

Annual Scientific Report Summary

'16



Barcelona Institute of Science and Technology

LETTER FROM THE DIRECTOR



Dear friends,

Thanks for browsing the 2016 ICIQ Scientific Report. I hope you find the information useful.

2016 was a busy, but at the same time really exciting year for me. In September 2016 I committed to become the general director of the Barcelona Institute of Science and Technology (BIST) for a one-year term, to start the deployment of this young institution. However, as you can imagine, ICIQ's life kept going. We faced very important challenges, all of them key to our future: a new strategic plan for 2017-2021, the renewal of the Severo Ochoa accreditation of excellence, the application to the Human Resources Excellence in Research seal awarded by the European Commission, securing funds for the construction of our third building. This, of course, required a lot of dedication and effort. In sum, the design and implementation of activities associated to this dual appointment was a demanding task. I'm most thankful to my closest collaborators at ICIQ (Antonio, Ariadna, Gisela, Lluís, Lorena, Pau, Sara), at my research group (Carles, Esther, Sonia), and at BIST (Àlex, Jenny, Margarita, Núria, Òscar) for their help and support. Together we made it!.

In this website you will find comprehensive information on ICIQ achievements during 2016. I would like to highlight our success in obtaining ERC funding. Professor Paolo Melchiorre received an ERC Consolidator Grant and Professors Emilio Palomares and José Ramón Galán-Mascarós were each awarded an ERC Proof of Concept. Also, Professor José Ramón Galán-Mascarós received 8 million euros from the European Commission (FET projects) to coordinate and develop the A-Leaf project, the first European project coordinated by ICIQ. Moreover, ICIQ research groups obtained funding from MINECO for a total of 14 projects. Once again, ICIQ Group



Leaders were able to raise funding for all their promising projects and ideas. Congratulations to all of them!

With respect to research outputs, the institute continued being very active, publishing **172 scientific papers during the year (90% in the first quartile)** with an average impact factor of 7.8. The institute reached Hirsch index 114 in December and topped international rankings measuring scientific excellence like excellencemapping.net and http://www.natureindex.com.

Finally, I would like to stress the importance of the strategic reflection activities carried out during 2016. Thus, the annual meeting of the ICIQ Scientific Advisory Board was devoted to the analysis of future directions of the Institute with respect to space needs, improvement of our Group Leaders hiring methodology, and scientific orientation. The same discussion process was also performed internally, during our first retreat held in Falset. My personal analysis of these activities is extremely positive. These discussions paved the way for the preparation of ICIQ's Strategic Plan 2017-2021 and the renovation of the Severo Ochoa accreditation, now underway. Moreover, the overall experience was also a great opportunity for team building.

Best regards,

Miquel À. Pericàs

FACTS AND **FIGURES**

Scientific Production





HIGHLIGHTS OF THE YEAR



A-LEAF

8 milions to develop a full artificial leaf

A project coordinated by Prof. José Ramón Galán-Mascarós was awarded €8m by the European Commission.

The A-LEAF project will develop transferable technologies that will be a sustainable alternative to fossil fuels. The artificial leaf will combine the expertise of ICIQ and 12 more partner institutions from 8 different countries, including leading industrial partner COVESTRO. The project kicked-off in January 2017 and will last 48 months.

The main goal of the project is to achieve direct transformation of water and CO_2 into oxygen and organic matter through the action of sunlight. The organic products will the be used as fuels, extracting their stored energy and emitting the original feedstock closing an environmentally neutral cycle.



Prof. Paolo Melchiorre

ERC FUNDING

During 2016, ICIQ received 2,950,000 euros from ERC Grants, which represented around 14 % of the overall funding.

In 2016, three ICIQ researchers were awarded with grants funded by the European Research Council.

Paolo Melchiorre obtained an ERC Consolidator Grant to develop the project "Light-Driven Asymmetric Organocatalysis" (CATA-LUX). Prof. Melchiorre aims at providing novel reactivity frameworks for conceiving light-driven enantioselective organocatalytic processes.

Rubén Martín received an *ERC Proof of Concept Grant* for the project "Catalytic reductive carboxylation of unactivated olefins with carbon dioxide" (OLE-DIOX), which offers the opportunity to convert ubiquitous alkenes into carboxylic acids, building blocks of utmost importance in our chemical industry, thus representing an important contribution for our circular economy by effectively recycling bulk materials into valuable products in one-step operation.

José Ramón Galán-Mascarós was awarded an ERC Proof of Concept Grant for the project "A novel platform for user-friendly spectroscopy at very low temperatures and under strong magnetic fields" (U-SPEC), aiming at assessing the technical and economic feasibility of a new device for spectroscopic measures developed by his research group.



