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Notes on Professor Piet van Leeuwen

Prof. van Leeuwen retired from ICIQ on March 31st, 2015.

“He belongs to the rarest species of group leaders: He never pushes, he inspires! He inspires you to strive for the best you can be.” - Dr. Henrik Gulyas, URV researcher.

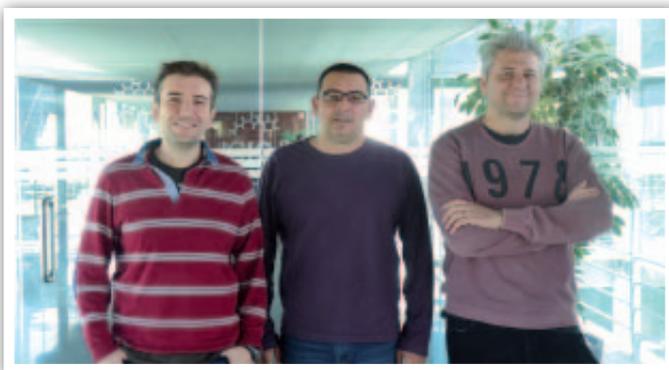
“ I worked with Piet for nine years (2001–2009), initially as post-doctoral researcher at UvA (Amsterdam), where I stayed for three years, and later on at ICIQ as group manager and Ramón y Cajal fellow. During that period I worked in perfect tandem, and I am indebted to him for letting me develop my own ideas and grow up whilst being under the umbrella of his advice, and protection.



Zoraida and Piet

Piet's capacity to work is overwhelming; I believe he arrives to the lab even before sunrise! But I was never there to check it out. He is the only one I know able to write a book in a systematic manner. When we were complaining for not having time to write he used to say, “Write just a page per day and in a year you have a 365 pages book...” and he is making it in this manner! Piet is always ready to enjoy either a good beer or a complicated ³¹P-NMR spectra — ideally both at the same time! — as he enjoys life and chemistry with equal intensity.” - Dr. Zoraida Freixa, Ikerbasque Research Professor **Continues on page 4**

ERC Funding for Three ICIQ Projects



Lloret-Fillol, Palomares and Galán-Mascarós

Dr. Julio Lloret-Fillol, ICIQ group leader since last November, received an ERC Consolidator Grant to develop the project: “Towards a Greener Reduction Chemistry by Using Cobalt Coordination Complexes as Catalysts and Light-driven Water Reduction as a Source of Reductive Equivalents” (GREENLIGHT_REDCAT). The project may open a newer and greener avenue towards the application of artificial photosynthetic schemes in fine catalytic transformations of organic molecules. ERC Consolidator Grants are worth up to € 2.75 million per grant for up to 5 years.

Prof. Emilio Palomares and Prof. José-Ramón Galán-Mascarós received a ‘Proof of Concept’ (PoC) grant. Worth up to €150.000 per grant, ‘Proof of Concept’ funding helps ERC grant holders to bridge the gap between their existing frontier research and its commercial applications.

Palomares' project aims to develop a demo system for cost effective, non-invasive device for rapid detection of cystic fibrosis in humans. Galán-Mascarós' project focuses on the determination of the technical and economic viability of a novel water electrolyzer technology based in inexpensive Prussian blue type catalysts.

Bridging the Valley of Death

One of the problems that we face today in the field of technological development is that in most cases, the research conducted in centers of excellence does not reach beyond a publication or a patent that has scarce possibilities to be exploited. So research results won't be applied to provide real benefit to society. This gap between research results and their application is what is known as the valley of death.

ICIQ aims to bridge this gap through the valorization of research results. *CSOL*, ICIQ's Catalyst Selection and Optimization Laboratory, is in charge of valorizing ICIQ's research results with the finance support of 'la Caixa' Foundation.

"The projects are funded by 'la Caixa' for a period of 1 year, although this funding can be extended by applying for in successive calls. The objective is that after this period, the projects move along the Technology Readiness Level metrics and are better positioned, so that

they can contribute to the creation of a spin-off company, be licensed more easily or achieve new sources of funding" says Dr. Fernando Bravo, CSOL manager.

