

**ICIQ**<sup>R</sup>

Institut  
Català  
d'Investigació  
Química



[www.iciq.es](http://www.iciq.es)

## CSOL, new ICIQ's technology development unit

Following the steps of Crysforma, ICIQ has launched CSOL: Catalyst Selection and Optimization Laboratory, its second technology development unit. "CSOL acts as a link between ICIQ's expertise in catalysis and the industry, and aims at developing ICIQ's discoveries into industrial applications", says Dr. Lluís Solà, ICIQ's strategic area manager.

CSOL offers innovative, tailor-made catalysts solutions for homogeneous transformations, including enantioselective reactions. For this purpose, CSOL counts with a

team of professionals with experience in pharmaceutical development, led by Dr. Fernando Bravo (CSOL unit manager). CSOL also benefits from the scientific advice of ICIQ's group leaders and group leaders from universities involved in the Consolider Intecat project.

 [More info: www.catalytic-solutions.com](http://www.catalytic-solutions.com)



## SIR World Report 2010 lists ICIQ among the best research institutions

According to the Second Edition of Scimago Institutions Ranking World Reports, ICIQ holds a Normalized Impact (NI) value of 2.69, the second highest one among the Spanish Institutions (and the 5th and 27th rank at the European and International levels, respectively). Normalized Impact scores indicate the scientific impact that institutions have over the scientific community, and show the ratio between the average scientific impact of an institution and the world average impact of publications of the same time frame, document type and subject area.

The report also considers the High Quality Publications (Q1) criteria. This ratio shows ICIQ holding a Q1 value of 83.89, which is the third highest one among the Spanish Institutions (and the 9th and 34th at the European and International levels, res-

pectively). This value refers to the ratio of publications an institution publishes in the world most influential scholarly journals.

SIR World Report 2010 is the most exhaustive and comprehensive ranking of Worldwide Research Institutions, and the ranking includes 2,833 institutions that together are responsible for 80.55% of worldwide scientific output during the term 2004-2008 as indexed in Scopus database.

 [More info: Scimago Institutions Ranking webpage](#)



## The Obra Social “La Caixa” supports ICIQ’s Summer Fellowships program

Last December Dr. Miquel Àngel Pericàs, ICIQ director, and Mr. Enric Dalmau, director of “La Caixa” business area in Tarragona, signed a collaboration agreement for the funding of the 2011 ICIQ Summer Fellowships program. Through this agreement, Obra Social “La Caixa” is committed to fund 10 fellowships for undergraduate students to spend three-months (from July to August) in one of the research laboratories at ICIQ.

The aim is to give the students the chance to work in the research areas of ICIQ (catalysis, supramolecular chemistry and renewable energies) and to participate in daily research tasks. “I was really impressed by the rigorous and at the same time pleasant way of working that the people have in this place, and I finally decided to stay here for my PhD” says Crisa Vargas, summer fellow in 2009.

The ICIQ Summer Fellowships program kicked off in 2008 and throughout this time more than 30 students have participated in this program. For some of these students, their stay at ICIQ has also represented an opportunity to start a research career by choosing ICIQ as the place to do their PhD in Chemistry.

**i** [More info: ICIQ Summer Fellowships Program](#)



Mr. Dalmau and Dr. Pericàs sign the agreement.

## Briefs

**PhD Thesis Defence:** Drs. Marta Santiago, M<sup>a</sup> Dolores Segarra, Anna Reynal, Miquel A. Planells, Torstein Fjermestad, Verónica López-Castillo, Laura P. Hernández, Mihai Raducan and Jaime Gómez, pre-doctoral students at ICIQ, have defended their PhD thesis recently. All seven were awarded the highest honors for their work.

**Science Week at ICIQ:** As it has become a tradition, last November ICIQ organised several activities in the frame of the 2010 Science Week in order to get Chemistry closer to Society. Throughout a week ICIQ offered guided tours to ICIQ facilities, a workshop in Chemistry (“Familiar Chemistry”) and fun experiments at the R&D Fair from the URV.



Participants in ICIQ's workshop in Chemistry.

### Step forward of the Campus of International Excellence Southern Catalonia:

**CEICS:** In the frame of the 2010 Call for the Campus of International Excellence of the Education Ministry, the project Campus of International Excellence Southern Catalonia (CEICS), promoted by the *Universitat Rovira i Virgili* (URV) and in which the ICIQ is a member, has received the qualification of “Campus of International Excellence” in the regional category. ICIQ’s participation is key in the proposal of the future PhD School in the field of Chemistry together with the URV, the *Universidad de Zaragoza* and the CSIC. Thanks to this acknowledgement, the CEICS project will get € 3 M.

**i** [More info: www.ceics.eu](http://www.ceics.eu)

## Challenging research

Oier Lakuntza is a predoctoral student under the supervision of Prof. Jesús Ugalde at Universidad del País Vasco. When he decided to study Chemistry, many people advised against it, and even some members of the National Organization of Spanish blind people (ONCE). At the beginning of its bachelor's degree, when his blindness was not complete, he took his own notes using a pen and magnifying glasses, but later on he had to make use of computers and software such as Braille 'n Speak and screen lectors, or ask his classmates for their notes (specially if there were a lot of formulae).



