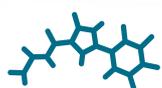




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**ICIQ**<sup>R</sup>

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Química



www.iciq.es

## ICIQ-IPMP Looking for talent

The ICIQ international postdoctoral mobility programme (ICIQ-IPMP) in 2012 offers 10 postdoctoral positions in 10 different research groups. The programme is partially funded by the Marie Curie Co-funding of Regional, National and International Programme (COFUND) action of the European Commission. The ICIQ-IPMP aims to set up a training programme addressed to highly talented and motivated experienced researchers to give them the opportunity to develop their research career at the Institute.

The postdoctoral researchers will have the opportunity to join one of the research groups at the Institute, and will follow an individual research project under the supervision and mentoring of an internationally renowned group leader in a stimulating and multidisciplinary scientific environment.



International  
PostDoctoral  
Mobility  
Programme



They will have access to the Institute's scientific facilities and scientific life and will follow hands-on training activities on the use of scientific instrumentation

The programme will consist of 4 calls for an average of 10 positions for a two year postdoctoral stay.

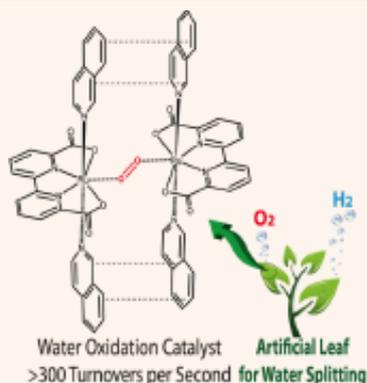
 [More info: http://ipmp.iciq.es](http://ipmp.iciq.es)

## Research Results

### Prof. Antoni Llobet publishes in Nature Chemistry:

Prof. Llobet, along with an International team of scientists, have designed a ruthenium catalyst for the most effective oxidation of water to date.

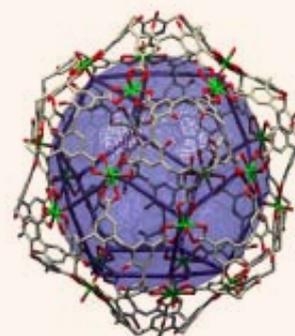
 [More info: Access to the abstract](#)



### Prof. Javier de Mendoza and his team in Nature Communications:

Prof. De Mendoza's team have synthesised unique octahedral and icosahedral anionic UOFs (Uranyl Organic Frameworks) from calixarenes, carboxylates and uranyl at room temperature.

 [More info: Access to the abstract](#)



UOF with an inscribed sphere of ca. 7238 Åms

## Intecat Project: The final balance



The project "INTECAT: Design of Catalysts for Green Chemistry. An Integrated Approach" Consolider (MICINN) ended in December 2011 and results achieved are very positive.

The INTECAT project, coordinated by ICIQ, was focused on developing an integrated approach to catalysis, with the aim of contributing to the discovery of new chemical processes that make a better use of raw materials minimizing energy input and the generation of wastes. The project included participation of research groups from ICIQ, Universidad de Valladolid, Universidad de Huelva, Universidad de Zaragoza and Universitat Rovira i Virgili.

INTECAT has more than fulfilled the objectives outlined in the project implementation agreement:

**Scientific output:** INTECAT has generated a total of 549 articles, of which 50% are articles in journals with IF > 5 and 76% in journals with IF > 4. It is noteworthy that 45 papers have been published in J. Am Chem Soc (IF 9,012), 39 in Eur J Chem (IF 5,476) and 30 papers in Angew. Chem Int Ed (12,730).

**Academic productivity:** During the the project INTECAT, 68 doctoral theses have been defended by members from the groups of the Universidad de Valladolid, Universitat Rovira i Virgili, Universidad de Zaragoza and ICIQ.

**A successful example of technology transfer:** INTECAT project has generated a new technology development unit, CSOL, which provides selection and optimization of catalysts for the chemical industry.

**Scipio:** Storing Comprehensibly Interesting Pieces of Inputs and Outputs (SCIPIO) is a new software platform that solves the problem of storing, managing and processing the most relevant results of computational studies.