This year *CSOL* will develop the following projects:

- 'Hydrogen production by water electrolysis using renewable energies' (under the scientific supervision of Prof. J. R. Galán-Mascarós)
- 'Methanol formation by hydrogenation of carbon dioxide at high pressures' (under the scientific supervision of Dr. A. Urakawa)
- 'In-silico studies for the formation of pharmaceutical co-crystals' (under the scientific supervision of Crystforma and Prof. C. Bo)



CSOL researchers

BBVA Frontiers of Knowledge Award to Professor Buchwald

Professor Stephen L. Buchwald, chairman of ICIQ's Scientific Advisory Board and Camille Dreyfus Professor of Chemistry at MIT, received the 2014 BBVA Foundation Frontiers of Knowledge Award in basic sciences. The award recognizes Buchwald's work on "the development of catalytic routes based on palladium and copper to construct carbon-nitrogen and carbon-carbon molecular bonds," according to the jury.



i [BBVA Foundation Frontiers of Research Awards](#)

i [The Buchwald Research Group](#)

Journal Covers

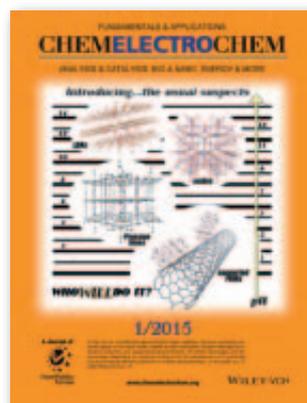


"Phosphinothiolates as Ligands for Polyhydrido Copper Nanoclusters"

i [Access to the abstract](#)

Chem. Eur. J., **2014**, 20, 16121-16127

Miguel A. Huertos, Israel Cano, Nuno A. Bandeira, Jordi Benet-Buchholz, Carles Bo, Piet W.N.M. van Leeuwen



"Water Oxidation at Electrodes Modified with Earth-Abundant Transition-Metal Catalysts"

i [Access to the abstract](#)

ChemElectroChem, **2015**, 2, 37-50

José Ramón Galán-Mascarós

Our First Severo-Ochoa PhD Promotion

They are the first ones to receive one of [ICIQ's Severo-Ochoa predoctoral grants](#). Their names are Marcos Rellán (López's group), Marta Borges (Urakawa's group), Ilario Gelmetti (Palomares' group), Elena de Orbe (Echavarren's group), Ignacio Funes (Maseras' group) and Giacomo Filippini (Melchiorre's group).



Ilario, Marcos, Marta, Elena and Ignacio

"Since I just entered the Severo Ochoa programme I'm still learning the ropes. But of course, I'm really pleased to have received such an excellence grant in such an excellence institute," says Ilario Gelmetti.

They're doing research in the frame of ICIQ's Severo Ochoa programme which develops a strategic project in the area of catalysis. Particularly in the fields of solar fuels through light-induced water splitting and activation of small, carbon-based inert molecules.

"In the future I would like to continue doing research for the industry. At ICIQ there are several collaboration projects with companies. So this is a very good place where to continue my academic formation", says Marta Borges.

Solid State + Impurities Workshop

News in brief

PhD theses defended: Drs. Jordi Ampurdanés, Carla Obradors, Giuliano Carchini, Anna Homs, Berta Camafort, Andrea Henseler, Fedor Miloserdov and Sasa Korom, predoctoral students at ICIQ have defended their PhD thesis. They were all awarded the highest honours for their work.

Mario Lorenzo, ICIQ's new HR Manager: Mario joins ICIQ with the mission to strengthen the HR department by establishing HR policies and with the commitment of implementing new tools that may help us to manage HR processes in a more professional and modern way. He has a bachelor's degree in Labor Studies from the Universidad de Huelva and has pursued a career of more than 12 years in the HR area in different sectors. He has worked for small, medium and large companies at the national and multinational level, thus he provides a broad experience to address his new challenge at ICIQ.



RSEQ awards ICIQ group leaders: Núria López, Ruben Martín and Kilian Muñoz were awarded with the Premio Excelencia Investigadora. The [Real Sociedad Española de Química](#) also awarded Julio Lloret-Fillol with the Premio Jóvenes investigadores.