He decided to do research in computational chemistry because he liked the field and because for a blind person it is easier to focus on the theoretical aspects of chemistry (while it is impossible to carry experimental work in the lab). An intriguing question for many people might be how he can imagine the chemical systems which he is studying, and the answer is through the "z-matrix" coordinate systems, which allows him to mentally represent molecular structures. Still, the chemical systems he deals with are generally small, even though he has sometimes worked with bigger systems (of about 36 atoms). The main topic of his research project is the study of methane activation through the Nickel hydroxy-hydride cation ( $\text{HNiOH}^+$ ). This reaction is known to take place experimentally, and Oier is studying the singlet and doublet surfaces, as well as their crossings.

He considers that his stay at ICIQ has been a very profitable experience, since he learnt new and useful things for the study of his system. Moreover, from a personal point of view he says this stay has

been excellent, and has been pleased with the good vibrations in the group. But apart from being a very positive experience for him, Oier's visit has been highly enriching for the rest of the people working in the theoretical and computational lab. When asked about Oier's daily work, Maria stays that he is in fact very independent (he writes his own papers and makes his presentations using pdfLaTeX), and in fact the only thing in which he needs some help is in drawing. Moreover, Maria says that before Oier's stay, she thought there were many things that would be very difficult or even impossible for a blind person, and she realized it is not true. Thanks to his optimistic attitude, Oier faces challenges in a positive way and with a good sense of humor, which is something that undoubtedly makes him go on with his projects. As the Monty Python would sing, always look on the bright side of life!

## Briefs

**Calix 11:** The 11th International Conference on Calixarenes, organized by Prof. Javier de Mendoza and Prof. Pau Ballester (ICIQ group leaders), will be held at ICIQ from June 26th to June 29th, 2011.



The program will consist on 30 keynote lectures, 10 short presentations selected among the abstracts submitted as contributors for the poster sessions, and 2 poster sessions.

**i** [More info: www.calix2011.org](http://www.calix2011.org)

**Young ICIQ researchers awarded:** Dr. Héctor Fernández (laboratory coordinator of Prof. Vidal's research group) and Dr. Vanesa Lillo (laboratory technician of Dr. Galán-Mascarós' research group) both received the PhD Extraordinary Award for their doctoral thesis.

On the other hand, the research works of Verónica López and Nicolas Delpont (predoctoral students at Prof. Echavarren's group) were also recognized by Lilly awards.

## Looking for alternative fuels

Dr. Atsushi Urakawa (Fukuoka, 1976) joined ICIQ as a group leader in January 2010, after having spent 4 years as an Oberassistent (senior scientist/lecturer) at the ETH (Zurich). His research group at ICIQ aims the rational improvement and design of heterogeneous catalytic processes, making use of an interdisciplinary experimental-theoretical approach (*in situ* spectroscopy and theoretical modelling).

Among others, one of the major reactions they currently focus on is the heterogeneous catalytic conversion of CO<sub>2</sub> into fuels and useful chemicals at a high efficiency. This way, the carbon-cycle, which has generally an open end due to burning of fossil fuels and release as CO<sub>2</sub> into atmosphere, can be closed for sustainable development.

### ■ Which is the most direct application of your research?

Design of new catalysts and improvement of energy- and cost-efficiency of current catalytic processes are typical results of our research. Also, we employ and develop various *in situ* spectroscopic tools for heterogeneous catalytic reactions occurring at solid surfaces; therefore our tools are often useful to investigate chemical species at solid-fluid (gas, liquid, supercritical fluid) interfaces.

### ■ Do you think the chemical industry will ever be able to use CO<sub>2</sub> instead of petroleum or oil-derived compounds as raw material?

I strongly believe so. I even consider it mandatory for mankind to utilize CO<sub>2</sub> as an important feedstock to produce valuable and useful chemicals. The chemical industry is under social pressure related to CO<sub>2</sub> emission and more actions will be surely taken in the future. The major challenge is to chemically reduce the stable CO<sub>2</sub> molecule at high efficiency without producing CO<sub>2</sub> by the conversion process. The use of renewable energy sources such as sun light should be maximally exploited for CO<sub>2</sub> conversion processes. Various forms of energy exist and they are inter-convertible; sun light can be used to reduce CO<sub>2</sub> by photocatalysis, by electrocatalysis using elec-

tricity generated by solar cells, or by thermocatalysis heated by the sun or by the electricity. CO<sub>2</sub> from chemical plants is often available in a highly energetic form (high temperature and pressure) and such conditions should be beneficially utilized. Another important point is the hydrogen source (e.g. molecular hydrogen and methane) for the reduction, which should also be produced by renewable energy. Because of this background, we currently develop efficient thermo-, photo-, and electrocatalytic CO<sub>2</sub> reduction systems using heterogeneous catalysts. Fossil fuel has an end; it is, without a doubt, the task and responsibility of the current generation to find more sustainable ways of life by carbon recycling based on renewable energy.