Last INTECAT project meeting in Huelva (Oct. 2011)

- <http://www.proyectointecat.es>
- <https://scipio.iciq.es/LabBookWeb/>
- More info:** [Web CSOL](#)

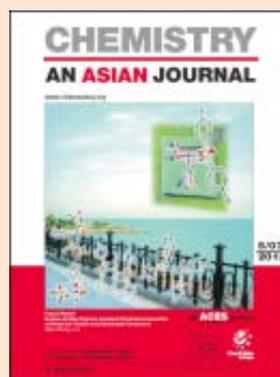
## ICIQ-SCP (Starting Career Programme)

2012 has seen the launch of this new programme to help young talented researchers (Postdoc level) to start their careers in chemistry research. ICIQ-SCP will work on a yearly basis. Application for this year's position has been closed. Next July, several members of our Scientific Committee will come to ICIQ to interview the short-listed candidates.



## News in brief

**PhD theses defence:** Drs. Ana Escribano, Josep Albero and Abel Locati, pre-doctoral students at ICIQ, have defended their PhD thesis. They were all awarded the highest honors for their work.



**Journal Cover: Iodine(III)-Promoted Intermolecular Diamination of Alkenes**

José A. Souto, Yolanda González, Alvaro Iglesias, Debora Zian, Anton Lishchynskyi, Kilian Muniz  
*Chem. Asian J.*, 2012, 7, 1103.

[access to the abstract](#)

## Where are they now?



**Torstein Fjermestad:** I started my Ph.D. at ICIQ in 2005 and my project concerned computational studies on systems related to the Pauson-Khand reaction. The project was supervised by Prof. Feliu Maseras and Prof. Miquel Pericàs. During my time at

ICIQ I gained a lot of experience and I learned to tackle problems in computational as well as organometallic chemistry. After I defended my thesis in 2010, I moved to Oslo, Norway, and I worked one year as a post doc. at SINTEF. There I studied mechanisms of Au catalyzed transformations. I am now doing my second post doc at the University of Oslo. I have changed field of research slightly, and I am currently working in materials science. In particular I am involved in a project where I look at how zeotype catalysts behave under operational conditions. My ICIQ-project on the Pauson-Khand reaction might seem rather specialized, but it has been gratifying to see that the methods used in that project are generally applicable.



**Cati Ferrer:** After I left ICIQ in 2008 I started a postdoctoral stay at the IRB in Barcelona in the group of Professor Antoni Riera. There I spent one year and a half after which I moved to Groningen, in the north of the Netherlands. I obtained a grant from the Spanish government and I could start another postdoctoral stay in the group of Professor Minnaard. After one year I got the opportunity to start working at Syncom, a spin-off company of the University of Groningen. I am now working at Syncom for almost one year, where we do contract research and custom synthesis. The company already exists for about ten years and has around a hundred employees. I am happy to see how the ICIQ has grown over the past years. I started at the ICIQ in 2004, the very beginning, when the labs were still being settled and there was not even an NMR machine! A lot of things were still being arranged and sorted out and it is nice to see that all this work has given such a good result.

But the best things I take from the time I spent at the ICIQ are the very good friends I made and all the great people I met there (including my future husband)!



**Elisa Huerta:** I started my PhD with Javier de Mendoza at the ICIQ at the end of 2004, when the institute was working for only a few months. At that time, we were just a few and there were still empty labs. During the six years I spent there, I have seen how

more people were arriving, the empty labs were filled and the institute was growing until needing a second building. I still remember when the parking was nothing else but a sandy esplanade that became a muddy hole as soon as a bit of rain showed up. During my PhD I focused my research on the synthesis and study of the properties of hydrogen-bonded self-assembled systems for the recognition of fullerenes. It spent a great time there and I met awesome people but, as the song says, "all the good things come to an end" and in October 2010 I moved to the group of Bert Meijer in Eindhoven where I'm currently working as Marie Curie postdoctoral fellow. Here I am working in the field of single-chain polymer nanoparticles with application in catalysis. The final goal of the project is to create enzyme mimicking catalysts.