Tarragona's "Chemical Experience Center": On February 4th, the mayor of Tarragona, Josep Fèlix Ballesteros, made the official announcement of the creation of a museum of chemistry in the site of the former Banco de España building in Tarragona.



ICIQ will participate in this project by offering its expertise on chemistry outreach. We will lead the outreach activities programme of this challenging new science center. Being part of this project and reaching out to Tarragona right from the city center, will facilitate our educational task towards the general public.

ICIQ-UniCat Summer School: Registration is now open for the [ICIQ-UniCat Summer School](#) to be held at the TU Berlin from July 6th to 9th. The ICIQ-UniCat Summer School will bring together graduate and postdoctoral researchers from all over the world to attend lectures of top-level speakers in molecular catalysis.

Good luck Vlad! Dr. Vladimir Grushin, ICIQ group leader, left ICIQ on March 20th, 2015. He joined ICIQ in 2010 and during his time at ICIQ he has made important contributions in the development of practical catalytic methods for selective fluorination.

Notes on Professor Piet van Leeuwen

“ Piet is definitely a great boss. He takes time to provide the necessary information to carry out tasks, his deadlines are usually very reasonable, as he likes to anticipate work, he values initiative and appreciates effort, he always comments on well done work. Even when he is under stress he manages to keep calm and decide on priorities. On the personal level, he can integrate all parts within one whole, as if with all the atoms (co-workers) he could create the perfect molecule (work team). His passion for good food, nature and birds is certainly contagious. One learns a lot from working with Piet, both as a person and as a brilliant scientist.” - *Marta Moya and M^a José Gutiérrez, Piet’s administrative support at ICIQ*



M^aJosé, Marta Serrano and Marta Moya

“ Piet is an awesome boss. After five years in his lab, I can say that he is a brilliant scientist and an amazing person. He is a demanding person and he likes the work well done. He always acknowledges and congratulates researchers for their hard work.

His time in ICIQ is over but we must follow in his steps because I’m completely sure he will certainly surprise us with scientific accomplishments!!” - *Marta Serrano, technician at ICIQ’s CRTU unit.*

“ I left Piet’s group a few years ago. I only have words of gratitude to Piet. In April 2004 he entrusted me to set up and organize his ICIQ lab from scratch. Piet, apart from teaching us his deep and extensive knowledge in chemistry, has always been very interested in giving continuous training to his researchers and in keeping the group’s cohesion through



Josep Maria, Piet and Zoraida

lunches, dinners and group travels. Moreover, he always remembers his former group members in many celebrations. For instance, he invites us every year for his birthday! I wish him luck in his new project.”- *Josep Maria López Valbuena, Science teacher at Col·legi Bon Salvador (Sant Feliu de Llobregat, Barcelona).*

“ I worked with Piet for three years (2012–2015). Until I started in his group, I was “two hands,” I needed 100% supervision and daily instructions from my bosses. Three years later, and under Piet’s supervision, I have learned to develop the projects proposed and my own projects independently, to



Piet and Israel

write papers and to give talks in English (the last two not very well). Currently, and thanks to Piet, I feel I am a “real” scientist. Similarly, he always treated me as a co-worker, and not as a subordinate. This is not strange, because he is passionate with chemistry, but also with culture, life, and beer. We have worked together in one of his steps, ICIQ, but it will continue in the next step of a long list, in Toulouse, as my boss, but most importantly, as my friend.” - *Dr. Israel Cano, postdoctoral student.*

Notes on Professor Piet van Leeuwen

Proust Questionnaire

A chemical element:

Palladium, the chameleon amongst the metals as I wrote somewhere.

Favourite scientist:

Djerassi, because he started a second career as a writer.

Your favourite invention:

Hard to get around without internet!

If you had not been scientist...

I might have been a cook or a plumber.

Favourite destination:

The Pyrenees, a bit chauvenistic, long time ago I would have said the Alps.

A book:

Javier Marías, the trilogy Tu rostro mañana (Your face tomorrow).