Prof. Rubén Martín



Prof. José Ramón Galán-Mascarós

A TASTE OF OUR 2016 HARVEST

Radical route for the synthesis of chiral molecules

Prof. Paolo Melchiorre's group developed a new methodology for the selective formation of chiral molecules. The work, published in *Nature*, combines two strategies which require very mild reaction conditions – enantioselective iminium ion chemistry and photoredox catalysis- to set quaternary carbon stereocentres with high enantioselectivity. The work represents a breakthrough in the synthesis of chiral molecules as it manages to perform the selective synthesis of the desired molecule via a new radical route that combines the action of a photocatalyst activated by visible light with a chiral organic catalyst.



Prof. P. Melchiorre (left), Dr. J. J. Murphy, Dr. D. Bastida, and Dr. S. Paria



The different CeO₂ reconstructions



a) STM image displaying the formation of quasi-unidimensional polymers.

b) STM image and models of the majority of products between coupled monomers.

Calculations predict disorder in the surface of certain materials

The group of **Professor Núria López** published a paper in **Nature Materials** explaining how massive simulations prove that certain surfaces are more disordered than previously thought. DFT calculations – more than 50000 simulations – carried out on the Mare Nostrum supercomputer at the Barcelona Supercomputing Center allow the introduction of all the complexity in these systems.

Based on the concept of configurational entropy, ICIQ researchers could classify different surface rearrangements according to their stability. They also demonstrated that CeO_2 surfaces are dynamic and the rearrangements are interchangeable. The new terminations show different patterns on the materials surface, affecting their mechanical and catalytic properties and their properties as sensors.

New reaction for the synthesis of nanostructures

The collaboration between the research groups of **professors Pau Ballester and José Ramón Galán-Mascarós** at ICIQ and the group of Dr. David Ecija at Institute IMDEA Nanoscience allowed the development of a new chemical reaction for the synthesis of low-dimensional polymers that can be rationalized as phthalocyanine derivatives. The results obtained were published in *Nature Communications*.

Surface-mediated synthesis of low-dimensional polymers from simple molecular precursors is a rapidly emerging field. In this work, the researchers introduce surface-confined thermally tunable reaction pathways as a route to select intramolecular versus intermolecular reactions yielding either monomeric phthalocyanines or low-dimensional phthalocyanine polymers, respectively.

BIST

First lines of research and new director

The Barcelona Institute of Science and Technology (BIST) presented its first lines of research.

- **Big data:** development of IT platforms to manage big data, incorporating new technological developments quickly and effectively.
- **Super-resolution microscopy:** technological development and promotion of applications common to biology, nanomedicine and materials of super-resolution optical microscopy and electronic microscopy.
- **Graphene:** applications of graphene and 2D materials (materials consisting of a single layer of atoms) in an interdisciplinary manner.
- **Chemical biology:** study and understanding of biological problems by applying the techniques and tools of chemistry.

Prof. Miquel A. Pericàs, Group Leader and ICIQ Director, took over as general director of BIST in October. Prof. Pericàs stressed the importance of the BIST project: "BIST brings together six of the best centers in Catalonia, multiplying their capacity to promote excellence in research, new lines of multidisciplinary research, training and career support programs for researchers, and science outreach. By making significant progress in these areas, we will be doing a great service to our country."



The BIST team



Prof. Miquel A. Pericàs, BIST and ICIQ director

A NEW ICIQ-INDUSTRY PROJECT

ICIQ and Esteve team up to promote innovation

The R&D teams of **Esteve** and **Esteve Química** teamed up with ICIQ's **technology development unit ERTFLOW** to kick-off an ambitious research pro-



ject dubbed **FLOW4HEALTH**. This project will develop new continuous-flow chemical processes to prepare new drugs and molecular leads useful for the pharmaceutical industry.

FLOW4HEALTH's continuous-flow processes will allow chemists to work with extreme reaction conditions and dangerous reagents in a safer, more predictable way. The project will accelerate the first stages of drug development by designing innovative laboratory equipment towards quicker purifications, enhanced productivity and more sustainable methodologies.

NEW OUTREACH ACTIVITIES Summer Camp: Let's do chemistry

At the ICIQ's chemistry summer camp we made visible the chemistry that surrounds us. **'Let's do chemisty'** is an introductory course to the world of chemistry. Participants have the chance to carry out experiments in our learning laboratory, doing group work and learning how to present their work and results obtained in public. The objective was to carry out a programme of experiments that explained and promoted understanding of our daily life from the perspective of chemistry. The activity was addressed to children finishing 5th and 6th year of primary education and it was held at ICIQ's Learnening Laboratory on July 25th – 29th.