**Ataualpa Braga:** My name is Ataualpa, I am from Brazil and former postdoc researcher at ICIQ for almost six years. I am deeply grateful to my supervisor Prof. Maseras and his group for giving me the opportunity to grow professionally in a very friendly environment. During that

time Catalunya has become my second country, ICIQ my home and the Colla Jove an extension of my very family. In early 2011 I returned to Brazil to work as a researcher at UNICAMP, my former university in Campinas. Finally, in the last months I got a permanent position at USP - University of São Paulo - where I'll begin a new stage in my career as professor and group leader. I am very happy with my new life in Brazil and I'm aware that much of this success I owe to my period in ICIQ. Moltes gràcies i fins aviat.

## Pau Ballester Interview

### ■ When did you decide to become a scientist, a chemist in your case, and why?

It was when I finished high school. I liked science, however I found both mathematics and physics to be too abstract. Chemistry had the right experimental and theoretical balance. I was fascinated by the possibility of transforming one substance into another via chemical reaction and the clever use of molecular structure. I also had a very good teacher and the opportunity to study in Palma de Mallorca.

### ■ What do you like and enjoy the most in your job?

I really enjoy being able to help those who are new to the world of research. I also like the challenge of designing new molecules and then seeing if they behave as we previously predicted they would. Now, I can do some of the chemistry that fascinated me as a student but I was not able to perform. Another thing I appreciate about ICIQ is its fantastic research support area that helps us develop our chemistry. We are privileged.

### ■ What do you see as the greatest achievements in your career to date?

My goal when I started my post-doc in 1985, which was when the area of molecular recognition and encapsulation emerged, was to design a molecule, a capsule, able to encapsulate other molecules. Recently, we have successfully designed a group of 'encapsulating' molecules and I am very proud of it.

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

We should all work in order to change the negative perception that society has on chemistry. We should invest money in programs and projects to help people understand that chemistry is actually very positive for society and our welfare.

In terms of research, I am a convinced supporter of basic and fundamental research, especially in academic centres. Investment in applied research is also necessary but it should perhaps be conducted in non-academic environments with interdisciplinary groups and professional and experienced researchers.



Prof. Pau Ballester, ICIQ group leader and ICREA professor, has been awarded the RSEQ Award of Organic Chemistry 2012.

We must differentiate between applied research aimed at more specialized technological centers and the fundamental research developed in academia. You can not stop funding basic research because it has no immediate applications. Fundamental research advances the frontiers of knowledge and plays a very important role in future applications. In addition, basic research provides the training for investigators and the knowledge and skills to face real problems they may find in future investigations.

### ■ Can you tell a funny story about you or your career?

I will tell you an anecdote about my PhD studies. I studied my PhD in the 80's in a very small university where we did not have nuclear magnetic resonance facilities. I experienced the rigors of classical organic chemistry.

We used IR and UV spectroscopy to characterize our molecules, we purified compounds by crystallization or distillation because we did not have column chromatography systems, the purity of our compounds was based on melting points and elemental analysis... Today this would be foolish, but back then it was heroic.

### ■ What do you do in your spare time?

Unfortunately, I don't have much free time. I like jogging, being with my family, cooking and going to buy fish at the market, which is something I did when I lived in Mallorca. I also really like sports cars and I would love to have a Ferrari!

### ■ PROUST / ICIQ questionnaire:

A chemical element: *Carbon*

Favourite Scientist: *Linus Pauling*

An invention: *Nuclear Magnetic Resonance*

If you had not been scientist... *I would have been an engineer to be able to design things*

Favourite destination: *My home*

A book: *"The third Chimpanzee" by Jared Diamond*

A movie: *Blade Runner*

A dream: *That the values of effort, responsibility and professionalism are not lost and remain important.*

Science is... *magic*

## SCIPIO: A new tool for scientific computation

S C I P I O

The Computational Groups at ICIQ have released, after 3 years of intensive work, SCIPIO (Storing Comprehensibly Interesting Pieces of Inputs and Outputs), a new software platform that solves the problem of storing, managing and processing the most relevant results of computational studies.