A music CD:

Lana del Rey, Born to die.

A dream:

Travel in space and time as in science fiction!

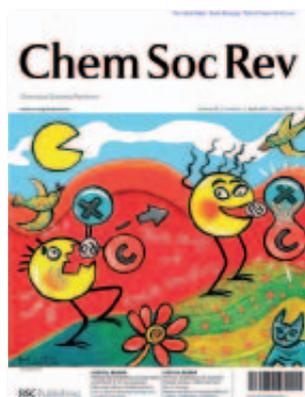
Science is...

no longer a gentleman's passtime.

Piet's Farewell Symposium

On February 20th, the ICIQ community and friends joined professor Piet van Leeuwen for a symposium in his honor. Professor van Leeuwen retires from ICIQ to start a new research adventure as a visiting professor in the UFRGS (Porto Alegre, Brazil) and he will be also holding a Chair in the Chaires d'Attractivité programme of the Université de Toulouse, France.

The symposium's invited speakers were professors Joos Reek (Amsterdam University), Dieter Vogt (University of Edinburgh), Carles Bo (ICIQ), Carmen Claver and Sergio Castellón (Universitat Rovira i Virgili). Professor van Leeuwen closed the event with a review of the soundtrack of his life as a researcher and as Piet.



"Bite angle effects of diphosphines in C-C and C-X bond forming cross coupling reactions"

M.-N. Birkholz (née Gensow), Z. Freixa, P. W. N. M. Van Leeuwen

Chem. Soc. Rev., **2009**, 38, 1099-1118



"SPOs as new ligands in Rh(III) catalyzed enantioselective transfer hydrogenation"

P. M. Castro, H. Gulyas, J. Benet-Buchholz, C. Bo, Z. Freixa, P. W. N. M. Van Leeuwen

Catal. Sci. Technol., **2011**, 1, 401-407



"NHC-stabilized ruthenium nanoparticles as new catalysts for the hydrogenation of aromatics"

D. Gonzalez-Galvez, P. Lara, O. Rivada-Wheelaghan, S. Conejero, B. Chaudret, K. Philippo, P. W. N. M. Van Leeuwen

Catal. Sci. Technol., **2013**, 3, 99-105



Piet received a 3D molecule as a present

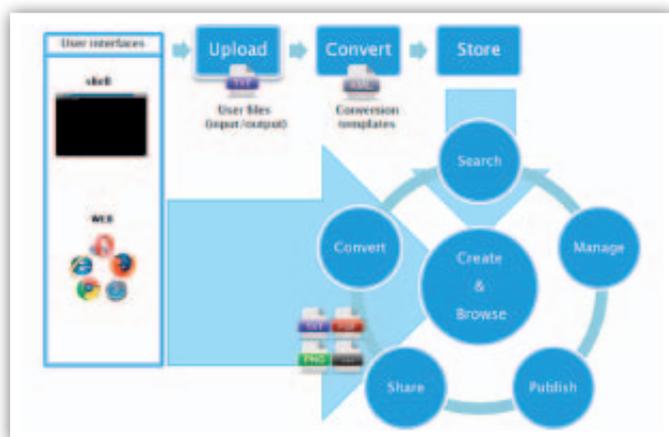
[Symposium's photo gallery](#)

Playing Big Data

The problem of managing huge amounts of data appears in many scientific research fields. The volume of information that is generated daily, coming from the results of scientific calculations is increasing exponentially and researchers need to have tools to manage it.

In the search for solutions to this problem, researchers at ICIQ and at URV have developed the [ioChem-BD platform](#), a multi-headed tool aimed at managing large volumes of computational chemistry results from a diverse group of already common simulation packages. The platform automates the extraction of relevant data and its conversion into fully tagged information in a distributed database. It provides tools for the researcher to validate, enrich, publish and share information, and tools in the cloud to access it and view it.

“We have developed a useful tool with the intention of it becoming a standard. We already have a data collection, but our idea is that other research groups, once they have published their work, incorporate their data to the platform. Thus results of published research projects



will be available almost immediately” –says professor Carles Bo, leading researcher in this project.