*Dr. Urakawa, ICIQ group leader.*

### ■ Which factors influenced your decision of coming to work at ICIQ? Are there any advantages regarding facilities, equipment, etc?

Sun, beach, fish... to name a few. Seriously, the major one is the research directions of ICIQ. It matched very well with my personal one. ICIQ is young and dynamic, giving a great momentum for research. Also, I greatly appreciate the centralized research facilities and equipments in Research Support Area, which offer great possibilities for all ICIQ researchers. This unique mixture convinced me that ICIQ is the right place.

 [More info: Urakawa research group](#)

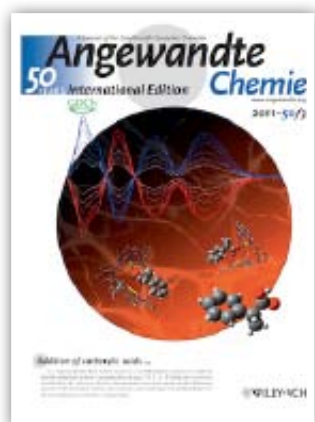
## Journal Covers



Ni-Catalyzed Reduction of Inert C-O Bonds: A New Strategy for Using Aryl Ethers as Easily Removable Directing Groups

**i** [Link to the article](#)

(*J. Am. Chem. Soc.* **2010**, *132*, 17352-17353) Authored by Paula Álvarez-Bercedo and Rubén Martín, cover of the Journal of the American Chemical Society.



Effective Chirogenesis in a Bis(metallosalphen) Complex through Host-Guest Binding with Carboxylic Acids

**i** [Link to the article](#)

(*Angew. Chem. Int. Ed.* **2011**, *50*, 713-716), authored Sander J. Wezenberg, Giovanni Salassa, Eduardo C. Escudero-Adán, Jordi Benet-Buchholz, and Arjan W. Kleij. Back cover of *Angewandte Chemie International Edition*.

## International Year of Chemistry 2011

ICIQ, the URV (Universitat Rovira i Virgili) and AEQT (Associació Empresarial Química de Tarragona) will coordinate the events programmed in Tarragona to celebrate the 2011 IYC. All the information can be found in a blog that has been created for the occasion.

**i** [More info: Events in Tarragona to the 2011 IYC](#)

ICIQ is also part of the Catalan Commission for the Coordination of the IYC 2011 led by the SCQ (Societat Catalana de Química)

**i** [More info: Blog SCQ](#)



**i** [More info: International Year of Chemistry 2011](#)

## 2011 ICIQ Summer School:



**Prof. Amos B. Smith III**  
Department of Chemistry,  
Penn Center for Molecular Discovery  
University of Pennsylvania, Philadelphia

**Prof. John F. Hartwig**  
Department of Chemistry,  
University of Illinois, Urbana

**Prof. F. Dean Toste**  
Department of Chemistry,  
University of California, Berkeley

**Prof. Oliver Baudoin**  
Institut de Chimie et Biochimie Moléculaires et  
Supramoléculaires  
Université Claude Bernard Lyon 1

**Prof. Richmond Sarpong**  
Department of Chemistry,  
University of California, Berkeley

**Prof. Polly Arnold**  
School of Chemistry,  
The University of Edinburgh

**Prof. Dr. Jeffrey W. Bode**  
Lab. für Organische Chemie Departements Chemie  
und Angewandte Biowissenschaften, ETH Zürich

**Prof. Dr. Paul Knochel**  
Department of Chemistry and Biochemistry  
Ludwig-Maximilians-Universität

**Dr. Rubén Martín**  
Institute of Chemical Research of Catalonia  
(ICIQ) Tarragona

## Last Christmas



## Agenda

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### Saló de l'Ensenyament

23 - 27 March, Barcelona

[www.ensenyament.com](http://www.ensenyament.com)



### 9<sup>a</sup> Edició Fira Recerca en Directe 2011

5 - 7 April, Barcelona

[www.pcb.ub.cat/recercaendirecte](http://www.pcb.ub.cat/recercaendirecte)

### ICIQ Seminar Program (January/April)

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

- Feb. 11th:** Prof. Yoshiaki Nakao (Graduate School of Eng., Kyoto University)  
"C-C bond forming addition reactions by Nickel/Lewis acid catalysis"
- Feb. 25th:** Prof. Fraser Armstrong (University of Oxford)
- Mar. 4th:** Prof. Stuart MacGregor (Heriot Watt University)
- Mar. 7th:** Prof. Kalman Szabo (Stockholm University)
- Mar. 22nd:** Prof. Stefan Matile (Université de Genève)
- Mar. 25th:** Prof. Jianliang Xiao (Liverpool University)
- Apr. 1st:** Dr. Mark Ford (Bayer)  
"Agrochemical Process Research: Searching for the holistic solution"
- Apr. 8th:** Prof. S. Höger (Universität Bonn)
- Apr. 18th:** Prof. K. C. Nicolau (University of California)
- Apr. 28th:** Prof. Dieter Seebach (ETH Zürich)  
& 29th