BIYSC

BIYSC (Barcelona International Youth Science Challenge) is an international scientific challenge event, that aims to connect the most passionate science students with the best researchers.

The ICIQ was one of the research centres participating in BIYSC. We offered the research project entitled **'From molecules into electricity'**, a workshop where participants learned to prepare organic molecules and devices that can be used to transform the sunlight into electrical power.



ICIQ Summer Camp



Participants in the project "From molecules into electricity."

In 2016, the web application Mapping Scientific Excellence ranked ICIQ in third 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.

ICIQ's privileged position in this list confirms the Institute's strong evolution towards scientific excellence since the beginning of its research activities in 2004. Since then, ICIQ has published more than 1500 scientific articles. About 90% of them have been published in the most influential chemical research journals in the world, those ranked in the first quartile (Q1- journals within the top 25 % of journals with highest IF).



SCIENTIFIC PRODUCTION

Articles in 2016 172Total articles (2004-2016) 1568 h-Index 14 Citations in 2016 9530 Total citations (2004-2016) 64,506 Average citations (2004-2016) 386

KNOWLEDGE AND TECHNOLOGY TRANSFER



Transfer of knowledge and technology to the industrial sector is an integral part of the institute's activities. During 2016, the technology development unit **CSOL** was involved in one collaborative project with industry in the field of homogeneous catalysis as well as performing seven valorization projects to develop the inventions made by ICIQ's research groups into technologies that are closer to an industrial application.

As for **Crysforma**, it continues expanding its capabilities in the field of pharmaceutical solid state development. During 2016, Crysforma continued with its own internal research lines, in this case in collaboration with the group of Prof. Carles Bo, in the area of prediction of co-crystal formation.

ERTFLOW, which works in the area of flow chemistry, started its first collaborations with industry, including a "Retos Colaboración" project with the pharmaceutical group Esteve.

Globally, **14 research projects with industry were active during 2016**, including the **Esteve-ICIQ and Henkel-ICIQ joint units**. Finally, **4 new patents** were applied for, arising from the research results from ICIQ's groups.

PREPARING THE NEXT GENERATION OF TOP RESEARCHERS

ICIQ has a strong commitment to offer training programmes for undergraduates, graduate students and doctoral researchers. We prepare a new generation of researchers with the skills and knowledge needed to tackle the most important challenges in chemical research. We are also eager to prepare graduate and post-graduate students to undertake research careers in chemistry. Our Complementary Training Programme offers complementary training such as weekly scientific seminars, technical workshops, international research stages, language courses, ICIQ Summer School, and other soft skills courses and activities.

Programmes



ICIQ Summer Fellowship UNIVERSITAT ROVIRA I VIRGILI

ICIQ-URV SO-ICIQ Master in International Synthesis, Graduate Catalysis and Students Molecular Programme Design



ICIQ-International PostDoctoral Mobility Programme



CELLEX-ICIQ Postdoctoral Programme on High Throughput Experimentation

ADVANCED TRAINING

15

Summer fellows:

Master students:

3

PhD students

113

Postdoctoral researchers

87

PUBLIC ENGAGEMENT

ENGAGING YOUTH TO PURSUE A CAREER IN CHEMISTRY

ICIQ seeks to raise public awareness of chemical research as a key factor for the progress of our society. Our purpose is to sensitize citizens to the benefits of chemistry research in terms of health, energy and environmental sustainability. We are also committed to engaging and encouraging youngsters to pursue a career in chemistry research. To this end in 2016, we have displayed a science outreach programme addressed to audiences of all ages as a way to position the joy of chemistry within reach of many more people and to explain the research we're carrying out at ICIQ.



For the first time we organized the ICIQ Summer Camp that included **'Let's do chemisty'**, an introductory course to the world of chemistry. We also participated in the Catalunya-La Pedrera Foundation programme **BIYSC** (**Barcelona International Youth Science Challenge**) with the research project entitled **"From molecules into electricity"**.

Moreover, we carried out our traditional **"Química en família"** workshop for children; scheduled weekly chemistry workshops addressed to high school in the **ICIQ Teaching and Learning Laboratory**; carried out the **"From the Lab to the Classroom Programme"** to inspire and train teachers in new



topics and methodologies to teach chemistry; and our PhD students delivered talks about their research within the frame of the **"Science at School"** programme of FCRI. We also participated in science fairs and visits to primary schools to perform chemistry experiments.

Finally, we organized the third edition of **"Crazy about Chemistry".** A yearlong course in chemistry addressed to high school students with a special interest and talent on chemistry and research. This training activity is funded by the "Crazy about Science" programme of Fundació Catalunya-La Pedrera.



"Química en família" workshop



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