The initial design of the platform has been made according to the demands of computational chemistry. But once it is established, it could be applied to any field in which large amounts of data are generated.

[Managing the Computational Chemistry Big Data Problem: The ioChem-BD Platform](#)

M. Álvarez-Moreno, C. de Graaf, [N. López](#), [F. Maseras](#), J. M. Poblet, [C. Bo](#)
J. Chem. Inf. Model., **2015**, 55, 95-103

Past and Future Meetings

RedIntecat



Kick-off meeting on February 12th, 2015. The [RedINTECAT](#) network has the goal of contributing to the discovery of new chemical processes that make a more rational use of feedstocks, require less energy consumption, and take place without the generation of environmentally harmful by-products.

Technion-ICIQ Joint Symposium



ICIQ, February 23-25, 2015. The symposium gathered experts in the field of catalysis from ICIQ and [Technion](#) working on the study of new catalytic transformations that can be employed successfully in novel synthetic pathways. The meeting aimed to search synergies and detect potential collaborations that could trigger possibilities of funding.

COST Action- Carisma



March 18, 19 and 20, 2015. - ICIQ and URV organized the meeting for the COST Action “Catalytic Routines for Small Molecule Activation (CARISMA).” CARISMA will set the stage for an unprecedented Action that will provide new processes for the selective and sustainable transformation of small and pervasive molecules like H₂O, CO₂, NH₃ into high-value chemical feedstocks and energy resources.

May 29th, 2015

[Celebration of Professor Echavarren's 60th Anniversary](#)

June 21st-23rd, 2015

[Japan-Spain Joint Symposium on Heterogeneous Catalysis](#)

June 28th-July 2nd, 2015

[OMCOS 18](#)

Reaching out

New Crazy Students on Board

Our new 2015 Crazy about Chemistry students have already learned the ropes. They have attended several theoretical sessions and they move around the lab with total confidence.

Crazy about Chemistry is a year-long course funded by Fundació Catalunya-La Pedrera addressed to Catalan students in their first year of high school. The course includes a mixture of theoretical lectures and hands-on experimental activities, covering 12 different chemistry topics, including the main chemical reactions. Participants also have the opportunity of learning from ICIQ group leaders about the latest in chemistry research.



A Different Way of Looking

“The X-rays: Our eyes! was the workshop ICIQ offered to visitors of *Recerca en Directe* at CaixaForum (April 8th-11th, Barcelona). Dr. Laia Pellejà, ICIQ’s education and outreach manager, and Eduardo Escudero, laboratory manager of ICIQ’s X-Ray Diffraction Unit, performed live crystallizations under the astonished faces of high-school students and their teachers. They used a digital microscope to project the crystallization of substances such as menthol, glycolic acid and vanillin. For the little ones, they grew a chemical garden and they showed them crystallisations of many frequently used products: Sugar, salt and alum.



Teacher Training

ICIQ collaborates with the *Education Department of the Generalitat de Catalunya* with the course “Methods of analysis of organic compounds,” organised by Dr. Gisela Colet, manager of ICIQ’s research support area, with the support of unit managers and technicians from this area: Drs. Noemí Cabello, Jordi Benet-Buchholz and Fernando Bozoglian. This course is part of the selection of optional training courses for high school teachers.



Dr. Bozoglian and course participants

ICIQ’s Chemistry Workshop Tour



Col·legi L’Estonnac (Tarragona)



CEIP Pau Delclòs (Tarragona)



Escola Cèsar August (Tarragona)

Office Space



Sports

Intermón-Oxfam Trailwalker

Two ICIQ teams, Sixto Trail and Topillos Atómicos Team (TAT) participated in the [Intermon-Oxfam Trailwalker](#) (Girona April 19th, 2015). Congratulations to our brave colleagues!

Zumba and Cardiotone Master Class

Sunday, March 15th, 2015 – Trainers from the Women Center Gym at Sant Pere i Sant Pau (Tarragona) made everyone move back and forward/up and down at ICIQ Auditorium.

Calçotada

Saturday, April 7th, 2015 - ICIQ people gathered for a calçotada at El Llorito picnic zone (Tarragona).

