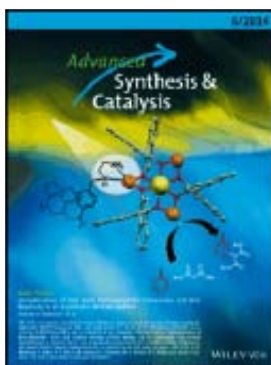
Journal Covers



The Energy Landscape of Uranyl-Peroxide Species.

[Access to the abstract](#)

Chem. Eur. J., **2014**, 20, 3464-3651
Eitan Tiferet, Adrià Gil, Carles Bo, Tatiana Y. Shvareva, May Nyman, Alexandra Navrotsky

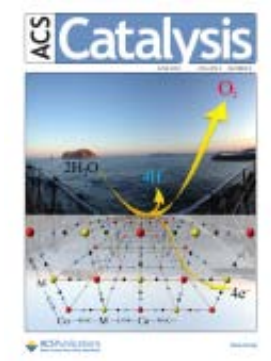


Non-Covalent Immobilization of Rare Earth Heterobimetallic Frameworks and their Reactivity in an Asymmetric Michael Addition.

[Access to the abstract](#)

Adv. Synth. Catal., **2014**, 356, 1243-1254
Jerome R. Robinson, Jagjit Yadav, Xinyuan Fan, Gretchen R. Stanton, Eric J. Schelter, Miquel A. Pericàs, Patrick J. Walsh

BACK COVER



Light-Driven Water Oxidation with Metal Hexacyanomethylate Heterogeneous Catalysts.

[Access to the abstract](#)

ACS Catal. **2014**, 4, 1637-1641
Sara Goberna-Ferrón, Willinton Y. Hernández, Bárbara Rodríguez-García, José Ramón Galán-Mascarós



From the Lindlar Catalyst to Supported Ligand-Modified Palladium Nanoparticles: Selectivity Patterns and Accessibility Constraints in the Continuous-Flow Three-Phase Hydrogenation of Acetylenic Compounds.

[Access to the abstract](#)

Chem. Eur. J., **2014**, 20, 5926-5937
Gianvito Vilé, Neyvis Almora-Barrios, Sharon Mitchell, Núria López, Javier Pérez-Ramírez

News in brief

H-Index: The current h-index for ICIQ is 88, according to the Web of Knowledge database.

Phd theses defences: Drs. Antony Pitaval, Pinar Kasaplar, Atul Bansode, Laura Osorio, Xu Tian, Ignacio Mon, Philipp Reeh, Takashi Ono, Laia Pellejà, Joan Gallardo, Núria Fernández, Charles Goehry, Lídia Cabau, Antonio Bazzo and Yahui Wang, pre-doctoral students at ICIQ have defended their PhD thesis. They were all awarded the highest honors for their work.

Bayer funds two ICIQ PhD grants: Bayer Material



Science gives funding for two pre-doctoral fellowships within ICIQ's PhD Fellowship Programme, for a period of

two years. This agreement is an example of collaboration within the framework of MedChem, the chemical cluster of Tarragona, which has among its objectives to foster collaboration between industry in Tarragona and knowledge-generating institutions.

[Jobs and Grants published in ICIQ's website](#)



Pablo Garrido gets a grant from Obra Social "La Caixa": Pablo, from Llobet's group, has received 1 of the 25 grants awarded by Obra Social "La Caixa" to pursue doctoral studies in Spain. A great privilege!

Mapping Scientific Excellence In its third release, time period 2007-2011, the web application Mapping Scientific Excellence ranks ICIQ in first position on "Best Paper Rate" (proportion of highly cited papers published by an institution) and second on "Best Journal Rate" (ratio of papers published in the most influential journals) in the field of Chemistry worldwide. In its second release ICIQ ranked first on "Best Journal Rate" and second on "Best Paper Rate". So it clearly shows that ICIQ keeps on performing great research. ICIQ did not appear in the first release for the time period 2005-2009 because the institute had not yet published 500 papers.

The web application Mapping Scientific Excellence visualizes the scientific performance of institutions (universities or research-focused institutions) within specific subject areas as ranking lists and on maps.

[Mapping Scientific Excellence](#)

Kids Around

ICIQ always gets younger on July even as we know deep inside that we're getting older when we come across any of the high school students doing a summer placement at ICIQ. They come in different ways and with different purposes:

- Andrea Ruiz and Sergi Rafel are in the Galán-Mascarós lab doing research as part of the Joves i Ciència programme
- Thanks to the Societat Catalana de Química, José Andrés Ballester is spending time with ICIQ's computational groups
- About 15 high school students will come in and out to get their research project supervised by Dr. Laia Pellejà, ICIQ's science outreach person

"Doing research in one of these labs is a great experience. My parents would prefer I become an engineer but what I like is chemistry" says Andrea.



Sergi and Andrea in the lab

"We have seen what's electrolysis, we have discovered the organic solar cells... My friends don't understand that I want to be here during my holidays" adds Sergi.

Whatever their reasons for coming here, we are glad they are here! Seeing the youths around and feeling their excitement about chemistry makes us – the day-to-day ICIQ inhabitants – believe that the future is in great hands.

Career Development: CSOL's Seminar

On June 13th, Dr. Fernando Bravo, CSOL's unit manager, delivered an open seminar about the use of Design of Experiments for reaction optimization. He showed a real example of the use of DoE for reaction optimization using the software Design Expert v8. This was a good opportunity to follow up complement the DoE training that was organized last year at ICIQ.



CSOL's seminar at ICIQ's auditorium

Science Showcase!

ICIQ's "Light as a source of chemical energy" workshop at the Science fair of Barcelona.



 [More info](#)

Welcome!



2014 ICIQ Summer Fellows

Outdoors!



Agenda

ICIQ Seminar Program

All seminars at 12p.m. in the ICIQ Auditorium

- Sep. 4th** **Dr. Oscar Delgado**
Jansenn Research & Development (Spain)
- Sep. 19th** **Dr. Dimas G. De Oteyza**
Universidad del País Vasco (Spain)
- Sep. 25th** **Prof. Masahiro Murakami**
Kyoto University (Japan)
- Sep. 26th** **Prof. Miguel Angel Miranda**
Universitat Politècnica de València (Spain)
- Oct. 1st** **Prof. Donna Blackmond**
The Scripps Research Institute (USA)

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- Oct. 10th** **Prof. Martin Albrecht**
University College Dublin (Ireland)
- Oct. 17th** **Prof. Kenneth Caulton**,
Indiana University (USA)
- Oct. 31st** **Prof. Luis A. Oro**
Universidad de Zaragoza (Spain)