### Unique features:

- Both command line interface (transparent to Linux bash shell) and Web interface.
- Data extractor engine fully independent of database structure and user interfaces.
- Almost no recoding is needed for new types of output files.
- Molecular substructure searches
- Computing and plotting reaction energy profiles from raw data.
- Straightforward generation of Supporting Information PDF or text files.

**i** [More info: https://scipio.iciq.es/LabBookWeb](https://scipio.iciq.es/LabBookWeb)

## At School

ICIQ researchers visited some schools (*Pau Delclòs* in Tarragona and *El Roquissar* in Altafulla) as part of our commitment to stimulate students' curiosity and interest in chemistry.



Nùria Huguet and Claudia de León (*Echavarren group*) at CEIPS Pau Delclòs, in Tarragona.

## News in brief

**CEICS Campus Nobel:** The "Southern Catalonia Nobel Campus" will take place from 1st to 4th July at Port Aventura Convention Centre. The event will bring together six Nobel Prize-winners in chemistry, world-class scientists, leaders in R&D&I in chemical companies and outstanding students and researchers. The goal of the Nobel Campus is to encourage interaction, discussion and experiences between the participants of the event.

**i** [More info: CEICS Campus Nobel](#)



### **Bayer sponsors two ICIQ PhD Fellowships:**

In the frame of ICIQ's PhD Fellowships Programme,

Bayer has agreed to support two of these fellowships. Deadline for application submission: October 30th, 2012

**i** [More info: ICIQ website](#)

**ICIQ Social Networks:** A new and more 'social' platform for Scientific Communications is coming soon.



'ICIQ Inter@ctions' will be a space to communicate the science and activities that take place at ICIQ. It will contain scientific news, interviews, blogs, a press office and an exclusive platform for science outreach. You can also contribute to this initiative by becoming a blogger for ICIQ Blogs. Voice your ideas and experiences on your personal blog! If you are interested contact Lorena [ltomas@iciq.es](mailto:ltomas@iciq.es).



### **BASF sponsors the ICIQ Seminars' Programme:**

BASF Española sponsors the ICIQ Seminars' Programme intended for training

researchers. The agreement reflects BASF's commitment to make an annual donation to ICIQ for a period of three consecutive years, from this year until 2014.

**ICIQ Summer Fellowships:** The selection of candidates for the 2012 ICIQ Summer Fellowships has been specially challenging this year. We have received nearly 90 applications, the highest number of applications since the fellowships programme started. The list of awardees is in our website. Congrats to all of them!

**i** [More info: ICIQ website](#)

## ICIQ's Ping-Pong Championship



## Agenda

7th Asian European Symposium on Metal-Mediated Efficient Organic Synthesis / ICIQ Summer School

July 22-27, ICIQ Auditorium

 [More info and registration](#)



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ICIQ Seminar Program (June/July/September)  
 All seminars at 12p.m. in the ICIQ Auditorium

- Jun. 1st:** Prof. Michael Famulok  
 LIMES Program Unit Chemical Biology & Medicinal Chemistry, University of Bonn, Germany  
*Oligonucleotide-Based Tools For Pharmacology And Nano-Engineering*
- Jun. 15th:** Dr. Rebecca Goss  
 University of East Anglia, Norwich, United Kingdom  
*Exploring and Harnessing Biosynthesis*
- Jun. 22nd:** Prof. Suzanne A. Blum  
 University of California, Irvine, USA  
*Single-Molecule Tools for Synthetic Chemists & Dual Catalysis with Gold*
- Jul. 05th:** Prof. Makoto Fujita  
 The University of Tokyo, Japan  
*Emergent Self-Assembly of Giant Coordination Polyhedra*
- Sep. 07th:** Prof. May Nyman  
 Sandia National Laboratory, New Mexico, USA
- Sep. 14th** Prof. Lawrence T. Scott  
 Merkert Chemistry Center, Boston College, USA